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Hyperspectral radiative transfer modeling to explore the combined retrieval of biophysical parameters and canopy fluorescence from FLEX – Sentinel-3 tandem mission multi-sensor data

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ABSTRACT

The *FLuorescence EXplorer* (FLEX) satellite mission, selected as ESA's 8th Earth Explorer, has been designed for the measurement of sun-induced fluorescence (*F*) spectra emitted by plants. This will be accomplished through a multi-sensor approach by placing it in a common orbit in tandem with the Sentinel-3 (S3) mission, which will have two optical sensors on board, OLCI (Ocean and Land Colour Instrument) and SLSTR (Sea and Land Surface Temperature Radiometer) to complement FLEX. These S3 instruments will be used in combination with the imaging spectrometers on board FLEX to provide data useful for atmospheric correction of FLEX data. However, a fully synergetic approach, i.e. by exploiting the spectral and directional information from all tandem mission instruments together, is an attractive alternative which is explored in this paper. By employing all combined top-of-atmosphere (TOA) spectral radiance data, one can (i) characterize the relevant optical properties of the atmosphere, (ii) retrieve biophysical canopy properties including the associated reflectance anisotropy, and (iii) retrieve a more accurate and consistent canopy *F*.

Regarding retrieval methods, Fraunhofer Line Depth (FLD) and Spectral Fitting (SF) are well-known techniques applied to hyperspectral data. Both methods depend on a high spectral resolution and assume a Lambertian (isotropic) canopy reflectance. However, most vegetation canopies are non-Lambertian. This implies that, in particular when ignoring the anisotropic surface reflection, substantial retrieval errors can occur due to the interaction between atmospheric absorption bands and surface reflectance anisotropy. In this paper, a novel method based on spectral radiative transfer (RT) modeling is proposed, in which coupled RT models are used to simulate TOA radiance spectra. These are then matched with 'measured' spectra in order to retrieve surface fluorescence, along with a suite of biophysical parameters, by model inversion through optimization. By applying coupled RT models of the soil-leaf-canopy and the surface-atmosphere systems, TOA radiance spectra can be simulated for all optical sensors of this tandem mission. In this way, complex effects due to surface reflectance anisotropy and the spectral sampling by the various instruments, which are difficult to compensate for in the end products, are properly taken into account by their incorporation in the forward modeling. Next, by model inversion of TOA radiance data via optimization, the most accurate *F* retrievals can be achieved in a consistent manner, along with important canopy level biophysical parameters that may help interpret the *F* spectrum, such as chlorophyll content and leaf area index (LAI). The potential of this approach has been explored in a numerical experiment, and the results are presented in this paper. We find that, with the assumed well-characterized and plausible FLEX/S3 instrument performances, the simultaneous retrieval of biophysical canopy parameters and *F* spectra would be possible with a remarkable accuracy, provided the correct atmospheric characterization is available.

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1. Introduction

1.1. Significance of F retrievals

Sun-induced chlorophyll fluorescence (*F*) emitted by plant leaves and vegetation canopies is a sensitive indicator of plant physiological functioning, including photosynthetic activity (Lee et al., 2013). There is considerable interest in *F* for use as a direct measure of actual, rather than potential, photosynthetic activity, and possibly also as a unique early warning signal for detection of vegetation stress conditions that reduce primary production (Verhoef et al., 2014; ESA, 2015).

1.2. Results from course spatial resolution satellite sensors

Among the multitude of current or future satellite missions and/or sensors that are intended for atmospheric chemistry observations, one can identify several that might suffer from biased greenhouse gas retrievals due to interference by chlorophyll fluorescence. These include the Greenhouse Gases Observing Satellite GOSAT (Kuze et al., 2009; Yoshida et al., 2011; Hamazaki et al., 2005), the SCanning Imaging Absorption SpectroMeter for Atmospheric CHartographY SCIAMACHY (Gottwald et al., 2006; Joiner et al., 2012), the Orbiting Carbon Observatory OCO-2 (Crisp et al., 2004), the Global Ozone Monitoring Experiment GOME-2 (Callies et al., 2000) and the TROPOspheric Monitoring Instrument TROPOMI (Butz et al., 2012). Atmospheric chemistry missions make use of high spectral resolution sensors that resolve atmospheric absorption lines in the region of the oxygen A band (O_2-A, 759–770 nm) to retrieve the photon path length and aerosol optical thickness. However, this retrieval can be biased by fluorescence (*F*) emitted from the surface, since both aerosol scattering and fluorescence have an in-filling effect on the depth of atmospheric absorption lines. Fortunately, and this has been shown to work fairly well (Frankenberg et al., 2012; Joiner et al., 2012; Guanter et al., 2012; Joiner et al., 2011), *F* at one or a few wavelengths can also be estimated due to its in-filling effect at solar Fraunhofer lines outside of the O_2-A band. Next, the retrieved *F* can be applied inside the O_2-A band to correct aerosol retrievals. Since the *F* signal is very weak, its retrieval at solar Fraunhofer lines at an acceptable precision is non-trivial and can only be achieved from these coarse spatial resolution sensors by aggregating multiple observations over time and space, leading to a very modest spatial and/or temporal sampling and still a limited precision (Frankenberg et al., 2012; Joiner et al., 2011, 2016).

