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A model and measurement comparison of diurnal cycles of sun-induced chlorophyll fluorescence of crops

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ABSTRACT

In this study, measurements of solar induced chlorophyll fluorescence (SIF) at 760 nm (F_{760}) are combined with hyperspectral reflectance (R) measurements collected in the field over agricultural crops in order to better understand the fluorescence (ChlF) signal of the vegetation. The 'Soil-Canopy Observation Photosynthesis and Energy fluxes' (SCOPE) model, which combines radiative transfer and enzyme kinetics of photosynthesis with turbulent heat exchange in vegetation canopies, was partly inverted to obtain model parameters from R taken over healthy (unstressed) crops during the growing season. Reflectance spectra between 400 and 900 nm obtained at midday on different days in the growing season were used to obtain pigment concentrations, leaf area index and leaf inclination. These parameters were then used to simulate diurnal cycles of half-hourly ChlF spectra, using measured weather variables as input. Three scenarios were simulated: (i) a constant emission efficiency of ChlF (at the photosystem level), (ii) a variable emission efficiency calculated per half hour with an electron transport, photosynthesis and ChlF model for the photosystem, and (iii) a constant emission efficiency that was set to a theoretical maximum value for fully blocked photochemical electron transport of photosystem II and minimal non-photochemical quenching. The simulations of the first two scenarios were compared to ChlF retrieved from field measurements in the O_2-A band with the spectral fitting method in unstressed rice and alfalfa. This comparison and a sensitivity analysis showed that SCOPE reproduces most of the seasonal variability of SIF after tuning to R even if the ChlF emission efficiency is kept constant, and F_{760} values are mostly determined by chlorophyll content, dry matter, senescent material and leaf area and leaf inclination, whereas leaf water and carotenoid content had small effects. Diurnal variations in the ChlF emission efficiency at photosystem level were small in these crops. The simulations of the third scenario were compared to measurements of grass that was treated chemically to block electron transport and to provoke maximum ChlF. This comparison showed that the observed increase in F_{760} can indeed be explained by a change in the ChlF emission efficiency at the photosystem level. It is concluded that hyperspectral reflectance and the ChlF signal together can reveal both the dynamics of vegetation structure and functioning.

1. Introduction

The emerging data of airborne and satellite solar induced chlorophyll fluorescence (SIF) create opportunities for obtaining new information about vegetation status through remote sensing. Chlorophyll fluorescence (ChlF) is the emission of energy in the red and far-red region of the electromagnetic spectrum by pigments that are involved in light harvest and photosynthetic electron transport in plants. Photochemical quenching was first mentioned as a cause of variability in ChlF in the literature in the 19th century (Müller, 1874), and ChlF measurements in controlled conditions on algae and terrestrial plants have been undertaken for many years using both active and passive techniques (for reviews, see Baker, 2008 and Meroni et al., 2009). The Fraunhofer Line Discrimination (FLD) method to decouple SIF from R of terrestrial vegetation was introduced by

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Plascyk (1975), but the possibility to apply this method at large area, from airborne or satellite platforms, is relatively new. The first papers presenting global satellite maps of SIF were published only a few years ago from data of GOSAT, GOME-2 and OCO-2 (Frankenberg et al., 2011, 2014; Guanter et al., 2012; Joiner et al., 2013, 2011). Retrievals of SIF from airborne sensors using medium spectral resolution non-imaging sensors (Damm et al., 2014) and high spectral and spatial resolution imaging sensors (Rascher et al., 2015) have been demonstrated recently as well. In addition, the Fluorescence Explorer satellite mission FLEX has been selected by the European Space Agency (ESA) as the 8th mission in the Earth Explorer series. FLEX will carry a hyperspectral instrument allowing SIF retrievals at different wavelengths in addition to hyperspectral reflectance, and it will be complemented with the optical and thermal bands of Sentinel-3 with which FLEX will fly in tandem.

It has been empirically demonstrated that SIF is a good indicator of photochemical activity in terrestrial vegetation (Damm et al., 2010), even better than indices based on reflectance (R) (Meroni et al., 2008a,b; Guanter et al., 2014). Indeed, there is evidence that SIF provides different information than reflectance spectra (Rossini et al., 2015), because SIF only originates from the parts of the vegetation that photosynthesize. This is further supported by the fact that SIF responds to a range of physiological stresses exerted on the vegetation (Ač et al., 2015).

