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# Exploring the physiological information of Sun-induced chlorophyll fluorescence through radiative transfer model inversion

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ABSTRACT

A novel approach to characterize the physiological conditions of plants from hyperspectral remote sensing data through the numerical inversion of a light version of the SCOPE model is proposed. The combined retrieval of vegetation biochemical and biophysical parameters and Sun-induced chlorophyll fluorescence ($F$) was investigated exploiting high resolution spectral measurements in the visible and near-infrared spectral regions. First, the retrieval scheme was evaluated against a synthetic dataset. Then, it was applied to very high resolution (sub-nanometer) canopy level spectral measurements collected over a lawn treated with different doses of a herbicide (Chlorotoluron) known to instantaneously inhibit both Photochemical and Non-Photochemical Quenching (PQ and NPQ, respectively). For the first time the full spectrum of canopy $F$, the fluorescence quantum yield ($\Phi_F$), as well as the main vegetation parameters that control light absorption and reabsorption, were retrieved concurrently using canopy-level high resolution apparent reflectance ($\rho^*$) spectra. The effects of pigment content, leaf/canopy structural properties and physiology were effectively discriminated. Their combined observation over time led to the recognition of dynamic patterns of stress adaptation and stress recovery. As a reference, $F$ values obtained with the model inversion were compared to those retrieved with state of the art Spectral Fitting Methods (SFM) and SpecFit retrieval algorithms applied on field data. $\Phi_F$ retrieved from $\rho^*$ was eventually compared with an independent biophysical model of photosynthesis and fluorescence. These results foster the use of repeated hyperspectral remote sensing observations together with radiative transfer and biochemical models for plant status monitoring.

## 1. Introduction

In the last years, Remote Sensing (RS) of Sun-induced chlorophyll fluorescence ($F$) emerged as a novel and promising scientific field for studying the dynamic behavior of photosynthesis (for a review of this topic see Meroni et al., 2009 and Porcar-Castell et al., 2014). $F$ is a physical side product of light absorption that is emitted as an electromagnetic radiation in the red and far-red spectral regions ($\approx$ 640 nm to 850 nm), and it is related to the energetic status of the photosystems.

The feasibility of consistent retrievals of $F$ from ground based platforms (Rossini et al., 2016; Yang et al., 2015), Unmanned Aerial Vehicles (UAVs) (Garzonio et al., 2017; Zarco-Tejada et al., 2013), airplanes (Rascher et al., 2015; Rossini et al., 2015) and satellites (Cogliati et al., 2015; Guanter et al., 2015, 2010; Joiner et al., 2016) has been successfully investigated in the last years, with a strong impulse given by the activity supporting the Earth-Explorer 8 FLuorescence EXplorer (FLEX) satellite mission, of the European Space Agency (ESA), specifically intended for global-scale $F$ retrieval from space (Drusch et al., 2017). Nevertheless, due to the concurrent influence of physiology, leaf and canopy structure, pigment concentration and weather conditions on $F$ (Porcar-Castell et al., 2014; Verrelst et al., 2015b), it's unambiguous interpretation in terms of the quantification of vegetation photosynthesis and stress detection is a largely unsolved challenge. Several authors (*e.g.*, Damm et al., 2010, Guanter et al., 2014, Lee et al.,

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2013) exploited the conceptual scheme of the Light Use Efficiency (LUE) model, proposed by Monteith (1972) for the Gross Primary Production (GPP), to express $F$ as:

$$F(\lambda) = PAR \times fAPAR \times \Phi_F(\lambda) \times f_{esc}(\lambda) \quad (1)$$

where PAR is the Photosynthetically Active Radiation, fAPAR is the fraction of PAR that is absorbed by vegetation (*i.e.*, the fraction of PAR that is transformed into Absorbed Photosynthetically Active Radiation (APAR)), $\Phi_F(\lambda)$ the fluorescence yield (also $LUE_F(\lambda)$, *i.e.*, the fraction of absorbed PAR emitted as fluorescence at wavelength λ), and $f_{esc}(\lambda)$ the "escape probability" (*i.e.*, the probability that an emitted fluorescence photon escapes the canopy in the direction of the sensor). These three processes together (*i.e.*, the absorption of light, the emission as fluorescence, and the escape of $F$ from the canopy) determine the directional $F$ flux emitted at the top of the canopy.

Given these definitions, the effective fluorescence quantum yield ($\Phi_F$) can be defined as:

$$\Phi_F = \frac{F_{int}^{TOT}}{APAR} = \frac{\int_{640}^{850} \frac{F(\lambda)}{f_{esc}(\lambda)} d\lambda}{fAPAR \times PAR} \quad (2)$$

with $F_{int}^{TOT}$ being the total emitted fluorescence by all photosystems in the leaves. $\Phi_F$ is modulated by changes in the physiological status of plants, and represents the fraction of absorbed energy that is not used for Photochemical (PQ) and Non-Photochemical Quenching (NPQ).

Although the potential of $\Phi_F$ to monitor photosynthesis has been demonstrated, it is not trivial to quantify it from canopy level measurements, with increasing complexity when moving from field to airborne and satellite observations. In particular: i) the calculation of $F_{int}^{TOT}$ requires the retrieval of the full spectrum of emitted $F$, but only few attempts have been made so far to retrieve it at canopy level from ground measurements (Zhao et al., 2014; Liu et al., 2015), airborne (Cogliati et al., 2016) or simulated satellite data (Cogliati et al., 2015; Sabater et al., 2015); ii) it is not possible to directly measure $f_{esc}$; iii) the proper quantification of the components of APAR from RS is still challenging (cfr. Garbulsky et al., 2010, Gitelson and Gamon, 2015). Apart from ground or near ground measurements, any retrieval of PAR or fAPAR from RS platforms is mediated by a model, and the disagreement between currently available fAPAR products is high (Meroni et al., 2013; Pickett-Heaps et al., 2014). This fosters the implementation of a flexible and robust framework able to tackle these three issues concurrently, by means of an appropriate modeling of light interception, absorption and emission, and to eventually consistently retrieve $\Phi_F$ at canopy level from RS data. This parameter could offer an additional observational constraint on modeled carbon uptake (MacBean et al., 2018) independent of canopy structure and illumination conditions.

