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Linking canopy scattering of far-red sun-induced chlorophyll fluorescence with reflectance

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ABSTRACT

Remotely sensed sun-induced chlorophyll fluorescence (SIF) has been used as an indicator of global terrestrial vegetation photosynthesis. The connection between SIF and photosynthesis allows its use for improving estimates of gross primary production (GPP) and monitoring plant stress. In these analyses, up-scaling of the relationship between SIF and photosynthesis from the photosynthetic level to the canopy, regional or global scale has been one of the main challenges. The scaling is strongly affected by the radiative transfer of emitted SIF, notably scattering and re-absorption of SIF. It is essential to understand these processes in order to differentiate effects of canopy structural variation from effects of photosynthesis functional variation on SIF. In this study, we derive the relationship between canopy scattering of SIF and top-of-canopy (TOC) reflectance analytically, by investigating the radiative transfer of incident light and emitted SIF. The similarity of radiative transfer of intercepted incident light and emitted SIF results in a simple relationship between reflectance and canopy scattering of SIF. In particular, we find that the ratio of far-red reflectance (R) to the product of canopy interceptance (i_0) and leaf albedo (ω) is an accurate estimate of canopy scattering of far-red SIF (i.e.,). SCOPE model simulations are used to validate our findings. The relationship we found provides an easy and accurate approach for rapid decoupling canopy structural and functional regulation of SIF, and correction of SIF for bidirectional effects. This will improve estimates of canopy photosynthesis from SIF.

1. Introduction

Sun-induced chlorophyll fluorescence (SIF) is a novel remote sensing signal for monitoring vegetation photosynthesis. It takes place in the pigment beds of photosystems, and SIF is an indicator of the efficiency by which photons are transmitted to photochemical reaction centers (Grace et al., 2007; Meroni et al., 2009). It is therefore closely related to the light harvesting process and responds timely to rapid changes in photosynthesis (Krause and Weis, 1991; Baker, 2008). In recent studies SIF was used to estimate vegetation photosynthetic capacity (Zhang et al., 2014) and for tracking dynamic changes of photosynthesis (Rossini et al., 2015). The connection between SIF and photosynthesis allows its use for improving the estimation of global or regional gross primary production (GPP) (Frankenberg et al., 2011; Guanter et al., 2014), and as an early warning signal of vegetation stress (Ač et al., 2015).

Apart from photosynthetic activity, SIF observations from remote sensing are strongly affected by the structure of vegetation canopies (Grace et al., 2007; Migliavacca et al., 2017; Damm et al., 2015). SIF observed at top of canopy is only a portion of the total emitted SIF, due to re-absorption and scattering (i.e., they are complementary to each other) (Porcar Castell et al., 2014). The scattering and re-absorption of SIF from the moment of emission to the moment of escape from the canopy in observation direction, is (among other factors) sensitive to canopy leaf area index (LAI) and leaf orientation (Verrelst et al., 2015; Verrelst et al., 2016). Scattering and re-absorption effects are spectrally dependent. SIF at 760 nm (far-red SIF) is scattered more and re-absorbed less than SIF at 687 nm (red SIF) (Porcar Castell et al., 2014) and therefore the portion of SIF reaching the sensor is higher for far-red SIF than for red SIF. As a result, the ratio of red and far-red SIF from canopy observation differs from that of leaf-level measurements (Fournier et al., 2012; Cendrero-Mateo et al., 2015).

Understanding of canopy scattering of SIF is crucial, especially when a quantitative link between SIF and photosynthesis is desired for GPP estimates. In a regional SIF to GPP comparison, Guanter et al. (2014) assumed a canopy scattering coefficient of unity (i.e. no absorption) of far-red SIF due to lack of effective ways to quantify the scattering, but acknowledged the potential importance of accurate estimates of this process. Simulations with radiative transfer models (RTMs) confirmed that the scattering is an important aspect: They show

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that the relation between photosynthetic activity and SIF is canopy structure dependent (Damm et al., 2015; Verrelst et al., 2016) and that a substantial portion of the variability of SIF at different spatial and temporal scales is due to canopy structure rather than photosynthetic functioning (Koffi et al., 2015; Van der Tol et al., 2016; Migliavacca et al., 2017).

One way to study the effect of the scattering is to compare leaf-level and canopy-level measurements. Cendrero-Mateo et al. (2015) found that top-of-canopy (TOC) fluorescence of a wheat canopy measured in a growing season differed from leaf-average fluorescence, and that they developed differently over the growing season. The asymmetric evolution of leaf and canopy SIF may be attributed to seasonal changes in the scattering of fluorescence. Spectral differences between leaf and canopy SIF have also been reported. Fournier et al. (2012) reported that the ratio of red to far-red SIF of grass decreased by a factor of two from the leaf to the canopy level. This confirms that canopy scattering for the red and far-red SIF are different.

The empirical method (i.e. comparing leaf and canopy measurements) can reveal the magnitude of the effect of scattering in specific cases, but it is challenging to generalize the results. The need to sample a representative number of leaves that account for the variability of incident light and leaf properties makes the method labor intensive (Zarco-Tejada et al., 2003; Cendrero-Mateo et al., 2015). Furthermore, it is not easy to control the experiment and to identify and isolate the different effects on scattering, such as those of soil background, viewing and solar illumination angles.

