OBSERVATION OF DIFFERENT PHYTOPLANKTON GROUPS AND BIOMASS USING DIFFERENTIAL OPTICAL ABSORPTION SPECTROSCOPY ON SCIAMACHY DATA AND COMPARISONS TO IN-SITU, NASA OCEAN BIOGEOCHEMICAL MODEL AND MERIS ALGAL-1 DATA

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ABSTRACT

In order to understand the marine phytoplankton's role in the global marine ecosystem and biogeochemical cycles it is necessary to derive global information on the distribution of major functional phytoplankton types (PFT) in the world oceans. In our study we use instead of the common ocean color sensors such as CZCS, SeaWiFS, MODIS, MERIS, with rather low spectral resolution, the Differential Optical Absorption Spectroscopy (DOAS) to study the retrieval of phytoplankton distribution and absorption with the satellite sensor Scanning Imaging Absorption Spectrometer for Atmospheric Chartography (SCIAMACHY). SCIAMACHY measures back scattered solar radiation in the UV-Vis-NIR spectral region with a high spectral resolution (0.2 to 1.5 nm). We used in-situ measured phytoplankton absorption spectra from three different RV Polarstern expeditions where different phytoplankton groups were representing or dominating the phytoplankton composition in order to identify these characteristic absorption spectra in SCIAMACHY data in the range of 430 to 500 nm. In addition also SCIAMACHY data were analysed with DOAS in the range of 530 to 590 where absorption from cyanobacterial photosynthetic pigment phycoerythrin was identified. Our results show clearly these phytoplankton assemblage absorptions in the SCIAMACHY data. The conversion of these differential absorptions by including the information of the light penetration depth (according to Vountas et al. 2007) leads to globally distributed concentrations for these characteristic phytoplankton groups, but also for a well mixed phytoplankton assemblage (corresponding to ocean chl a). Phytoplankton concentrations have been determined for three monthly periods (Feb-March 2004, Oct-Nov 2005 and Nov 2007). The information retrieved by DOAS from SCIAMACHY on phytoplankton groups and chl a is compared to collocated in-situ measurements, MERIS algal-1 data and to the global model analysis with the NASA Ocean Biogeochemical Model (NOBM from http://reason.gsfc.nasa.gov/OPS/Giovanni/) according to Gregg and Casey 2006). Results are of great importance for global modelling of marine ecosystem and climate change studies regarding changes in the ocean.

1. INTRODUCTION

The aim of this study is to substantially improve the estimation of global marine primary production and phytoplankton distribution by retrieving until today missing biooptical parameters from space in the world's ocean case-1 waters. This is a major contribution for a better understanding of the marine food web, CO_2 sinks and sources, and climate change since phytoplankton is a major player within the marine food web and marine biogeochemical processes. Opposed to other retrievals of ocean color data, the information of the spectrally high resolved SCIAMACHY data was used. In conjunction with highly precise field and laboratory measurements for comparison and for reference spectra for satellite retrievals, for the first time the spectral dependent parameters of phytoplankton absorption and light penetration depth were retrieved. This information is used to:

- Improve satellite retrievals of phytoplankton biomass
- Identify globally different phytoplankton groups (phytoplankton functional types) from satellite phytoplankton absorption fits
- Establish a data base on biooptical parameters, phytoplankton functional types and biomass and make it available to the wider community for the purposes of optical and ecosystem modeling
- Improve regional and global primary production estimates by incorporating the additional biooptical information
- Improve the retrievals of atmospheric trace gases from UV-VIS satellite spectra by incorporating ocean optics.

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2. PHYTODOAS

Within this study the method used often in atmospheric remote sensing of Differential Optical Absorption Spectroscopy (DOAS) by Perner und Platt (1979) was applied to extract information on ocean optics; in particular on phytoplankton absorption and distribution (results have been published in Vountas et al. 2007). The key innovation in the DOAS analysis for phytoplankton retrieval is the introduction of the in-situ measured specific spectrum of phytoplankton absorption measured in the Antarctiv Circumpolar Current (ACC) region plotted in Fig. 1. The method then is called PhytoDOAS.

