# Remote sensing of coccolithophore blooms in selected oceanic regions using PhytoDOAS method applied to hyper-spectral satellite data

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## Abstract

Phytoplankton, as the main oceanic primary producers, play a crucial role in the marine food-chain, as well as playing an important role in the global carbon cycle, due to photosynthesis and biological carbon pumping. On the other hand, because of their sensitive responses to ecological impacts, they are reliable indicators for monitoring the variations of climate factors and anthropogenic contributions. Ocean color remote sensing often utilizes satellite data providing continuous observations of phytoplankton biomass on a global scale. As different phytoplankton species cause different bio-geochemical impact, the identification of phytoplankton groups using satellite data has been recently of great interest (e.g., Bracher et al., 2009). Studying the bloom cycles of specific phytoplankton functional types (PFTs, Nair et al., 2008), in terms of spatial and temporal variations of their abundance, is now regarded as a method to follow annual and inter-annual variations in climate impacts (Winder et al., 2010). Among different phytoplankton blooms, coccolithophore blooms, dominated by *Emiliania huxleyi* species, are very important due to their wide coverage and frequent occurrence (Holligan et al., 1983), as well as their unique bio-optical and bio-geochemical properties (Brown et al., 1997). In this study the PhytoDOAS method (according to Bracher et al., 2009 and improved by Sadeghi et al., submitted in 2010) has been applied to the satellite data of the sensor SCIAMACHY (a hyper-spectral sensor on-board ENVISAT) to detect coccolithophore E. huxleyi blooms in three selected oceanic regions. To monitor the bloom cycles, eight years of SCIAMACHY data have been processed, classifying the blooms based on a threshold value for monthly averaged chl-a concentration. The retrieval results, shown as time series, were also compared to corresponding satellite data.

Keywords: PhytoDOAS, Phytoplankton Functional Types (PFTs),

Preprint submitted to Elsevier

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coccolithophore bloom,  $Emiliania\ huxleyi,$ Particulate Inorganic Carbon (PIC), MODIS-Aqua, GlobColour Chla

# 1. Introduction

## 1.1. Background

Oceanic phytoplankton are considered to play a vital role in marine primary production and marine ecosystem, as well as in oceanic biogeochemical cycles, including carbon cycles (Raven et al., 1999), through which they have a major influence on global climate. Because of these features, it has been in recent decades of great interest to monitor regularly the distribution and development of marine phytoplankton on a global scale, which corresponds to a large research framework, called ocean-color remote sensing (e.g., Platt et al., 1988). In this field mainly bio-optical empirical algorithms (e.g., O'Reilly et al., 1998) and semi-analytical algorithms have been developed to retrieve water chlorophyll-a content, as an indicator of phytoplankton biomass (Falkowski et al., 1998), using water-leaving radiance detected by satellite sensors at specific wavelengths. However, due to phytoplankton biodiversity and differences in optical properties of phytoplankton groups, improving current algorithms or developing new retrieval methods have been often demanded, in order to identify remotely different phytoplankton functional types (PFTs; see summary by Nair et al., 2008). This would help have better estimation of total phytoplankton biomass, as well as reach a deeper understanding of oceanic biogeochemical cycles. Based on this demand, PhytoDOAS method was established (Vountas et al., 2007) as an extension of DOAS into aquatic media to retrieve specific phytoplankton groups. This is done by including absorption spectra of target PFTs and applying the method to hyper-spectral satellite data, which is provided by SCIAMACHY sensor (on-board ENVISAT). Using PhytoDOAS method Bracher et al. (2009) were able to obtain global distribution of two main phytoplankton groups: diatoms and cyanobacteria and later on, by improving the method, another major PFT, coccolithophores, was successfully distinguished (Sadeghi et al., submitted in 2010).