RTMs offer a comprehensive complementary method to investigate the effects of canopy structure on TOC SIF. They provide an estimation of canopy scattering of SIF by simulating the light-canopy interaction. The SCOPE model (Van der Tol et al., 2009) simulates leaf fluorescence emission and TOC SIF, reflectance and photosynthesis of homogeneous canopies, while the mSCOPE model (Yang et al., 2017) simulates these for vertically heterogeneous canopies. For more complex canopies, 3D models have been developed, such as the DART (Gastellu-Etchegorry et al., 2017), FluorWPS (Zhao et al., 2016), and FluorFLIGHT (Hernández-Clemente et al., 2017). All these models require prior inputs of canopy structure and leaf properties. These are unknown in most remote sensing applications, but they can be retrieved by means of inverting a RTM using measured reflectance data (Houborg et al., 2007; Jacquemoud et al., 2009). The retrieved properties can then be used in a fluorescence RTM to quantify the SIF scattering. In this way, RTMs for reflectance and fluorescence can be used to interpret observed SIF signals.

Van der Tol et al. (2016) retrieved key biophysical and biochemical parameters from the reflectance data of rice canopies, and applied these parameters to simulate TOC SIF by using SCOPE. Such retrievals have a number of limitations. First, they are computational demanding. Second, both the retrieval of properties and prediction of SIF scattering are model dependent, and uncertainties in the estimation of canopy properties may be introduced due to ill-posed retrievals that may propagate into error in the prediction of canopy scattering of SIF. Nevertheless, Van der Tol et al. (2016) found that most of the variability of SIF could be reproduced after retrieval of parameters from reflectance. This not only confirms the dominating role of canopy scattering on seasonal variations of SIF, but also suggests that reflectance data can be used to estimate this scattering.

The idea that reflectance can explain the canopy scattering of SIF is promising. Reflectance data are widely available as many satellites have the capability to detect vegetation reflectance in many bands. The quantification of SIF scattering through reflectance measurements provides a way to decouple canopy structural and photosynthetic regulation effects on remotely sensed SIF.

Two recent studies provide experimental evidence of a close link between canopy scattering of SIF and reflectance. Badgley et al. (2017) reported that far-red reflectance times NDVI strongly correlates with SIF through the vegetated fraction of the surface. Liu et al. (2016) reported a bidirectional effect on SIF measurements that was similar to the effect on reflectance.

In the present study, we aim to link reflectance and canopy scattering of SIF by investigating the radiative transfer of incident light and emitted fluorescence with a minimum set of assumptions about the representation of canopies in models. We provide a detailed derivation of the canopy scattering of SIF and its relation to TOC reflectance. SCOPE model simulations are used to validate our findings. The relationship we found will allow rapid decoupling of canopy structural and functional regulation of SIF, which is useful for improving estimates of canopy photosynthesis from SIF.

2. Theoretical basis

2.1. Definitions and aim of study

The objective of the study is to relate the scattering of SIF (σ_{FC}) to TOC (directional) reflectance (R). R and σ_{FC} describe, respectively, the scattering of incident light and that of total emitted SIF to the viewing direction. They are defined as

$$R = \pi L_o / E \tag{1}$$

$$\sigma_{FC} = \pi L_o^F / E_F \tag{2}$$

where L_o and L_o^F are the radiance of observed reflected solar radiation and of observed fluorescence at top of canopy, respectively, and E and E_F are the irradiance of incident flux at top of canopy and emitted fluorescence from all the leaves in the canopy (i.e., fluorescence emission), respectively. Note that an observation is always the sum of L_o and L_o^F, and in remote sensing applications, they need to be separated with for example the FLD method (for a review, see Meroni et al., 2009). In radiative transfer modelling, they are separately simulated.

As mentioned, our objective is to express the canopy scattering of SIF σ_{FC} as a function of reflectance R:

$$\sigma_{FC} = f(R) \tag{3}$$

Reflectance and canopy scattering of SIF, and their relationship can be obtained if we know the observed radiance (L_o), observed fluorescence radiance (L_o^F), incident irradiance (E) and canopy total fluorescence emission (E_F). The incident irradiance is known in most cases either from measurements or from atmosphere radiative transfer models (e.g. MODTRAN, Berk et al., 2005), but E_F cannot be estimated easily.

In what follows, we derive an explicit expression of Eq. (3) in four steps, the final result of which is Eq. (12). First, we explain the interaction between incident flux and a vegetation canopy. Second, we provide an expression of canopy fluorescence emission. Third, we compare the equation for the observed reflected flux to that of the observed fluorescence flux. Finally, we link canopy scattering of SIF to TOC reflectance (Eq. (12)).

2.2. Flux interaction with vegetation canopy

Photons entering the canopy from the top will either go through the canopy via gaps or interact with leaves (or needles). The portion of photons from the incident beam that will not interact with leaves is known as the zero order transmittance (t_0). The complementary portion, the canopy interceptance (i_0), is the portion of photons that will interact with leaves (Smolander and Stenberg, 2005; Huang et al., 2007) (Fig. 1). The sum of the zero order transmittance and canopy interceptance is unity. The interception is the first order interactions between incident light and the canopy.

In the first order interactions, photons can either be scattered or absorbed by a leaf, depending on leaf albedo (ω), which is the sum of leaf reflectance (ρ) and transmittance (τ). Photons in the photosynthetically active radiation (PAR) range (i.e., from 400 to 750 nm)