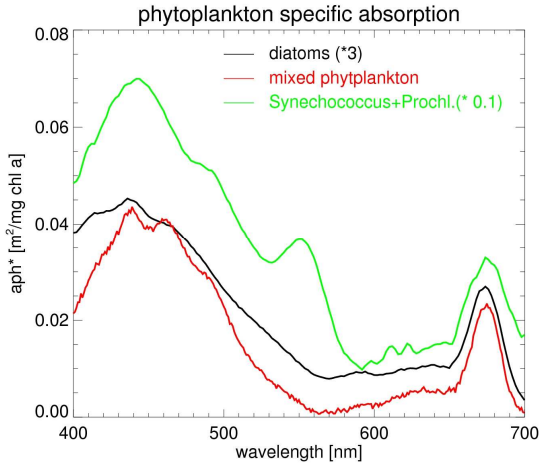

Fig. 1: Spectra of pigment-specific phytoplankton absorption determined in water samples of three different ship cruises with RV Polarstern within the Atlantic Southern Ocean: A phytoplankton absorption spectrum of a phytoplankton community dominated by over 80% diatoms measured during EIFEX cruise in March 2004 (Diatoms = black), a spectrum from phytoplankton community with a mixed phytoplankton population from ANTXIII/2 cruise in Jan 1996 (red) and of only Synechococcus and Prochlorococcus from ANTXXIII/1 in Oct 2005 (green). Figure from Bracher et al. submitted to Biogeosciences.

In a non-linear least squares fit, they are scaled by the slant column S_{phyto}, which is estimated simultaneously with the slant columns of the atmospheric trace gases included in the analysis (in our case O_3, NO_2, O_4, H_2O, plus a pseudo-absorber for the Ring effect (from Vountas et al. 1998). In addition, we included liquid water absorption cross sections in the analysis, which was performed in the wavelength window 428-496 nm. A typical result for the specific phytoplankton absorption fit is depicted in Fig. 2. The solid line represents the phytoplankton reference spectrum, scaled by the result for S_{phyto} and reduced by the low-order polynomial in wavelength. Adding the fit residual yields the broken line. The agreement between the two curves is a measure of how well the observations fit the reference spectrum used in the analysis. As we see from the plots, the space-borne observations match the in-situ measured reference spectra remarkably well (Fig. 2). The analysis of the fit quality suggests that the under-water absorption signal from photosynthetic pigments in phytoplankton is sufficiently strong to be detected by SCIAMACHY. They can be well distinguished from contributions of atmospheric constituents, which allows for a quantitative retrieval of the phytoplankton amount along the under-water light path.

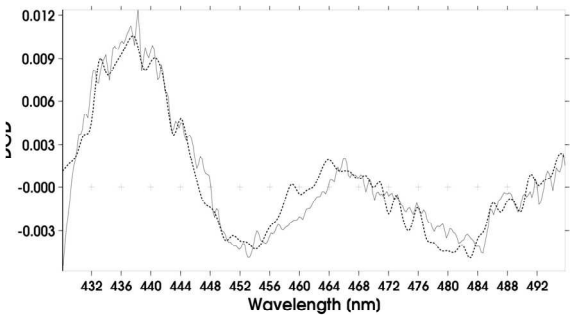

Fig. 2: Spectral DOAS fit for phytoplankton using the phytoplankton absorption cross sections from the ACC plotted in Fig. 1 for a SCIAMACHY pixel with high chl a conc. (>3 µg/l at 25°N and 16°W, left). Figures from Vountas et al. 2007.

