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Retrieval of sun-induced fluorescence using advanced spectral fitting methods

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ABSTRACT

The *FLuorescence EXplorer* (FLEX) satellite mission, candidate of ESA's 8th Earth Explorer program, is explicitly optimized for detecting the sun-induced fluorescence emitted by plants. It will allow consistent measurements around the O_2-B (687 nm) and O_2-A (760 nm) bands, related to the red and far-red fluorescence emission peaks respectively, the photochemical reflectance index, and the structural-chemical state variables of the canopy. The sun-induced fluorescence signal, overlapped to the surface reflected radiance, can be accurately retrieved by employing the powerful spectral fitting technique. In this framework, a set of fluorescence retrieval algorithms optimized for FLEX are proposed in this study. Two main retrieval approaches were investigated: i) the optimization of the spectral fitting for retrieving fluorescence at the oxygen absorption bands; ii) the extension of the spectral fitting to a broader spectral window to retrieve the full fluorescence spectrum in the range from 670 to 780 nm. The accuracy of the retrieval algorithms is assessed by employing atmosphere-surface radiative transfer simulations obtained by coupling SCOPE and MODTRAN5 codes. The simulated dataset considers more realistic conditions because it includes directional effects, and the top-of-atmosphere radiance spectra are resampled to the current specifications of the *FLuORescence Imaging Spectrometer* (FLORIS) planned to serve as the primary instrument aboard FLEX. The retrieval accuracy obtained at the O_2-A band is strongly affected by directional effects, and better performance is found in cases where directional effects are lower. However, the best performing algorithms tested provided similar performance, the RMSE (RRMSE) is 0.044 mW m^{-2} sr^{-1} nm^{-1} (6.2%) at the O_2-A band, 0.018 mW m^{-2} sr^{-1} nm^{-1} (2.9%) at the O_2-B band, and 6.225 mW m^{-2} sr^{-1} (6.4%) for the spectrally integrated fluorescence emission. The promising results achieved open new perspectives extending fluorescence studies not only in limited absorption bands, but its spectral behavior in relation to different plant species, photosynthetic rates and stress occurrences.

1. Introduction

Satellite remote sensing provides fundamental data to study and monitor vegetation state variables and processes. Most Earth Observation missions rely on the analysis of the reflected radiance in the solar domain to derive bio-physical (i.e. fractional cover (FC), leaf area index (LAI)), and bio-chemical constituents of vegetation (i.e. chlorophyll, water and nitrogen). In the last few years, the remote sensing of sun-induced fluorescence (SIF) represents a novel approach to provide new insight into plant photosynthetic activity. SIF is a faint light signal released by the photosynthetic apparatus that plant canopies add continuously to the reflected radiance in the visible and near-infrared wavelength range. The strong interest and the various efforts ongoing by scientific community are prompted by the close link between SIF and the actual plant photosynthetic rate (Baker, 2008; Papageorgiou & Govindjee, 2004). The exploitation of this signal at continental and global scale for examining the atmosphere-vegetation carbon exchanges estimations (Guanter et al., 2014; Lee et al., 2013; Parazoo et al., 2014), and its parametrization into the Community Land Models (Lee et al., 2015), represent recent applications.

In the last few years, global scale maps of SIF in the far-red region have been generated by exploiting high spectral resolution sensors on board current space-borne mission, primarily devoted to atmospheric chemistry. Joiner et al., (2011), Frankenberg et al., (2011) and Guanter et al., (2012) produced the first global maps of far-red SIF by exploiting the data produced by the *TANSO Fourier Transform Spectrometer* on board the Japanese GOSAT satellite (Hamazaki, Kaneko, Kuze & Kondo, 2005; Kuze, Suto, Nakajima & Hamazaki, 2009). Afterwards, global