# 1.2. Why coccolithophore bloom?

Coccolithophores are a large group of marine phytoplankton with the characteristic of building calcium carbonate (CaCO3) plates, called coccoliths, which makes them the main planktonic calcifer in the ocean (Westbroek *et al.*, 1985). Through building and releasing coccoliths, coccolithophores have an important role in total content of Particulate Inorganic Carbon (PIC or CaCO3) in open oceans (Milliman, 1993). PIC represents about 1/4 of all marine sediments (Broecker and Peng, 1982), for which it is regarded as a major oceanic sink for atmospheric CO2. PIC also has interaction with the rate of ocean acidification due to the change in the total amount of pCO2 (Balch & Utgoff, 2009). In the same context, increased oceanic CO2, which is a response to increase in antropogenic CO2 in the atmosphere, affects the rate of calcification by coccolithophores, as defecting the supersaturation state of carbonate ion (Riebesell et al., 2000). Moreover, falling down through water column and getting deposited in sediment (either directly as coccoliths and detritus or after dessolving into PIC), coccolithophores are considered to be one of the main drivers of biological carbon pump (Thierstein & Young, 2004). Increased CO2 affects the rate of calcification CoccolithophoresIncreased CO2 affects the rate of calcification Coccolithophores On the other hand, due to having bright calcite shells (coccoliths), coccolithophores cause a very high reflectance from the ocean surface. Coccolithophores are also known because of forming large scale and frequent occurrence of blooms (Holligan et al., 1983), where they impact widely the light field in upper ocean (Ackleson et al., 1988; Balch et al., 1989). Moreover, it was shown that large blooms of diatoms are replaced by coccolithophores blooms due to the limitation of nitrate or silicate through the former blooms (Holligan et al., 1983). The dominant species within the coccolithophore group is *Emilia*nia huxleyi. E. huxleyi is known to be a significant producer of dimethylsulfide, DMS (Keller et al., 1989; Malin et al., 1993), which affects the planetary albedo (Charlson *et al.*, 1987). All these aspects justifies those studies who attempt to exploit and develop remote sensing methods for monitoring distribution of coccolithophore on a global scale, as well as studying corresponding blooms on regional scale.

## 1.3. Objectives

Two sets of objectives have been conducting this study. Firstly, as we are developing a new retrieval method for remote identification of phytoplankton groups (PhytoDOAS: Bracher et al., 2009), a cocolithophore bloom is indeed an appropriate target for us to test this method and expand it to another important PFT, i.e., E. huxleyi. In this respect taking coccolithophores, as the next retrieval target for expanding PhytoDOAS method, was motivated by the study suggesting that coccolithophores succeed diatoms in response to increasing stabilization and nutrient depletion of surface waters (Margalef 1978). This would also compensate, to some extent, the shortage of in-situ data. Secondly, due to the crucial role of coccolithophores in oceanic biogeochemical cycles, we are aiming to establish a new detection method for their blooms, which in contrast to current methods (mostly based on band-ratio algorithms), would take other factors as well into account, including: PFTs' absorption spectra, existence of multiple PFTs and water penetration depth. For instance, while other phytoplankton pigments cause a decrease in backscatter radiance mostly in the blue part (slightly in the green), coccolithophores, due to their calcite plates, affect the solar radiance uniformly in both the blue and green (Gordon *et al.*, 1988). Thus remote sensing of coccolithophores requires an understanding of the actual water-leaving radiance rather than just radiance ratios. Furthermore, as coccolithophore blooms cause flattening of the reflectance spectrum, the standard ratio pigment algorithms (Gordon and Morel, 1983) will not provide correct pigment retrievals within the blooms (Balch et al., 1989; 2004).