In addition, also inelastic scattering of seawater in ocean waters (vibrational Raman scattering, VRS) and its impact on trace gas retrievals from satellite data was studied and detected in GOME (Vountas et al. 2003) and SCIAMACHY data (Dinter 2005). VRS slant columns/fit factors from SCIAMACHY data are obtained by using the DOAS method described for phytoplankton absorption fits in the range of 349.5 nm and 382 nm and fitting to a modelled VRS spectra (details described in Dinter 2005). It has been found, that over clear ocean waters, photons scattered within the water body contribute significantly to the upwelling flux. In addition to elastic scattering, inelastic Vibrational Raman Scattering (VRS) by liquid water is also playing a role and can have a strong impact on the spectral distribution of the outgoing radiance.

The above described retrieval technique has been applied for fitting both, spec. phytoplankton absorption and VRS, to several SCIAMACHY groundpixels of one month (July 2005) and global maps of these fits are shown in Fig 3. Both approaches, fitting VRS or phytoplankton absorption spectra, exhibit expected clear correlations to global chl *a* from other satellite measurements (see Fig 5). Obviously both methods could be used to retrieve this quantity. An optimized retrieval technique would take advantage of a hybrid approach: VRS fits strongly in regions where low chl *a*

prevail whereas direct fitting of phytoplankton behaves vice versa.

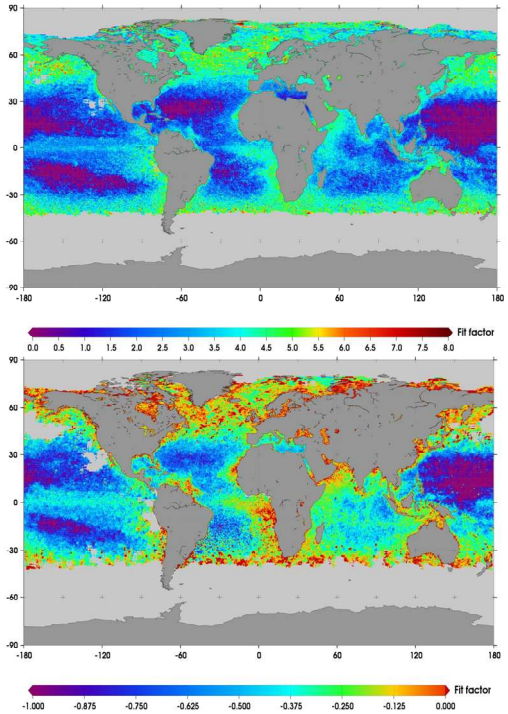

Fig. 3: Monthly global averages for July 2005 of phytoplankton (left) and vibrational Raman Scattering (VRS, right) fit factors derived from SCIAMACHY data using DOAS; figures from Vountas et al. 2007

3. PHYTOPLANKTON BIOMASS FROM SCIAMACHY AND COMPARISON TO MERIS ALGAL-1

In order to retrieve chlorophyll conc. from SCIAMACHY measurements we used the combined information from the fits to VRS and specific phytoplankton absorption as described in detail in Vountas et al. (2007). The fit factor S_{chl} for phytoplankton (or to be precise for the specific absorption spectrum) is given in [mg/m^2] which is a mass column. If the penetration depth δ of light for the wavelength window considered is known this column can be converted into a concentration by the ratio:

$$C = S_{chl} / \delta \qquad (1)$$

VRS is strongly related to δ and serves therefore as a proxy: A single vibrational Raman scattering event is always accompanied by an elastic scattering process. Therefore the fit factor of VRS, S_v, is directly related to the same quantity for elastic scattering only. As described above (and in more detail in Vountas et al. 2003) a bio-optical model from Morel (1988) has been used to describe the dependence of the elastic backscattering coefficient b_b. The backscattering coefficient scaled with the same factor as the VRS spectrum S_v can be understood as the true b_b for the real situation considered. As b_b is the modelled penetration depth, $S_v * b_b^{-1}$ can be associated with the measured one. For the whole retrievals of S_{chl} for July 2005 (as described above) all corresponding values of S_v have been used within Eq. (2) to model a global map of chl *a* (*C*), which is displayed in Fig. 4.