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maps of far-red fluorescence have also been produced by exploiting the *SCanning Imaging Absorption SpectroMeter for Atmospheric CHartographY* (SCIAMACHY) aboard of ENVISAT (Joiner et al., 2012), and the *Global Ozone Monitoring Experiment 2* (GOME-2) flying on the operational European meteorological (MetOp) satellite (Joiner et al., 2013). Future advancements for the far-red SIF region are expected from NASA's OCO-2 (Frankenberg et al., 2014) launched in July 2014, and the forthcoming *TROPOspheric Monitoring Instrument* (TROPOMI) to be aboard the Sentinel-5 Precursor (Guanter et al., 2015). The SIF retrieval algorithms from atmospheric space-borne satellites are mostly based on the analysis of the absolute in-filling of fluorescence in the solar Fraunhofer lines (740–755 nm). Even though the contribution of SIF is lower in such narrow lines compared to broader and deeper telluric oxygen bands, the main advantage of this approach relies in a simplified radiative transfer modeling of the atmospheric scattering and absorption effects in such spectral window. The SIF global maps derived from the atmospheric sensors can be very useful for a global assessment of SIF, but their coarse spatial resolution (between few up to tens of kilometers) do not provide optimal data to study terrestrial ecosystems. In fact, the heterogeneity of the natural land surface cannot be properly represented at these spatial resolutions in most of the cases. Furthermore, the spectral configurations of the existing atmospheric missions (mostly between 757 and 775 nm) do not allow the retrieval of red SIF, thus limiting the analysis to the far-red SIF only.

The *FLuorescence EXplorer* (FLEX) mission, candidate to the 8th Earth Explorer program, is currently under Phase A/B1 study by the European Space Agency (ESA). FLEX is explicitly optimized for detecting the SIF emitted by plants at a unique spatial resolution of 300 m (ESA, 2015). It will fly in tandem with the ESA's Sentinel-3 (S3) (Donlon et al., 2012) to take advantage of complementary measurements from the *Ocean and Land Color Instrument* (OLCI) and the *Sea and Land Surface Temperature Radiometer* (SLSTR). The FLEX/S3 tandem mission will provide numerous advantages including an accurate atmospheric correction, the consistent measurements of both red and far-red fluorescence peaks, the detection of the photochemical reflectance index (PRI) (Gamon, Peñuelas & Field, 1992), and estimation of bio-physical and biochemical canopy parameters. All these sources of information are essential in this mission for a better understanding and interpretation of sun-induced fluorescence, canopy variables and their relationships. Moreover, the canopy temperature delivered by S3 in combination with these information can allow parameterizing photosynthesis models to derive higher level products.

The *FLuORescence Imaging Spectrometer* (FLORIS) to fly aboard the FLEX satellite consists of two spectrometers explicitly designed to provide systematic high-resolution spectral radiance observations (0.3 nm) around the O_2-A (760 nm) and O_2-B (687 nm) absorption bands together with the continuous spectral coverage in the visible to near-infrared spectrum (500–780 nm, ≤3 nm). The technical specifications of FLORIS, in terms of spectral coverage, spectral resolution (SR), spectral sampling interval (SSI) and signal to noise ratio (SNR), are well suited for retrieving fluorescence by using spectral fitting methods (SFMs) (Mazzoni, Meroni, Fortunato, Colombo & Verhoef, 2012; Mazzoni, Falorni & Del Bianco, 2008; Mazzoni, Falorni & Verhoef, 2010; Meroni et al., 2010). These methods make use of proper mathematical functions to simultaneously model the surface reflectance (ρ) and fluorescence at different wavelengths within spectral windows confined to the oxygen absorption bands. However, FLORIS not only permits retrieving SIF at the two narrow O_2 bands with high accuracy, but it also offers a continuous spectral coverage over the entire spectral region where the fluorescence emission occurs. Taking advantage of this, spectral fitting approach can be further improved and tested over broader spectral windows with the aim of recovering the entire fluorescence emission spectrum. This could represent a relevant advancement because sun-induced fluorescence spectrum is a complex function which mainly depends on the specific emission of photosystem I (PS_I) and photosystem II (PS_{II}), and the successive re-absorption/scattering effects that occur at both leaf and canopy levels. The variability of SIF spectrum at leaf level in relation to different plant species, environmental conditions and plant's stress occurrence are documented in Agati (1998) and Van Wittenberghe et al. (2013). Therefore, the possibility of retrieving the fluorescence spectrum opens novel and promising perspectives to have a better understanding of fluorescence in relation to photosynthesis and other canopy state variables.