Comparisons of coarse resolution far-red *F* data retrieved from GOSAT have been made (Lee et al., 2013) with MODerate-resolution Imaging Spectroradiometer (MODIS) - based global maps of the enhanced vegetation index (EVI) to successfully estimate gross primary production (GPP), supported by simulations with the Soil-Canopy Observations for Photosynthesis and Energy balance (SCOPE) model (Joiner et al., 2011; Van der Tol et al., 2009). Global maps of far-red *F* have also been made using data from other satellite sensors like SCIAMACHY and GOME-2 (Joiner et al., 2012, 2013, 2016; Guanter et al., 2014). The utility of these very low spatial resolution satellite products, especially since they focus primarily on far-red *F*, is still under study.

1.3. The FLuorescence EXplorer mission

The FLEX mission is designed to provide the complete spectrum of red and far-red chlorophyll fluorescence, and additionally will do this at a high, ecologically relevant spatial resolution of ~300 m. The FLEX mission was selected in December 2015 as the Earth Explorer 8 by the European Space Agency (Drusch et al., 2008, 2016; ESA, 2015; Kraft et al., 2012). The FLEX instrument is called FLORIS (FLuORescence Imaging Spectrometer), which has two high resolution spectrometers covering different spectral ranges, one having very high spectral resolution referred to as the narrow band spectrometer (NBS, 0.3 nm resolution) and the other a wider band spectrometer (WBS, 2 nm). FLEX is specifically dedicated to the accurate retrieval of the whole fluorescence spectrum over land, and at an orders of magnitude better spatial resolution, when compared to 0.5°–1° grids or 50 km^2 blocks of the existing and proposed atmospheric chemistry missions. FLEX will fly in tandem with Sentinel-3 (S3) (Aguirre et al., 2007; Donlon et al., 2012; Drusch et al., 2016), to exploit the synergy among the sensors on board both satellites, and to retrieve not only the full *F* spectrum (650–780 nm), but also other important vegetation state variables like the leaf area index (LAI), the fraction of absorbed photosynthetically active radiation (fAPAR), the leaf chlorophyll content (LCC, indicated as C_{ab} in the remainder of this paper), the photochemical reflectance index (PRI) (Gamon et al., 1992), as well as surface temperature. This suite of measurements will enable the advancement of science through a meaningful and well-founded interpretation of the fluorescence signal. For the first time ever, the FLEX mission will provide continuous field local scale coverage for global surveys over land, monthly. This approach will enable the retrieval from space of the complete fluorescence spectrum at a sufficient precision and ground spatial resolution, to advance scientific understanding, as the FLEX mission tracks seasonal physiologic health in forests, grasslands, and agriculture.

1.4. Retrieval approaches

Changes in surface reflectance (*R*), solar induced chlorophyll fluorescence (*F*) and aerosol loads (*A*) in the atmosphere (Verhoef et al., 2014) are, in principle, simultaneously retrievable from space by spectral analysis methods, provided that these three components have spectrally distinct (linearly independent) effects on radiance spectra measured at the TOA. So, apart from good signal to noise ratio (SNR) characteristics of the sensor, the success of these retrievals will therefore also depend on the degree of linear independence of the respective spectral effects (Frankenberg et al., 2011a). This linear independence can be improved by using a wider spectral coverage and a finer spectral resolution. In particular, a high spectral resolution ($\leq$ 0.3 nm) is known to be beneficial for the retrieval of *F*, since changes in *F* can be distinguished from changes in both *R* and *A* due to its in-filling effect (Plascyk, 1975; Sioris et al., 2003) in either solar Fraunhofer or atmospheric absorption lines. Also, a wider spectral coverage sampled at a sufficiently high spectral resolution can enhance the linear independence, since over such a wider interval it becomes more likely that the effects of changes in *R*, *A* and *F* are spectrally distinct. For instance, the *F* spectrum extends over a well-defined 200 + nm range, from 640 to 850 nm, with distinct emission maxima (or peaks) at about 685 and 740 nm. The relative magnitudes of these peaks and the unique *F* spectral shape over this interval are unlikely to be found in any *A* or *R* spectra. This allows *F* effects to be distinguished from *R* and *A* effects. However, an interval of only 20 nm wide would be too narrow to examine these broad band features within the shape of the *F* spectrum, unless a very high spectral resolution is used to improve the detection of in-filling effects. But high spectral resolution must be balanced against a good SNR, which is also required to detect the weak *F* signal.

There are however several other factors which can affect the quality of *F* retrievals, such as those related to forward modeling deficiencies, instrumental defects, oversimplifications, et cetera, as pointed out by Frankenberg et al. (2011b) and Guanter et al. (2010). Modeling errors and incorrect assumptions can also have a negative effect (Frankenberg et al., 2012) on *F* retrieval accuracies when applied in practice, one of which is related to the surface anisotropy effect (expressed in the bidirectional reflectance distribution function, BRDF), which is briefly addressed in this contribution, as well as the finite width of spectral bands, which leads to an apparent violation of Beer's law, and might be confused with infilling effects. In Cogliati et al. (2015) the BRDF effect and the finite band effect on TOA radiance spectra was discussed and simulated in the context of *F* retrievals for the first time.

The FLD method (Plascyk, 1975; Sioris et al., 2003) typically makes