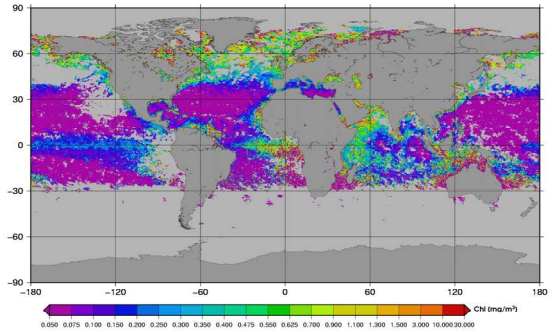

Fig. 4: Monthly global averages for July 2005 of chl-a conc. derived from SCIAMACHY (upper panel) data fitting to phytoplankton absorption (to derive slant column of specific phytoplankton absorption along the under-water light path) and to VRS (to derive penetration depth); figure from Vountas et al. 2007

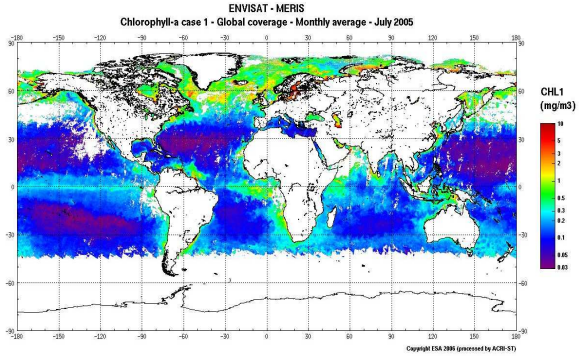

Fig. 5: Monthly global averages for July 2005 of chlorophyll conc. derived from level-3 products of MERIS algal_1 (right, figure from http://www.enviport.org/meris).

A first visual comparison of SCIAMACHY with MERIS global chl *a* of the same time period (Fig. 5) shows good agreement. Further studies will optimize this approach and will also include a thorough quantitative comparison. An important point of investigation must be the impact of the "saturation effects" (discussed in the paragraph above) on the chl *a* conversions. The patchy appearance of the mapped chl *a* is related to the fact that due to fitting failures, either

in case of VRS or phytoplankton fitting, not both corresponding quantities could be related.

4. PHYTOPLANKTON BIOMASS FROM SCIAMACHY AND COMPARISON TO MERIS ALGAL-1

In order to derive the information on the distribution of different types of phytoplankton groups the for a specific group characteristic absorption spectrum (see Fig. 1) is successively fitted with PhytoDOAS within the wavelength range of 430 nm to 495 nm. As pointed out before these absorption spectra and their relation to phytoplankton groups have been measured by the cooperation partners of this project on different ship cruises with RV Polarstern. Absorption measurements have been done by Rüdiger Röttgers (GKSS) using both, filter pad and PSICAM method (see Röttgers et al. 2005). The composition of phytoplankton has been determined by High-Liquid-Pressure-Chromatography (HPLC) by R. Röttgers (GKSS) and Ilka Peeken (IFM-Geomar) according to Hoffmann et al. (2006) and the dominant phytoplankton groups have been derived from marker pigments (done by Ilka Peeken) according to the method by Mackey et al. (1996).

