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Model-based analysis of the relationship between sun-induced chlorophyll fluorescence and gross primary production for remote sensing applications

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ABSTRACT

Remote sensing of sun-induced chlorophyll fluorescence (SIF) is a novel optical tool for the assessment of terrestrial photosynthesis or gross primary production (GPP). Several recent studies have demonstrated the strong link between GPP and space-borne retrievals of SIF at broad scales. However, critical gaps remain between short-term small-scale mechanistic understanding and seasonal global observations. Here, we present a model-based analysis of the relationship between SIF and GPP across scales for diverse vegetation types and a range of meteorological conditions, with the ultimate focus on reproducing the environmental conditions during remote sensing measurements. The coupled fluorescence-photosynthesis model SCOPE is used to simulate GPP and SIF at the both leaf and canopy levels for 13 flux sites. Analyses were conducted to investigate the effects of temporal scaling, canopy structure, overpass time, and spectral domain on the relationship between SIF and GPP. The simulated SIF is highly non-linear with GPP at the leaf level and instantaneous time scale and tends to linearize when scaling to the canopy level and daily to seasonal. These relationships are consistent across a wide range of vegetation types. The relationship between SIF and GPP is primarily driven by absorbed photosynthetically active radiation (APAR), especially at the seasonal scale, although the photosynthetic efficiency also contributes to strengthen the link between them. The linearization of their relationship from leaf to canopy and averaging over time is because the overall conditions of the canopy fall within the range of the linear responses of GPP and SIF to light and the photosynthetic capacity. Our results further show that the top-of-canopy relationships between simulated SIF and GPP have similar linearity regardless of whether we used the morning or midday satellite overpass times. Field measurements confirmed these findings. In addition, the simulated red SIF at 685 nm has a similar relationship with GPP as that of far-red SIF at 740 nm at the canopy level. These findings provide model-based evidence to interpret remotely sensed SIF data and their relationship with GPP.

1. Introduction

Gross primary production (GPP), the rate of CO_2 uptake by plants through photosynthesis, represents the largest carbon flux between terrestrial ecosystems and the atmosphere (Beer et al., 2010). Despite the critical importance of photosynthesis for the Earth system, understanding how factors such as climate variability, disturbance history, and water or nutrient availability affect it remains a challenge because of complex interactions and limited GPP measurements at various temporal and spatial scales (Schaefer et al., 2012).

Remote sensing methods have long been used for large-scale assessments of vegetation conditions and types, usually through vegetation indices and other vegetation parameters derived from spectral measurements of surface reflectance (e.g., Huete et al., 2002). Reflectance-based vegetation indices are proxies for vegetation "greenness" and photosynthetic capacity, as they represent a mixed signal from leaf chlorophyll content and canopy green biomass and structure. However,

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vegetation parameters derived from red and near-infrared (far-red) surface reflectance have no link to actual plant photosynthetic functioning (Grace et al., 2007). Only the photochemical reflectance index (PRI) (Gamon et al., 1992), based on the sensitivity of reflectance at 531 nm to xanthophyll pigments, has been shown to be sensitive to photosynthetic light use efficiency, although it has not yet been applied to studies at the global scale.

Recent instrumental and methodological developments in the field of space-borne spectroscopy have enabled the measurement of sun-induced chlorophyll fluorescence (SIF) from space, which promises to alleviate current limitations on the monitoring of terrestrial photosynthesis. The SIF signal is emitted by the photosynthetic machinery of healthy vegetation and is thus linked to actual plant photochemistry (Porcar-Castell et al., 2014). SIF observations can, therefore, provide a proxy for photosynthesis not available from any other remote sensing measurements of vegetation (Damm et al., 2010; Rossini et al., 2010; Guanter et al., 2014). Global data sets of SIF have been derived from GOSAT (Joiner et al., 2011; Frankenberg et al., 2011; Guanter et al., 2012; Köhler et al., 2015a), GOME-2 (Joiner et al., 2013; Köhler et al., 2015b; Wolanin et al., 2015), and SCIAMACHY (Joiner et al., 2012; Köhler et al., 2015b; Wolanin et al., 2015). The spatial coverage and resolution, wavelength, acquisition time and the amount of data available for analysis depend on the instrument from which they are derived. Single SIF retrievals from those systems are normally aggregated in space and/or time to reduce random retrieval noise.

The potential use of SIF as an indicator of large-scale GPP has been demonstrated for the relatively short period of available global SIF data. For example, high correlations between SIF derived from GOSAT and data-driven GPP estimates at the global and annual scale were shown by Frankenberg et al. (2011) and by Guanter et al. (2012). Lee et al. (2013) used GOSAT SIF data to investigate the seasonality of forest productivity in Amazonia and found that peak productivity occurs during the wet season, which indicates that productivity of the Amazon rainforest is driven by water availability rather than by solar radiation. Using GOME-2 SIF data, Guanter et al. (2014) have shown that SIF has a higher sensitivity to crop photosynthesis than to any other existing remote sensing parameter or model, which has been used to produce new maps of the productivity of the largest crop belts worldwide. More recently, Joiner et al. (2014) demonstrated good agreement between the seasonal cycles of GOME-2 SIF data and flux tower-based GPP estimates. Zhang et al. (2014) have also used GOME-2 SIF data over agricultural areas to demonstrate the feasibility of estimating crop photosynthetic capacity, suggesting the usefulness of SIF in a confined parameter space when certain main properties are known. On the other hand, Koffi et al. (2015) reported a relatively low sensitivity of SIF to photosynthetic capacity in global parameter space when used the Carbon-Cycle Data Assimilation System.