# 2. Method and Material

## 2.1. Method overview: Principles of PhytoDOAS

PhytoDOAS is an extension of DOAS (Differential Optical Absorption Spectroscopy) to water medium to retrieve marine phytoplankton in case I waters. DOAS, which is based on Beer-Lambert law and very sensitive to highly varying spectral features, is a method for retrieving atmospheric trace gases from their absorption cross-sections (Platt & Perner, 1979; Platt, 1994). However, in PhytoDOAS, in addition to the cross-sections of water vapor, all atmospheric trace gases active in visible range and the spectral signature of the Ring effect, the absorption spectra of target PFTs are also needed, which are mainly measured in lab after being sampled in oceanic campaigns. The optical behavior of other water components, like absorption and scattering of CDOM (colored dissolved organic matter) and non-phytoplankton particulates are simply covered by a polynomial, due to their spectral smoothness. On the other hand, according to Vountas et al. (2007), to have an estimation of water penetration depth, Vibrational Raman Scattering (VRS) of water molecules (inelastic scattering) is fitted separately for the region of study. Finally, for each water-pixel the average concentration of chl-a in water column for the target PFT is calculated by dividing the fit-coefficient of PFT absorption spectrum by corresponding fit-coefficient of VRS. The calculation core of PhytoDOAS is based on the leastsquare optimization. The optimization process here referes to the minimization of the residual difference between satellite measurement of optical depth and its retrieval counterpart from fitting process. Optical depth measured by satellite is obtained by dividing solar reference spectra and backscattered radiation from the earth. To rebuild the optical depth by retrieval, after including all existing absorbtion spectra along the light-path (extending into water body), their corresponding coefficients are adjusted via fitting process. (see Bracher et al., 2009) and Sadeghi et al., submitted in 2010).

# 2.2. Satellite data

Satellite data used in PhytoDOAS must be spectrally highly resolved. This requirement is met using the date collected by SCIAMACHY (SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY), a sensor onboard ENVISAT (ENVIronmental SATellite of European Space Agency, ESA) launched in 2002. This sensor was originally designed for atmospheric measurements and covers a wide wavelength range (from 240 nm to 2380 nm in 8 channels) with a relatively high spectral resolution, ranging from 0.2 nm to 1.5 nm for its scanning channels over the range 240 nm to 1700 nm (Bovensmann *et al.*, 1999). In this study, nadir-viewing geometry of SCIAMACHY data in UV and visible ranges have been used, for which the spectral resolution is ranging from 0.24 nm to 0.48 nm. These data include backscatter solar radiation from the Earth's surface, with a spatial resolution of about 30 km x 60 km, and solar radiation at the top of the atmosphere in the same wavelength range, the latter of which is regarded in the retrieval process as the reference measurement. Within the retrieval process of PhytoDOA, SCIAMACHY data

are exploited in the two following aspects: First, using the visible data, the absorption spectra of target PFTs are fitted within the fit-window of 429 nm to 521 nm. This provides us with the PFTs' absorption fit-factors; secondly, part of SCIAMACHY UV data, from 340 nm to 385 nm, are used to fit the VRS spectral signature of water molecules, which is needed for the calculation of light penetration depth. In addition to SCIAMACHY data, which are needed as the satellite input of PhytoDOAS, to copmare and evaluate the retrieval results, specific products of two other satellite sensors have been used: total chl-a from GlobColour data-bank and Particulate Inorganic Carbon (PIC) from MODIS-Aqua products. MODIS-Aqua is a NASA near-polar sun-synchronous sensor viewing the entire Earth's surface every 1 to 2 days, acquiring data in 36 spectral bands (for details see the webpage of MODIS: http://modis.gsfc.nasa.gov/). GlobColour is an ESA project of ocean-color data, providing merged data from 3 major ocean-color sensors: MODIS-Aqua, MERIS and SeaWiFS (for details see the GlobColour webpage:http://www.globcolour.info)

# 2.3. Reference spectral data

In addition to hyper-spectral satellite data, PhytoDOAS retrieval requires reference spectra of atmospheric and oceanic species. Atmospheric spectra, including absorption cross sections of ozone, NO2, glyoxal, iodine oxide, O4, water vapour and also the spectral signature of the Ring effect (used as a pseudoabsorber spectrum) were taken the same as in Bracher et al., (2009). The second set of reference spectra corresponds to oceanic components, including the VRS spectral signature of water molecules and the absorption spectra of target PFTs. The VRS spectrum used in this study has been obtained through a modeling approach (Vountas et al., 2003, 2007). The phytoplankton absorption spectra include the spectra of three different target species: *Emiliania huxleyi*, dinoflagellates and diatoms. The absorption spectrum of E. huxleyi was measured from a culture, with a Point-Source Integrating-Cavity Absorption Meter (PSICAM, see Röttgers et al., 2007). A dinoflagellate dominated sample (over 92%), taken from a bloom during the OOMPH field experiment (with RV Marion Dufresne on 2 February 2007, at  $59.88^{\circ} W$  and  $46.01^{\circ} S$ ), was used to obtain the corresponding absorption spectrum. As the third phytoplankton reference spectrum, the absorption spectrum of diatoms was acquired from the in-situ measurements conducted during a cross-Atlantic research cruise (EIFEX, with RV Polarstern, on 14 March 2004, at  $9^{\circ}W$  and  $46^{\circ}S$ , where diatoms were donminant (over 80%). The process of measurement of specific absorption spectra of dinoflagellates and diatoms has been explained in Bracher et al., (2009). This process mainly includes the HPLC pigment analysis (based on Hoffmann et al., 2006) and then applying the results into CHEMTAX program (Mackey et al., 1996) in order to specify taxonomic groups and their contributioning within the water samples. Fig. 1 shows the specific absorption spectra of the three PFTs used as the retrieval targets in this study and also their so-called differential absorption spectra, being used as input spectra in PhytoDOAS, after subtracting their low-order polynomials. terial in the water.