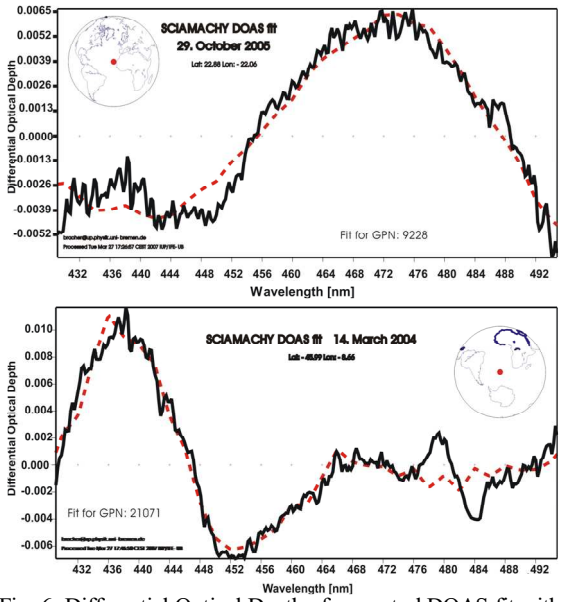

Fig. 6: Differential Optical Depth of a spectral DOAS fit with SCIAMACHY data (black) for a specific phytoplankton group (left: for cyanobacteria and right: for diatoms) using the phytoplankton group specific absorption cross sections from Fig. 7 and the scaled in-situ phytoplankton differential absorption (red) of the specific group. For the example left the in-situ measurement for cyanobacteria was taken on 29 Oct 2005 at 23°N and 22°W and the SCIAMACHY measurement was within 20 hours and 50 km of the in-situ measurement. For the example right the in-situ measurement for a community dominated by diatoms (right) was taken on 14 Mar 2004 at 46°S and 9°W and the SCIAMACHY measurement was within 2 hours and 200 km of the in-situ measurement. Figure from Bracher et al. submitted to Biogeosciences .

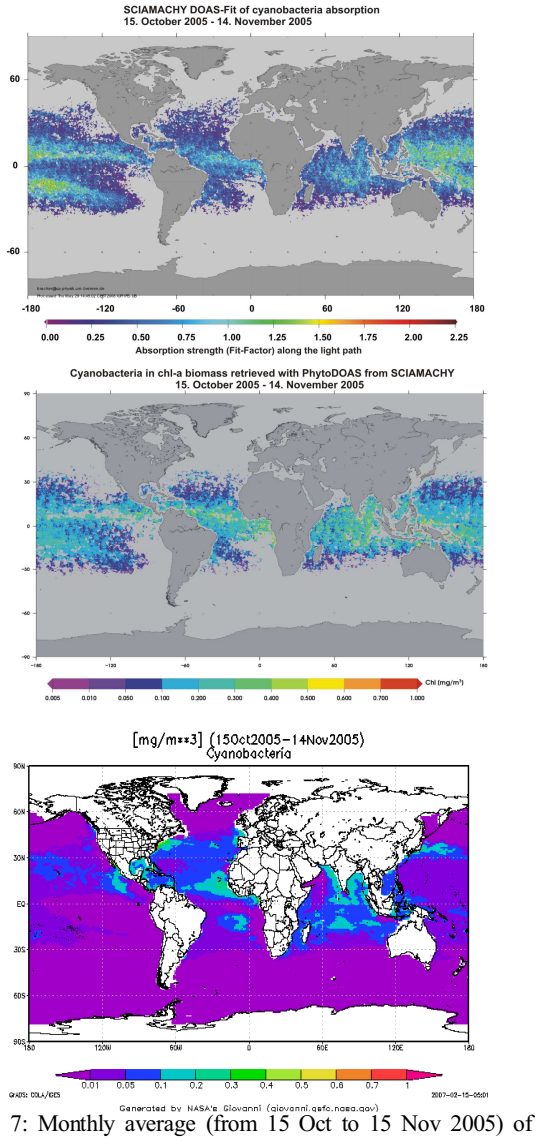

Fig. 7: Monthly average (from 15 Oct to 15 Nov 2005) of global distribution of cyanobacteria. Upper panel: obtained as "Strength of Absorption" by using PhytoDOAS with SCIAMACHY data. Middle panel: the conc. of chl-a of cyanobacteria as derived from Fig. 7 upper panel. Both figs. from Bracher et al. submitted to Biogeosciences) and fitting VRS. Lower panel: from calculations with NOBM model http://reason.gsfc.nasa.gov/OPS/Giovanni/ocean.modelDay.2.shtml [1]) by Gregg and Casey (2007).