In this framework, the main aim of this study is to develop SIF retrieval algorithms optimized for FLORIS, and suitable for similar high-resolution sensors, based on spectral fitting methods. The specific objectives consist of: i) optimizing existing SFMs in confined spectral windows around the O_2 absorption bands; and ii) developing a novel retrieval algorithm which allows estimating SIF spectrum. The paper is structured as follows: Section 2 describes the FLEX mission providing technical details on the FLORIS instrument. Section 3 describes the radiative transfer equations used, the SIF retrieval algorithms developed, and metrics used for evaluating the retrieval accuracy. Section 4 shows and discuss the results with emphasis on the impact of atmosphere-surface directional effects. Section 5 describes a number of indices that can be derived from FLEX. The main findings of the study are summarized in Section 6.

2. The FLEX/S3 tandem mission

The FLEX satellite is expected to fly in tandem with the Sentinel-3 in a Sun-synchronous orbit at an altitude of about 815 km to deliver imagery at 300 m spatial resolution with a swath of 150 km (ESA, 2015). The revisit time will be 27 days at the Equator and more frequent acquisitions (~19 days) over high latitudes due to orbital overlaps. The lifetime foreseen of the mission is 3.5 years. The *FLuORescence Imaging Spectrometer* (Kraft, Del Bello, Bouvet, Drusch & Moreno, 2012; Kraft et al., 2013), on board of FLEX, is a pushbroom imaging spectrometer designed to detect canopy fluorescence and reflectance within a spectral range between 500 and 780 nm. The current configuration of the FLORIS instrument consists of two spectrometers: i) the *Narrow Band Spectrometer* (NBS) which provides high-resolution radiance in defined spectral ranges around the O_2-A and O_2-B absorption bands, ii) the *Wide Band Spectrometer* (WBS) characterized by a broader spectral coverage from 500 to 740 nm, with a lower spectral resolution. The spectral bands are then resampled according to a defined binning scheme providing the proper SR, SSI and SNR over the different spectral ranges. The resulting characteristics expected for a typical spectral radiance observation by FLORIS are reported in Table 1. The required SNR values synthetized in the table refer to the spectral bands, therefore the expected actual values will be higher after the spectral binning.

The combination of NBS and WBS spectra will provide both the high SR for fluorescence retrieval at the O_2 bands, and a broader spectral coverage, at the same time (Fig. 1). This particular combination of variable SRs, SSI, and the binning-scheme will provide an unprecedented SNR, which is one key factor ensuring accurate retrieval of SIF.

3. Materials and methods

3.1. Radiative transfer simulations

A dataset of radiative transfer (RT) simulations has been initially created to develop the retrieval algorithms and to assess their performances. It consists of fluorescence, reflectance and total upward radiance at top of atmosphere (TOA) and bottom of atmosphere (BOA, assumed to be equivalent to TOC, top-of-canopy) calculated by coupling the *Soil Canopy Observation Photosynthesis Energy balance* (SCOPE) (Van Der Tol, Verhoef, Timmermans, Verhoef & Su, 2009) with the *MODerate resolution atmospheric TRANsmission* (MODTRAN) RT models. In particular, the forward model used relies on the four-stream radiative transfer theory (Verhoef & Bach, 2007, 2012) with the addition of the direct and diffuse fluorescence fluxes (Verhoef, van der Tol & Middleton, 2014). It