Physically-based Radiative Transfer Models (RTMs) of the vegetation have been used in the last decades to express mathematically the complex interactions between plant elements (*e.g.*, tissues, leaves, branches) and the electromagnetic radiation. RTMs inversion techniques have been widely used to retrieve vegetation parameters such as chlorophyll content ($C_{ab}$) or leaf area index (*LAI*) from RS data (for a review of methods and applications see Verrelst et al., 2015a), but so far few of them incorporated the $F$ signal within the modeling or the retrieval process. The 1-D (vertical) "Soil-Canopy Observation Photosynthesis and Energy fluxes" (SCOPE) model (van der Tol et al., 2009) is a state of the art integrated radiative transfer and energy balance model that enables the simulation of canopy leaving hyperspectral reflectance and fluorescence, modeling the full radiative transfer of light from the photosystem to the top of canopy, as well as the turbulent heat fluxes and photosynthesis. van der Tol et al. (2016) successfully exploited high resolution (Spectral Sampling Interval (SSI) = 0.24 nm and Full Width at Half Maximum (FWHM) = 1 nm) top of canopy reflectance spectra in the visible and near-infrared (VNIR) spectral region, to partially invert SCOPE to retrieve biochemical and structural parameters of the vegetation (*e.g.*, pigment concentration, canopy structure), and further simulate emitted $F_{760}$. Very recently, Verhoef et al. (2018) developed a scheme based on several routines of SCOPE and a $F$ retrieval based on principal components, to obtain $F$ together with important vegetation parameters out of FLEX/Sentinel-3 top of atmosphere synthetic data. Verhoef et al. (2018) showed that it was possible to reach a remarkable accuracy, given the correct atmospheric characterization. Hernández-Clemente et al. (2017) extended a 3-D radiative transfer model to simulate $F$ in complex canopies, and used this model (FluorFLIGHT) to account for the effects of sunlit/shadow pixels, vegetation structure and fractional cover on $F$ in an oak forest, highlighting the importance of a proper modeling approach to relate $F$ to forest health. Nevertheless, 3-D models are generally slower and require a larger number of input parameters than simpler 1-D RTMs, and this can be a limiting factor for their invertibility and their large-scale application.

In this work we propose a novel approach to improve the characterization of the physiological conditions of plants from hyperspectral RS data through the inversion of a light version of the SCOPE model. Compared to van der Tol et al. (2016) and to Verhoef et al. (2018), in this work we retrieve the full $F$ spectrum and $\Phi_F$ as direct products of the numerical inversion of a physically based model. This work aims at using these, together with other important vegetation biochemical and biophysical parameters consistently retrieved within the inversion process, to assess vegetation status in a case of induced stress. In order to evaluate the proposed approach, we compare the retrieved $F$ values with state of the art SFM and SpecFit algorithms (Cogliati et al., 2015) and we analyze the temporal evolution of the retrieved parameters during the controlled stress experiment. Finally, we compare the retrieved $\Phi_F$ values with an independent biochemical model of photosynthesis and fluorescence to sketch a conceptual use of $\Phi_F$ to inform on PQ.

## 2. Materials and methods

### 2.1. Experimental setup

The field campaign was conducted in a farm in Latisana (Udine, Italy; 13.013E, 45.779N) from 7th June 2014 to 3rd July 2014, during the ESA funded FLEX-EU campaign. Three parcels (9 m × 12 m) of a commercially produced lawn were treated with different doses of Dicuran 700 FW (Syngenta AG), a commercial formulation of Chlorotoluron (3-(3-chloro-p-tolyl)-1,1-dimethylurea). Chlorotoluron is an herbicide that interferes with the light reactions of photosynthesis, inhibiting the electron transport chain from photosystem II to photosystem I. This translates in a strong decrease of PQ, and in an accumulation of absorbed energy inside the reaction centers that has to be rapidly dissipated to avoid oxidative stress. Chlorotoluron is also known to inhibit NPQ, hence we expect a strong increase of $\Phi_F$, driven by an increase in $F$ emission, after the treatment. On the other hand, the vegetation biophysical and biochemical parameters should only be influenced at a later stage. Three additional non-treated plots were sprayed with water and used as control. A similar treatment was exploited in Rossini et al. (2015), with noticeable effects on both $F_{687}$ and $F_{760}$. The lawn was frequently irrigated during the campaign and was expected to never experience water limited conditions. A preliminary assessment of the full dataset showed i) no differences between the control plots and ii) that the effect of the lower doses of Dicuran was statistically comparable. Hence, for the sake of simplicity, data shown in this paper refer only to three plots, representative of the more (maximum dose, 24 ml l$^{-1}$) and less stressed (minimum dose, 1.5 ml l$^{-1}$) among the treated plots, as well as a control plot. Due to logistic constraints, the herbicide was applied on the two plots seven days apart (12th June 2014 and 19th June 2014, respectively) hence in this paper the Day After the Treatment (DAT), instead of the Day Of the Year (DOY) will be used.