[1] The images and data used to calculate the phytoplankton group distributions of cyanobacteria and diatoms with the NOBM model were acquired using the GES-DISC Interactive Online Visualization ANd aNalysis Infrastructure (Giovanni) as part of the NASA's Goddard Earth Sciences (GES) Data and Information Services Center (DISC)

In Fig. 6 the differential optical depths of the results of the SCIAMACHY separate fit of different phytoplankton groups and of the results of the in-situ measured differential phytoplankton spectrum scaled with the fit-factor are shown. For both major phytoplankton groups, the cyanobacteria and the diatoms, there is a good agreement between the differential spectrum obtained from the PhytoDOAS-fit with SCIAMACHY satellite data and the in-situ measurement.

Fig. 7 shows the "absorption strength" (upper panel) and chl-a conc. (middle panel) as monthly average of the global distribution of cyanobacteria during the northern hemispheric fall and southern hemispheric spring (Oct/Nov 2005) retrieved from SCIAMACHY data with PhytoDOAS using the phytoplankton absorption spectrum typical for cyanobacteria. Cyanobacteria appear mainly in the warmer seas of the subtropics and tropics, e. g. in larger parts of the Pacific, the Arabian Sea and off the West-African coast. The distribution of cyanobacteria retrieved from SCIAMACHY data agrees well with the distribution found from in-situ measurements and with the calculations made by the NASA Ocean Biochemical Model (NOBM, see Fig. 7 lower panel) developed by Watson and Gregg (2005). Not all, but quite a few, cyanobacteria are known to be able to fix elementary nitrogen and produce nitrate. By that the amount of biological available nitrogen within the ocean is increased and the nitrogen flux within the ocean is significantly influenced.

Fig. 8 shows for the same time period as Fig. 7 the global distribution of diatoms retrieved with PhytoDOAS from SCIAMACHY ("absorption strength" in the upper panel and chl-a conc. in middle panel) and from calculations made for diatoms with the NOBM Model (lower panel). As expected from punctual measurements on water samples during various ship cruises and as calculated by the NOBM model also the analysis of the SCIAMACHY data shows that during hemispheric fall and southern hemispheric spring diatoms are quite abundant and the dominant group in the Southern Ocean (blow 32°S) and at the coastal areas around up-welling regions at the West-American and West-African coasts. Former model studies calculated that diatoms contribute to about 30% of all phytoplankton and form blooms predominantly where there are sufficient nutrients, these are where cool and nutrient-rich waters come to the surface (mainly cool waters in the higher latitudes during spring-summer) and coastal areas. Diatoms cells are encased within a unique cell wall made of silica called a frustule which protect tem mainly from grazing. Because of this bloom-and-bust lifestyle, diatoms are believed to play a disproportionately important role in the export of carbon from oceanic surface waters (biological pump). Significantly, they also play a key role in the regulation of the biogeochemical cycle of silicon in the modern ocean.

