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Global retrieval of marine and terrestrial chlorophyll fluorescence at its red peak using hyperspectral top of atmosphere radiance measurements: Feasibility study and first results

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ABSTRACT

Chlorophyll fluorescence is directly linked to the physiology of phytoplankton or plants. Here, we present a new satellite remote sensing approach to retrieve chlorophyll fluorescence at its red peak (~685 nm) by using measurements from the hyperspectral instruments SCanning Imaging Absorption SpectroMeter for Atmospheric CHartographY (SCIAMACHY) and Global Ozone Monitoring Experiment-2 (GOME-2). This method, which is based on the Differential Optical Absorption Spectroscopy (DOAS) technique, was used to exploit narrow spectral structures resulting from the filling-in of the Fraunhofer Fe I line, which originates from fluorescence. The reference spectra for chlorophyll fluorescence were calculated by the coupled ocean–atmosphere radiative transfer model SCIATRAN. We compared our results on marine chlorophyll fluorescence observations with the MODIS Terra normalized Fluorescence Line Height (nFLH) product for the average of years 2003–2011 and year 2009. Our method also enables the retrieval of chlorophyll fluorescence above land vegetation scenes. The results for the fluorescence observed above terrestrial vegetation for July and December 2009 were compared to MODIS Enhanced Vegetation Index (EVI). The comparisons show good spatial agreement between different retrievals providing evidence for the good performance of our algorithm. The method presented is generic and can be applied to other hyperspectral instruments in the future. Having established the retrieval technique, extensive studies of chlorophyll fluorescence will improve global knowledge on physiology and photosynthetic efficiency, in both the marine and terrestrial realms, and its dependence on environmental factors.

1. Introduction

Marine and terrestrial carbon pools are important reservoirs in the carbon cycle, and they absorb a significant part of the emitted carbon dioxide from fossil fuel combustion (IPCC, 2013). It is clear that due to land-use changes worldwide, areas of pristine vegetation have been decreasing, *e.g.*, the deforestation of the rainforest. With respect to the oceanic biosphere, there is an ongoing discussion about the changes in health, composition and abundance of phytoplankton (Doney et al., 2012). It has been reported that the biomass of phytoplankton has declined significantly in the last decades at all scales (Boyce, Lewis, & Worm, 2010; Gregg, 2003) and this decline is expected to continue (Hofmann, Worm, Rahmstorf, & Schellnhuber, 2011; Olonscheck, Hofmann, Worm, & Schellnhuber, 2013). However, the results of Boyce et al. (2010) have been questioned (Mackas, 2011; McQuatters-Gollop et al., 2011; Rykaczewski & Dunne, 2011), and studies showing the opposite sign have been published claiming that phytoplankton has been increasing within the last years on both regional (*e.g.*, McQuatters-Gollop et al., 2007) and global scales (Gregg, Casey, & McClain, 2005). Other studies have also shown that the ocean regions should be studied separately, as there are opposite trends for different regions worldwide (Siegel, 2010; Wernand, van der Woerd, & Gieskes, 2013).

Phytoplankton is responsible for about half of the estimated global net primary production of carbon (Field, 1998). Moreover, because of a rather short turnover rate of phytoplankton organic matter, in the order of a week (Falkowski, 1998), and changing phytoplankton growth conditions in response to changing physical and chemical parameters of the ocean, phytoplankton abundance and community structure constantly change in time and space. Consequently, in order to assess accurately the amount of phytoplankton and to identify its change, global observations require a reasonable temporal and spatial resolution in order to resolve their intrinsic natural variability. Observations from instrumentation on polar orbiting sun synchronous satellites have facilitated the study of changes in the phytoplankton biomass having a temporal sampling of a day and a spatial resolution on the order of a km. Recently, in addition to chlorophyll concentration products, ocean color products of other oceanic parameters have also been retrieved from measurements made by satellite-based instrumentation, *e.g.*, particulate organic

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carbon, particulate inorganic carbon, euphotic depth, and fluorescence line height (*e.g.*, see http://oceancolor.gsfc.nasa.gov).