Despite the experimental evidence of a direct and highly linear correlation between spatiotemporal aggregates of remotely-sensed SIF data and large-scale GPP, the relationship between instantaneous photosynthesis and SIF is complex (Porcar-Castell et al., 2014; Verrelst et al., 2015) at both leaf and canopy levels. At the leaf level, this relationship is primarily driven by incoming solar radiation, which defines the relative amounts of energy used for photosynthesis, emitted as fluorescence or dissipated as heat in the process of non-photochemical quenching (NPQ). At light-limiting conditions, most photosynthetically active radiation (PAR, in the 400–700 nm spectral range) absorbed by chlorophyll is used for photosynthesis, termed as photochemical quenching (PQ), so that fluorescence and NPQ remain low. At high light levels, however, NPQ dominates, and the yields of photosynthesis and SIF decrease with light and tend to co-vary in green and healthy vegetation (van der Tol et al., 2009a). High-light conditions can generally be assumed for the morning and noon overpass times of satellite missions, but this may not apply, e.g., during some parts of the year at high latitudes. In addition, the roles of photorespiration, leaf structure and light scattering properties must also be considered when assessing the relationship between SIF and GPP at the leaf level (Porcar-Castell et al., 2014; van Wittenberghe et al., 2015).

At the canopy level, the effect of canopy structure must also be considered when using remotely-sensed SIF data to estimate large-scale GPP because of the reabsorption of SIF photons emitted in internal canopy layers by other leaves, which depends on leaf optical properties and orientation as well as on the leaf-area index (LAI) and the particular canopy structure. Canopy absorption has a substantial spectral component because red radiation is strongly absorbed by chlorophyll, whereas multiple scattering dominates in the near-infrared (Knyazikhin et al., 2012). Both physiological and canopy structure factors affect the top-of-canopy GPP-SIF relationship and can, therefore, explain the different scaling factors between the two (Guanter et al., 2012). The temporal trajectories of GPP and SIF might also differ throughout the year at a given location as a function of incoming light, temperature and canopy development stage. Field measurements are usually performed at the leaf level with active methods (Porcar-Castell et al., 2014). Recently, a few ground and airborne campaigns have begun to measure SIF at the canopy level in the field (Damm et al., 2010, 2015; Rossini et al., 2010; Rascher et al., 2015), but continuous, long-term measurements are limited due to technical issues (Meroni et al., 2011; Cogliati et al., 2015; Yang et al., 2015). In this regard, process-based models may be an alternative tool to investigate the complicated relationship between photosynthesis and fluorescence at the seasonal scale in the context of remote sensing SIF applications. As a coupled fluorescence-photosynthesis model, Soil Canopy Observation, Photochemistry and Energy fluxes (SCOPE) has demonstrated the feasibility of simulating SIF and GPP (van der Tol et al., 2009a, 2009b, 2014; Zhang et al., 2014), and can be used as a tool for this purpose.

In this context, the objective of this work is to investigate the relationship between SIF and GPP from a model-based perspective, with emphasis on aspects of special relevance for remote sensing applications. In particular, we explore the relationship between GPP and SIF with attention to their link to absorbed PAR (APAR) as well as to the impact of data acquisition time (as a surrogate for incoming radiation), temporal averaging (as needed to reduce noise in global SIF composites), canopy structure and SIF retrieval wavelength. Our analysis is based on the SCOPE model constrained by vegetation and meteorological data at a number of flux tower sites representing different ecosystems for a wide range of environmental conditions. Field measurements and satellite retrievals of SIF from GOME-2 were also used as validations. This analysis is useful for understanding the differences in the relationships between GPP and SIF from leaf level mechanistic understanding to ecosystem-specific observations.

2. Materials and methods

2.1. Satellite SIF retrievals from GOME-2

We used SIF data from the GOME-2 instrument onboard Eumetsat's MetOp-A platform. Details of the retrieval of SIF from GOME-2 measurements can be found in Köhler et al. (2015a, 2015b). We used SIF data from the period between 2007 and 2012 in this work. For each site, SIF values were extracted based on the coordinates of the flux tower and averaged to biweekly means when at least 5 SIF retrievals were available within each biweekly period. Although the footprint size of the flux tower (<1 km^2) does not match the coarse resolution of GOME-2, we assumed landscape homogeneity within the GOME-2 grid based on the criteria described in Section 2.2. We admit that this assumption of landscape homogeneity could lead to biases in the comparison. However, previous studies using the same SIF and flux dataset have demonstrated the overall performance of this assumption (Guanter et al., 2014; Zhang et al., 2014).