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Biogeosciences Discussions

Interactive comment on "Quantitative observation of cyanobacteria and diatoms from space using PhytoDOAS on SCIAMACHY data" *by* A. Bracher et al.

A. Bracher et al.

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We thank Reviewer 2, Steven Lohrenz, for his positive review and his critical comments. In the following we answer each of his comments and highlight where we made changes to the manuscript.The comments by Reviewer 1 are introduced with "R1" and our reply to these comments are introduced with "A:".

Response to general comments: R1: This manuscript examines the feasibility of applying Differential Optical Absorption (DOAS) Spectroscopy techniques to the Scanning Imaging Absorption Spectrometer for Atmospheric Chartography (SCIAMACHY). The authors evaluated the technique using in situ data and then applied the method to global observations. The basis for the approach involves discrimination of Vibrational

Raman Scattering spectral signature in backscattered radiation and its modification by absorption due to dissolved organic matter and phytoplankton. Additional considerations are made for contributions by weak atmospheric absorbers (e.g., ozone and other gases), as well as Raman scattering by air molecules, the effect of which is treated as pseudo-absorption (Vountas et al., 2007). The method is novel and has the potential to augment the arsenal of techniques for probing spatial and temporal patterns in phytoplankton functional groups on regional and global scales. The manuscript assumes a high degree of familiarity with prior literature describing the technique. The authors may wish to consider giving more background about the method and a concise, yet comprehensive explanation of how phytoplankton absorption is derived. As it stands, frequent cryptic references to terminology and methodology explained elsewhere makes this a difficult read. More detailed explanation of how results were derived would also be helpful. Possible inclusion of a diagram or an equation describing steps involved in processing and the fitting sequences for differential absorption might be helpful.

A: We now added a lot of information on the method as pointed out under response to specific comments 6-10.

R1: In general, the manuscript could be greatly improved by better organization and improved clarity in objectives and explanation of results. The authors might wish to consider including a short paragraph in the introduction explaining the organization of the paper.

A: We now restructured and shortened the introduction focusing more on the relevance of the PhytoDOAS approach. As suggested, at the end of the introduction we added now such an explanation. We also rewrote most parts of the results section to improve the clarity of the paper.

R1: The introduction provided a thorough review of the approaches for discerning phytoplankton taxonomic composition using pigment chemotaxonomy, as well as absorption-based and satellite ocean color approaches. While informative, the introduction tended to meander and its relevance to the PhytoDOAS method was not always apparent.

A: See comment above about that we changed the introduction.

R1: The authors provide preliminary results that appear consistent with in situ observations as well as with a NASA Ocean Biogeochemical Model patterns. The authors reference other work examining global distributions of taxa based on pigment and optical approaches. However, they failed to examine their findings in the context of patterns observed in these other studies. This would have been a useful comparison and provide further evaluation of the PhytoDOAS method as applied to the SCIAMACHY data

A: We now added these comparisons as pointed out under response to specific comment 11.

More specific comments are given below: Specific comments 1. Abstract, lines 16-18 R1: the authors' use of cryptic statements such as "including the information of the sensor's optical paths" and "DOAS fits of inelastic scattering" should be minimized in the abstract and throughout the manuscript, and replaced clear and understandable statements. As noted above, a reader must necessarily be familiar with the prior literature on this method, particularly Vountas et al. (2007), to be able to follow this manuscript and understand the terminology. The manuscript would be improved if descriptions of the approach were clear and succinct (see first paragraph in this review for suggestions).

A: This was changed in the abstract now as follows:"Results show clearly different absorption characteristics of the two phytoplankton groups in the SCIAMACHY spectra. Using these results in addition to calculations of the light penetration depth derived from DOAS retrievals of the inelastic scattering (developed by Vountas et al. 2007), globally distributed pigment concentrations for these characteristic phytoplankton groups for two monthly periods (Feb-Mar 2004 and Oct-Nov 2005) were determined."

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2. Introduction, p. 4561, lines 17-20 R1: the intensity of carbon fixation and its relationship to export is a function not only of the phytoplankton size and composition, but of the overall trophic community structure. This point should be acknowledged by the authors and note that differences in phytoplankton composition reflect a broader suite of associated differences in autotrophic and heterotrophic interactions.

A: This was changed accordingly in the text.