Information about chlorophyll fluorescence has been used to assess the physiological state of phytoplankton, as a result of its relationship to photosynthetic efficiency (Falkowski & Kolber, 1995). Photosynthesis is the process by which light energy is transformed into chemical energy and fixes atmospheric carbon dioxide into sugars. Oxygenic photosynthesis is responsible for virtually all of the biochemical production of organic matter (Field, 1998). The first elementary step in photosynthesis, the absorption of solar radiation in the visible part of the spectrum, takes place in the thylakoid membrane, where two pigmented functional units, photosystem II (PS II) and photosystem I (PS I), are located. Photosystems carry out the primary photochemistry of photosynthesis: the absorption of light and the transfer of energy and electrons. When chlorophyll-a (chl-a) molecules absorb light, a fraction of the energy absorbed is re-emitted as fluorescence. Although both photosystems contain chl-a pigments that contribute among other pigments to light absorption, the majority (95%) of fluorescence originates from chl-a of PS II and only a small contribution is emitted from PS I (Krause & Weis, 1991). However, for the second peak of fluorescence at longer-wavelengths (~735 nm), PS I can contribute up to 40% to the fluorescence signal (Agati, Cerovic, & Moya, 2000).

In vivo, the efficiency of fluorescence is around 1% (Behrenfeld et al., 2009; Maxwell, 2000 and references therein). The fluorescence signal is clearly stronger in regions with high phytoplankton biomass and low in depleted areas, as the fluorescence of chl-a occurs only when the molecule is present in the water column. The relationship between fluorescence and chl-a is curvilinear as a result of pigment packaging. This is because fluorescence is proportional to the concentration of the excited electronic state of chl-a, which depends on the number of photons absorbed by chl-a and the quenching and other reactions of this excited state. As incident irradiance is highly variable (due to clouds, surface wave focusing, *etc.*), phytoplankton use three processes to protect themselves from excessive solar electromagnetic radiation: photoadaptation, photoacclimation and photoregulation (Huot & Babin, 2010). When incident photosynthetically active radiation (iPAR) increases, the absorbed light energy proportionally increases, but the absorbed energy for charge separation and photochemistry is limited. As photochemistry saturates, the fluorescence increases; however, additional processes are invoked to dissipate the excess energy in order to minimize photodamage. These processes are collectively termed non-photochemical quenching (NPQ) and they dissipate excess absorbed energy as heat.

Chl-a fluorescence changes in response to phytoplankton physiology. Consequently, monitoring these changes could be helpful in the characterization of photosynthesis, health and the productivity of oceans at global scales (Babin, Morel, & Gentili, 1996; Lichtenthaler & Rinderle, 1988). For example, they reflect the effect of nutrient limitations, *e.g.*, macro-nutrients (Abbott & Letelier, 1999; Schallenberg, Lewis, Kelley, & Cullen, 2008) or iron (Behrenfeld et al., 2009). Chl-a fluorescence also depends on species composition (MacIntyre, Lawrenz, & Richardson, 2010) and growth irradiance, *i.e.*, irradiance that phytoplankton has experienced during the growth phase of the cells and hence to which it is acclimated (*e.g.*, Morrison & Goodwin, 2010; O'Malley et al., 2014).