Figure 1: Upper panel shows the specific absorption spectra of *E. huxleyi* (green), dinoflagellates (red) and diatoms (blue). The first one was obtain from a culture sample and the two latter spectra were obtained from in-situ measurements. The lower pannel depicts the differential absorption spectra of given spectra, after subtracting each of them from their two-order polynomial. The latter spectra are the target PFT input for the PhytoDOAS retrieval

# 3. Initial tests and Setup of the study

#### 3.1. Initial tests

Through a recent improvement to PhytoDOAS (Sadeghi *et al.*, submitted in 2010), the method was applied to several sets of PFTs and it was observed that for specific sets of PFTs, simultaneous fit (multi-target fit) would result in better retrievals within an opptimized fit-window. Furthermore, it has been shown that the combination of diatoms, dinoflagellate and *E. huxleyi* leads to better retrieval, especially for *E. huxleyi*. Based on this finding, single events of coccol-ithophore blooms have been detected successfully (e.g., a coccolithophore bloom near Chatham Islans reported by NASA in Dec. 2009 and another bloom south to Iceland in July 2005). Then long-term averages of *E. huxleyi*, as monthly and seasonal means, were processed globally (all derived by multi-target fit of SCIAMACHY data) and were compared to corresponding coccolithophore model data, e.g., NOBM. The comparisons showed good agreement in the magnitude of chl-a concentrations of coccolithophore monthly and seasonal means,

which was again an approval to the method improvement. A sample comparison is shown in Fig. 2, which depicts the globla distribution of PhytoDOAS E. *huxleyi* and NOBM coccolithophores based on seasonal means of chl-a.



Figure 2: Comparison of the PhytoDOAS retrieval result in triple-target mode for *E. huxleyi* from SCIAMACHY data (upper panel) to the NOBM assimilated data (lower panel, obtained from NASA Giovanni project), over the northern spring (Apr/May/Jun.) 2005.

# 3.2. Setup of the study

The basic idea was monitoring the development of coccolithophore blooms in regions of their most occurrence to track the cycles and intensities of the blooms and their probable variations. To select the appropriate regions to be focussed in this study, three sources have been used: first, a global distribution of coccolithophore, mapped by Brown & Yoder (1994) was considered; secondly, 9 years of variation in global distribution of Particulate Inorganic Carbon, PIC, (which is a good proxy for coccolithophores) have been studied from MODIS-Aqua level 3 monthly products; and finally some coccolithophore field studies have been regarded (e.g., Brown & Podesta, 1996; Balch *et al.*, 1991; Garcia *et al.*, 2010). Based on this pre-investigation, three regions have been selected, which, as shown in Fig. 3, are located in North Atlantic (south to Iceland), Southwest Atlantic (north to Falkland Islands) and South Pacific (southwest to New Zealand). For inter-comparison purpose, these selected regions all have the same area-size, 10°x10°, and they have been labled for simplicity as: nAtl, sAtl and sPAc respectively. Expectedly, two regions (sAtl and sPAc) are located in Great Calcit Belt (Balch 2010), a great belt of elevated PIC concentrations all the way around the Southern Ocean near the sub-Antarctic front and polar front (an latitudinal belt between about  $30^{\circ}S$  and  $60^{\circ}S$ , which contains over one-third of all global PIC). For each selected region, we applied PhytoDOAS multi-target fit, in the manner explained in previous section, to more than 8 years of SCIAMACHY data (from Aug. 2002 to Dec. 2010) to retrieve E. huxleyi. Using the retrieval results, a time-series of E. huxleyi for each region was built up in a monthly-mean basis over 8 years of data. Then we used PIC monthly data from MODIS-Aqua level 3 products, in order to produce corresponding time-seris for selected regions over the same period. Finally, we built up another time-seris using total chl-a, obtained from GlobColour daily products, after being processed into monthly means.