3. Introduction, p. 4562, lines 3-8 R1: differences in pigment absorption can be attributed not only to the "package effect" or self-shading of pigment molecules, but also due to molecular interactions of pigment molecules in their corresponding pigment-protein complexes (Johnsen et al., 1994).

A: This was changed in the text accordingly as follows: "Since certain phytoplankton groups are generally characterised by some diagnostic pigments (Jeffrey and Vesk, 1997) the chl-a normalized phytoplankton absorption differ in magnitude due to phytoplankton composition (e.g. Sathyendranath et al., 1987; Hoepffner und Sathyendranath, 1991, Bracher und Tilzer, 2001, Ciotti et al., 2002; as well see Fig. 1). However, the absorption spectrum can also be modified by variations in pigment packaging (described by Kirk, 1994) and molecular interactions of pigment molecules in their corresponding pigment-protein complexes (Johnsen et al., 1994)."

4. Introduction R1: a general comment about the introduction is that it is written more as an annotated bibliography. Relevance to the current work was not always apparent. The authors may wish to revise this to better express linkages between prior literature and their current work.

A: We now restructured and shortened the introduction focusing more on the relevance of the PhytoDOAS approach.

5. Methods, p. 4565, lines 1-3 R1: information about pixel size would be helpful here. It is mentioned later in the discussion, but would be appropriate to state in methods. The

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large pixel size of this instrument limits it application to open ocean and necessitates analyses over longer time periods than conventional ocean color sensors. This point should be acknowledged.

A: We add this information to this section "The draw back of the high spectral resolution is a rather large pixel size for the phytoplankton information retrieved in our study with an open ocean scene of 30 km by 30 km at best."

6. Methods, p. 4565, lines 18-22 R1: this section lacks clarity. The authors need to be more explicit in what is meant by high-frequency spectral structures (frequency of electromagnetic radiation or frequency of variability as a function of wavelength?). What criteria are used to define the low order polynomial, or is it a fit to residual variability not accounted for by other contributions? What is meant by "low-order"?

A. We gave now a larger explanation now of the whole DOAS method in the beginning of section 2.2 explaining this issue: "The DOAS algorithm determines the amount of a molecular absorber along the observed optical light path by least square fitting a linear combination of reference absorption cross-section spectra of trace gases, a Ring reference spectrum (RING), the Vibrational Raman Scattering (VRS) spectrum and in our case the phytoplankton absorption (phyto). That is, ..."

7. Methods, p. 4566, lines 7-18 R1: more explanation about the purpose of the eigenvector analysis would be helpful. Was this to account for unexplained variation in the sensor data? Presumably, the analysis in waters low in cyanobacteria and diatoms provided a baseline for correction of image data acquired in other regions. Correct?

A: This is correct and we added more information in the text: "As described in Vountas et al. (2007) we accounted for unclear instrumental effects in SCIAMACHY spectra prior to the DOAS fit of phytoplankton absorption applied to a global data set. SCIAMACHY data within the wavelength range of 425 to 499 nm were analysed by DOAS over a region with hardly any absorption by phytoplankton including the fitting of the Ring effect and atmospheric absorbers as specified below except for phytoplankton.

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Then an Eigenvector analysis by Principal Component Analysis (PCA) on the residuals of these regional DOAS fit was performed. This provides a baseline for correction of image data acquired in other regions. The region selected for analysing the residuals was selected based on the criteria that both, cyanobacteria and diatoms, have very small absorption and the total phytoplankton biomass is below 0.05 æg/l; the region chosen was 18øS to 28øS and 115øW to 125øW (as described in Morel et al., 2007)."

8. Methods, p. 4567, lines 7-8 R1: a brief explanation of the basis for the pseudoabsorbers and ring spectrum would be helpful.

A: We added this information in the text: "The Ring effect as the VRS causes filling-in of solar Fraunhofer lines observed in the backscattered radiation due to inelastic scattering by N2 and O2 molecules in the atmosphere for Ring (Vountas et al. 1998) and by liquid water in the ocean for VRS (Vassilkov et al. 2002, Vountas et al. 2003). These features relevant in the DOAS retrievals from UV/visible spectra must be accounted for and are therefore treated here as an effective absorber (named as pseudoabsorber) in the retrieval."