The marine chl-a fluorescence has been retrieved from space by the multispectral instruments MODIS and MERIS. The fluorescence line height algorithm (FLH) designed for MODIS (Abbott & Letelier, 1999), later also applied to the MERIS instrument (Gower, Brown, & Borstad, 2004), derives the strength of the fluorescence signal by comparing radiance in the fluorescence channel to background radiance. MODIS and MERIS are high spatial resolution low spectral resolution instruments, both having bands in the visible spectral region dedicated to fluorescence measurements. For MODIS, the radiances are measured in three channels in 10 nm windows, two of which are used to account for other effects (backscatter and Raman scattering) by calculating the 'baseline radiance' for fluorescence through interpolation of measurements at 667 nm (band 13) and 748 nm (band 15), the latter one being far from fluorescence emission due to water vapor absorption lines near 730 nm. The third band, the fluorescence band, is centered at 678 nm (band 14). This band does not cover the maximum of the fluorescence signal at 685 nm in order to avoid oxygen absorption features (Abbott & Letelier, 1999). Because of these limitations on band placement, the measured MODIS FLH will respond to only 57% of the actual fluorescence signal (Gower et al., 2004). In the case of the MERIS instrument, the FLH algorithm uses bands 7, 8 and 9, located at 665 nm, 681 nm and 709 nm, respectively, and hence measured MERIS FLH will respond to 78% of the actual fluorescence signal (Gower et al., 2004). FLH is calculated with water leaving radiances, while nFLH (normalized FLH) uses normalized water leaving radiances. The schematic of the algorithm and corresponding positions of relevant MODIS and MERIS bands are shown in Fig. 1. Using the following algorithm, nFLH for MODIS is calculated:

$$\mathrm{nFLH} = L_{WN,14} - L_{WN,15} + \left(L_{WN,13} - L_{WN,15}\right) * \left[\left(\lambda_{15} - \lambda_{14}\right)/\left(\lambda_{15} - \lambda_{13}\right)\right], \quad (1)$$

where L_{WN} are the normalized water leaving radiances of the MODIS band number given by the subscript; nFLH is currently a MODIS Level 3 standard product (available online at http://oceancolor.gsfc.nasa.gov/cgi/l3).

MODIS nFLH delivered the first global picture of marine fluorescence and initiated global studies of phytoplankton physiology and productivity (Behrenfeld et al., 2009; Huot, Franz, & Fradette, 2013; McKibben, Strutton, Foley, Peterson, & White, 2012; Morrison & Goodwin, 2010; Westberry, Behrenfeld, Milligan, & Doney, 2013). However, detecting a weak fluorescence signal accurately is challenging. Atmospheric correction applied to multispectral data makes several assumptions about atmospheric effects for different wavelength regions and the nFLH algorithm assumes the shape of the emission function. In case of the MODIS nFLH retrieval, further problems may arise from backscattered light by particulate matter that scatter light in the red wavelengths and from which some nFLH signals originate (Abbott & Letelier, 1999). Negative values of nFLH were also observed during blooms of some cyanobacteria species (Wynne et al., 2008), which was later used for a cyanobacterial bloom forecast system in Lake Erie (Wynne, Stumpf, Tomlinson, et al., 2013).

We present in this manuscript a new method for the detection of phytoplankton fluorescence utilizing hyperspectral measurements. Hyperspectral satellite data are not traditionally used in optical remote sensing of the oceans, but have already proven to be an interesting and useful tool in studies of the photic zone by identifying vibrational Raman scattering and phytoplankton composition (Bracher et al., 2009; Sadeghi et al., 2012; Vountas, Dinter, Bracher, Burrows, & Sierk, 2007). The hyperspectral instrument TANSO-FTS onboard the Japanese GOSAT satellite has been used to detect land fluorescence (Frankenberg et al., 2011; Guanter et al., 2012; Joiner et al., 2011) with promising results. Unfortunately, the method developed for fluorescence from terrestrial plants, cannot be used for marine chl-a fluorescence, because TANSO-FTS does not observe wavelengths of visible phytoplankton fluorescence emission. More recently, the land fluorescence signal was also retrieved from the GOME-2 instrument (Joiner et al., 2013), which also covers the spectral range of marine fluorescence.

We present in this manuscript a new approach to retrieve the chl-a fluorescence signal, emanating from the marine and the terrestrial biosphere, from measurements of nadir sounding hyperspectral passive remote sensing spectrometers. The retrieval has been developed using the level 1 SCIAMACHY (SCanning Imaging Absorption SpectroMeter for Atmospheric CHartographY) data, but has also been applied to data from GOME-2 (Global Ozone Monitoring Experiment-2). The method developed is generic and can also be applied to other hyperspectral instruments. In this feasibility study we demonstrate that the hyperspectral