Figure 3: Selected regions for monitoring the development of coccolithophore blooms in this study. These regions were chosen based on several coccolithophore field studies reported by Brown & Yoder 1996, Balch *et al.* 1991, Garcia *et al.* 2010, etc., and also after tracking ten years of global variation of PIC product from MODIS-Aqua reported in NASA OceanColor data-bank. For comparison purpose, each region has the same size of 10x10 and for simplicity, regions 1, 2 and 3 have been named as nAtl, sAtl and sPac respectively.

## 4. Results of coccolithophore bloom developments

# 4.1. Time series of 3 products in 3 selected region

Figures 4, 5 and 6 show the time-series of three retrieved products from Aug. 2002 to Dec. 2010 separately over selected regions. Each time-series is associated with a trend. In depicting these time-series and consequently in calculation of their corresponding trends, those data points either with low number of pixels or with high amount of standard deviation had been removed (in satellite remote

sensing, especially in visible range, the data can be simply spoiled by clouds over the study region or other source of obscureness). However, these timeseries comprise the core results of this study. Other subsidary results have been be extracted from these time series for beter description and analysis. When following the time-series, it should be noted that in x-axis the month index has been labled with a half-year interval.



Figure 4: Time-series of three retrieved products over region 1 (nAtl) from Aug. 2002 to Dec. 2010: PhytoDOAS *E. huxleyi* (green), GlobColour total chl-a (red) and MODIS-Aqua PIC concentration(blue)



Figure 5: Time-series of three retrieved products over region 2 (sAtl) from Aug. 2002 to Dec. 2010: PhytoDOAS *E. huxleyi* (green), GlobColour total chl-a (red) and MODIS-Aqua PIC concentration(blue)

# 4.2. Anomalies and Climatology of PhytoDOAS E. huxleyi

Figures 7, 8 and 9 show the anomalies of PhytoDOAS *E. huxleyi* over selected regions within the period of study. Here each *E. huxleyi* time-series is associated



Figure 6: Time-series of three retrieved products over region 3 (sPac) from Aug. 2002 to Dec. 2010: PhytoDOAS *E. huxleyi* (green), GlobColour total chl-a (red) and MODIS-Aqua PIC concentration(blue)

with errorbars corresponding to data points. Below each *E. huxleyi* time-series, corresponding anomaly curve has been depicted, for which each data point was acquired by subtracting current monthly-average value from total-average over whole 8 years data for that specific month.



Figure 7: Anomaly of PhytoDOAS *E. huxleyi* over region 1 (nAtl) from Aug. 2002 to Dec. 2010. Original time-series is depicted on the top in dark-brown and corresonding anomaly curve is shown below in black. Both curves are associated with related trends

Figure 10 shows three climatology curves of PhytoDOAS *E. huxleyi* results separately over selected regions. Each data point here depicts the difference between monthly average for each specific month over the whole 8 years and the total average, having all months included. This figure provides an overall comparison of bloom development in selected regions during a typical year (overall behaviour was extracted by averaging monthly chl-a values over 8 years).