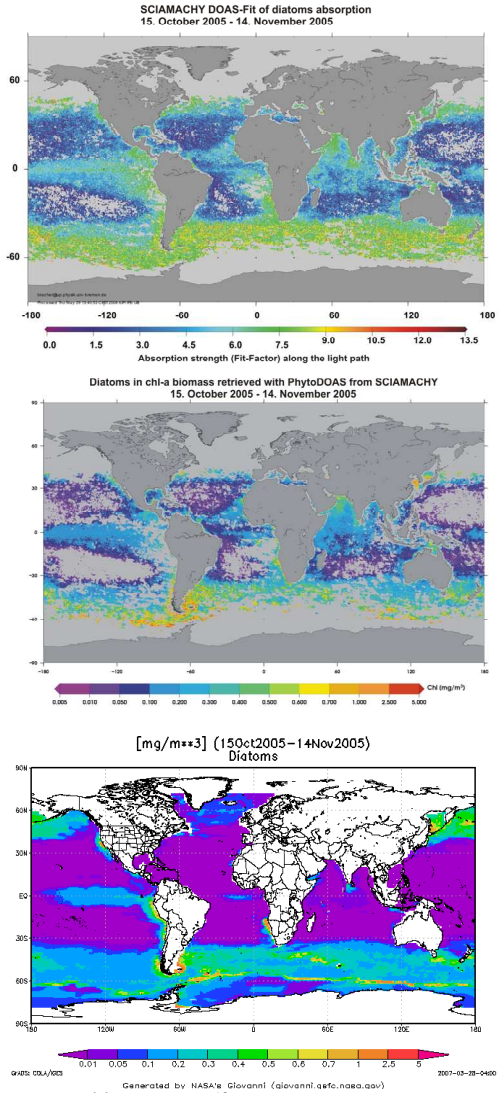

Fig. 8: Monthly average (from 15 Oct to 15 Nov 2005) of global distribution of diatoms. Upper panel: obtained as "Strength of Absorption" by using PhytoDOAS with SCIAMACHY data (fig. from Bracher et al. submitted to Biogeosciences). Middle panel: the conc. of chl-a of cyanobacteria as derived from Fig. 7 upper panel (fig. from Bracher et al. submitted to Biogeosciences) and fitting VRS. Lower panel: from calculations with NOBM model (http://reason.gsfc.nasa.gov/OPS/Giovanni/ocean.modelDay.2.shtml) by Gregg and Casey (2007).

5. CONCLUSIONS AND OUTLOOK

Within this study SCIAMACHY data were used to obtain information of the absorption, distribution and composition of phytoplankton. The results on phytoplankton overall biomass and absorption compare well with collocated in-situ measurements in the Atlantic Ocean and the global Ocean Colour data set obtained from MERIS and MODIS, respectively. Our SCIAMACHY satellite maps on the distribution of cyanobacteria and diatoms show overall a very good agreement with measurements on phytoplankton absorption and composition of these particular groups which are spatially and temporally collocated. Furthermore their global distribution is in qualitative agreement with the calculations based on the NOBM model. These model simulations combine global Ocean Colour biomass data with global data sets on nutrient distributions, sea surface temperature and current conditions. For the first time it is possible with using PhytoDOAS on SCIAMACHY data to produce a near-real time picture in the open ocean of the global distributions of two phytoplankton groups which each of them plays an important role within the global nitrogen or silicate budget, respectively, and also has a different function within the marine ecosystem.

The results of the project have already been used to improve trace gas retrieval from SCIAMACHY data; in particular improvements have been found for glyoxal (Myriokefalitakis et al. 2008) when in the DOAS retrieval inelastic scattering and phytoplankton absorption has been accounted for as developed in Vountas et al (2007). The objectives of future studies are to further work on the extraction of additional biooptical information by the synergistically using high spectrally (besides SCIAMACHY extend the analysis to the newer sensors GOME-2 and OMI) and high spatially resolved satellite data (MERIS, MODIS) in order to develop global data sets covering a time period of 10 + X years. In detail, it is planned to intensively validate the satellite biooptical data with ship-based measurements on phytoplankton samples and the above-surface and underwater light. This additional biooptical satellite information shall be used for developing near-real time picture of the distribution of other than cyanobacteria and diatoms major phytoplankton groups (e.g. coccolithophorids, dinoflagellates) and an improved MERIS phytoplankton biomass retrieval. This new information shall be used as an input basis for primary production modelling and for developing improved atmospheric trace gas retrievals by accounting for the oceanic optical signal. The maps on the distribution of major phytoplankton groups and marine primary production are planned to be used within several climate change studies (e.g. Identifying biogenic sources of greenhouse gas and short lived halogenated species, carbon cycle estimations).

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