A key aspect is how to best obtain useful information from SIF, and how to combine SIF and R data for better understanding of the vegetation status. ChlF depends on the actions of light harvesting pigments, the leaf area and leaf orientation, and the efficiencies of the main de-excitation pathways of chlorophyll, notably photochemical quenching via electron transport (PQ) and variable thermal dissipation or non-photochemical quenching (NPQ) (Porcar-Castell et al., 2014). These pathways compete with ChlF. Under low light, the excitation energy is efficiently used by photochemistry (PQ), while under high light excessive energy is dissipated as heat by unregulated thermal dissipation and by various physiological NPQ mechanisms (Krause and Weis, 1991). The ChlF emission efficiency usually peaks between these extremes. SIF is thus always a function of both vegetation leaf (pigment) composition, leaf area and leaf inclination on the one hand, and the biochemical regulation of the energy pathways on the other hand. The vegetation architecture and pigment composition can be retrieved from the spectral signature, i.e., the shape of the reflectance curve as a function of wavelength over the solar reflective range (Jacquemoud et al., 2009). It is also possible to detect subtle variations in the reflectance due to changes in epoxidation state of the xanthophyll cycle related to NPQ (Garbulsky et al., 2011), and this can be detected from airborne data (Zarco-Tejada et al., 2012) and from space as well (Coops et al., 2010; Hilker et al., 2009; Drolet et al., 2008; Hall et al., 2008). SIF may therefore be partly explained by reflectance, but also provide complementary information to the rich signal of reflectance.

In several studies in the last years, the model 'Soil-Canopy Observation of Photosynthesis and Energy fluxes' (SCOPE) (Van der Tol et al., 2009) has been used to interpret SIF. SCOPE combines radiative transfer in the canopy with a Soil-Vegetation-Atmosphere Transfer (SVAT) scheme for the energy balance and photosynthesis. It contains routines for radiative transfer of solar radiation and radiation emitted by the vegetation (thermal and ChlF), and a routine for PQ and NPQ. SCOPE has been used to, for example, investigate the seasonality of SIF and productivity in parts of the Amazonia (Lee et al., 2013) and to retrieve the photosynthetic capacity of crops (Zhang et al., 2014). Even with a tool like the SCOPE model it is not easy to unravel the signal of SIF and to understand how it is related to processes and interactions within the vegetation. The model is complex and inevitably has representation errors due to model abstractions, and uncertainty in parameters and driving variables (in this paper we treat all vegetation properties as parameters, and all weather data as variables). Verrelst et al. (2015) addressed the problem of model complexity by carrying out a sensitivity analysis of SIF, as simulated by SCOPE, in order to identify the most sensitive model parameters and variables. It was shown that irradiance, leaf composition, leaf area index and the carboxylation capacity V_{cmo} are the most influential parameters and variables affecting the signal of SIF. Most of the parameters and variables that affect SIF also influence reflectance. However, some, i.e., irradiance intensity, V_{cmo} and parameters for stomatal conductance, affect only SIF (not R), while others affect R rather strongly but have only a limited effect on SIF (leaf water content C_w). A practical question is thus, whether SCOPE can effectively explain the added value of SIF in understanding the functional status of vegetation. Up to now, a comparison between simulated SIF and field measurements of canopy ChlF has not been made in detail. To understand both simulated and observed diurnal and seasonal dynamics of ChlF is an important aspect. In this study we address this gap.

The objective of this investigation is therefore to utilize the SCOPE model to separately quantify the effects of leaf pigment concentrations and canopy architecture on SIF on the one hand, and the effects of PQ and NPQ on SIF on the other hand. We utilized existing datasets from published studies to obtain SCOPE parameter inputs. That work included measurements of reflectance in field crops using high-resolution (spatial, spectral) spectroscopy systems (Cogliati et al., 2015a; Rossini et al., 2010, 2015). Parameter retrieval from R determined the value of most of the model parameters that affect SIF, notably the parameters of the PROSPECT (Jacquemoud and Baret, 1990) and SAIL (Verhoef, 1984) models. This enabled the simulation of SIF with SCOPE, then simulated SIF was compared to corresponding field measurements. In the comparison between model outputs and observations, we focused on diurnal cycles of several days in the growing season of rice and alfalfa crops. The selected days spanned different phenological stages, so that the effects of canopy density and greenness could be evaluated. The diurnal cycles enabled us to study the effects of PQ and NPQ, which vary during the day, while canopy density and greenness can be considered constant. Finally, data of a manipulation experiment, in which PQ was inhibited (Rossini et al., 2015), were used to further assess the effect of PQ on SIF.

2. Materials and methods

2.1. SCOPE model description

The SCOPE model (Van der Tol et al., 2009) consists of several routines that are combined to simulate ChlF. Since the first publication the model has undergone several revisions. For the present paper we used version 1.61 as published on https://github.com/Christiaanvandertol under GNU General Public Licence.

The illumination by direct solar light and diffuse sky light is simulated with the turbid medium model SAIL (Verhoef, 1984). The SAIL model calculates the scattering and absorption by leaves with a user-defined inclination distribution. Inputs of the SAIL model are the illumination above the canopy and the reflectance and transmittance of the leaves. The latter were originally calculated with the PROSPECT model, but in later versions (including version 1.61) PROSPECT has been replaced by the model Fluspect. The incident light is converted into emitted ChlF spectra on each side (top and bottom) of the leaf by Fluspect (Verhoef, 2011; Vilfan et al., 2016). This is done for all leaf layers and inclination classes. The emitted ChlF is finally used in a radiative transfer model to calculate top-of-canopy (TOC) SIF in the observation direction and hemispherically integrated. The canopy radiative transfer model for SIF is similar to SAIL, but it simulates the fate of emitted radiation rather than the incident radiation. Thus three aspects determine SIF in the SCOPE model: the distribution of