Figure 8: Anomaly of PhytoDOAS *E. huxleyi* over region 2 (sAtl) from Aug. 2002 to Dec. 2010. Original time-series is depicted on the top in violet and corresonding anomaly curve is shown below in black. Both curves are associated with related trends

#### 4.3. Scatter plots and correlations

Here are the scatter-plots of all three retrieved products over selected regions from Aug.2002 to Dec. 2010:

### 5. Discussions and Analysis

From the time series (6.1), it can be clearly seen that all three methods indicate the bloom cycles in a regular order and fairly good accordance to each other. According to the main time-series (figures 4, 5 & 6), the best accordance between three methods (products) belongs to region 1 (nAtl), where all 3 quantities indicate positive trends. The intensity of blooms are lower in region 3 (sPac), where PhytoDOAS E. huxleyi in average has surprisingly higher values than GlobColour total chl-a. The cyclical period in each region is almost constant, with some annual variations for all 3 products in blooming time and their bloom intensities. This can be assigned basically to the inter-annual regional changes in ocean and climate conditions and also to some extent to the retrieval errors. For PhytoDOAS E. huxleyi this fluctuation in cycles together with monthly irregularities are shown in figures 7, 8 & 9, where monthly anomalies have been depicted. Interestingly, based on comparison of E. huxleyi climatology curves, it can be inferred that in southern oceans (regions 1 & 2) two coccolithophore blooms are observed annually; This phenomenon was referred by Balch (2010) as well. As a short overview to the trend results, all trends associated to the time-series are listed below in table 1 and all correlation coefficients between different retrievals are listed in table 2. The fact that PIC and total chl-a are better correlated with each other than each of them with E. huxleyi, can be explained by several reasons: first, in comparison of GlobColour total chl-a and PhytoDOAS E. huxleyi it should be noted that even in the best retrieval, very high correlation will not be expected, because



Figure 9: Anomaly of PhytoDOAS *E. huxleyi* over region 3 (sPac) from Aug. 2002 to Dec. 2010. Original time-series is depicted on the top in orange and corresonding anomaly curve is shown below in black. Both curves are associated with related trends

*E. huxleyi* is not the only PFT, whose chl-a pigment is accounted in total chl-a; secondly, this is also possible that, contrary to our pre-assumption, other species of coccolithophores is dominant in a coccolithophore bloom event; and finally, the third reason refers to the differences in the data sources: GlobColour total chl-a and MODIS-Aqua PIC product are obtained through similar retrieval algorithms, whereas PhytoDOAS is representing a completely different retrieval method. Additionally, GlobColour's merged data contain MODIS-Aqua data as one of its three data sources. Moreover, the SCIAMACHY sensor has a much coarser spatial resolution than MODIS-Aqua( 30 x 60 km compared to 9 km respectively).

#### 6. Conclusions and Outlook

The PhytoDOAS retrieval method can be reliably used for remote identification of E. huxleyi and tracking its bloom developments in global ocean. Based on the results for region 1, nAtl, where the 3 methods have their best correlation, we can infer (due to the positive trends) that at least for this region E. huxleyi and thus coccolithophores have been growing over the last decade. PhytoDOAS E. huxleyi retrieval will be validated with available in-situ measurements. The process will be repeated for some other regions, to check how important or casual are the different behaviours in region 2 (negative total trend) and region 3 (higher E. huxleyi than total chl-a). More investigation about the regional climate and oceanic conditions will be done, for better analysis and interpretation of the results for each region. for instance, it was already clear for us that around New Zealand, the dominant coccolithophore species is not E. huxleyi, but gephyrocapsa oceanica, which compared to E. huxleyi has much more chl-a pigment content in its cell. This fact could explain why in region 3 (sPac) the PhytoDOAS retrieved chl-a is surprisinglly higher than GlobColour total chl-a.



Figure 10: Climatology curves of PhytoDOAS *E. huxleyi* over 3 selected regions. region 1: nAtl (dark-brown); region 2: sAtl (violet) and region 3: sPac (orange)

Similarly, the irregularities observed in the time-series of region 2 (sAtl) might be correlated to the irregularities in the dost-loads originating from the Patagonian desert, which can change the nutrients' regime in the region of study. Both these probable influencing factors demand suplementary precise regional studies.

## Acknowledgements

We thank to: AWI, Helmholtz Impulse Fund (PHYTOOPTICS project); MODIS-Aqua and GlobColour teams for providing PIC and chl-a data respectively; We also thank ESA, DLR and SQWG for SCIAMACHY level-1 data, NASA-GSFC for NOBM data and SCIAMACHY group in IUP for technical supports. Many thanks to ESSReS research school and Klaus Grosfeld for suplementary supports to the first author.

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