9. Methods, p. 4567, lines 8-15 R1: reproduction of the Vountas et al. (2007) Eq. 1 would be useful here.

A: As pointed out in response to specific comment 7. we added this information now in section 2.2.

10. Results, p. 4570, lines 7-8 R1: another reference to subtraction of a low order polynomial, but no explanation given as to how this is derived. Is this the same polynomial referenced on p. 4565?

A: We now explained in the last paragraph of section 2.3 and in Fig. 2 how we applied the technique of the polynomial: "Within the DOAS analysis in order to perform the least square fit to the differential absorption of all relevant absorbers and to the low order polynomial, from each absorption spectrum the polynomial is subtracted. Fig. 2

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shows as an example for the diatom-like specific absorption spectrum, the 2nd order polynomial and the specific differential spectrum for the wavelength range of 429 nm to 495 nm which was used in the PhytoDOAS retrieval."

R1: What do the authors mean by the statement that the differential spectra are correlated with pure water absorption? What statistical basis is there for saying that these spectra are correlated?

A: We now give a explanation for it in the text (end of section 2.3):"As seen in Fig. 2 the differential spectrum of the diatom-like spectrum shows significant different structures to the cyanobacteria and the pure water spectra, while the differential absorption of cyanobacteria correlates between 435 to 475 nm with pure water absorption (obtained from Pope and Fry, 1997). The correlation is described in the sense of orthogonality which means that the scalar product of the two spectra is not equal zero."

R1: Are they saying effects of water absorption are embedded in the phytoplankton differential absorption spectra?

A: Exactly that is what we mean!

11. Discussion R1: the manuscript would be strengthened if the authors compared their global distributions to those generated by other pigment-based and satellite-derived approaches referenced in the manuscript.

A. We explained now in more detail why only comparisons to Alvain et al. Physat method are possible at this stage. We added in the text: "Comparison of SCIAMACHY PhytoDOAS diatom and cyanobacteria estimates to other methods retrieving information on PFTs from space is difficult for two reasons: a) different time periods of the year were analysed (Uitz et al. 2006; Aiken et al. 2007; Hirata et al. 2008; Raitsos et al. 2008), b) in all methods except for Uitz et al. 2006, only the dominant groups were identified and no quantitative value is given. Alvain et al. (2008) provide globally the mean monthly dominant PFTs determined by the PHYSAT method which allow

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comparison with the PhytoDOAS results. These monthly means show for the months Feb-March and Oct-Nov similar distributions of cyanobacteria (identified here as the PFTs "Synechococcus-like-cyanobacteria" and "Prochlorococcus") and diatoms in regions where SCIAMACHY PhytoDOAS identified the highest biomass for these two groups. Alvain et al. (2008) identified for Oct-Nov and Feb-Mar the dominance of diatoms in a circumpolar belt at 40øS-55øS and in the upwelling area off the coast of Peru. In November also diatoms also dominated the Benguela upwelling area. With the PhytoDOAS quantitative estimate and the NOBM estimate of diatoms additional areas are identified to be rich in diatoms for the investigated months, such as the whole West-South American coast, the West-African coast and the region around Japan. Our findings on the distributions of diatoms, the NOBM and the Physat method are also in accordance with previous studies based on in-situ sampling throughout the ocean: During hemispheric fall and southern hemispheric spring diatoms are quite abundant and the dominant group in the Southern Ocean and at the coastal areas around up-welling regions at the West-American and West-African coasts. This dominance and distribution of diatoms can be explained by their need for silicic acid (=silicate) to build their cell walls. Therefore, diatoms blooms predominantly occur, where there are sufficient nutrients (Treguer et al., 1995). Usually these areas are where cool and nutrient-rich waters come to the surface (mainly cool waters in the higher latitudes during spring-summer) and coastal areas. Also for the cyanobacteria, SCIAMACHY PhytoDOAS, PHYSAT by Alvain et al. (2008) and the NOBM show that they 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, typical regions of low nutrients."

12. Discussion, p. 4574, lines 9-18 R1: the argument that the PhytoDOAS method is not "empirical" is questionable. The method does provide a different approach to discrimination of cyanobacteria and diatoms as generally classified by the shape spectra given in Fig. 1. Perhaps the authors could emphasize this aspect as a fundamental difference from other approaches. Additionally, the statement that the method "directly" retrieves chl concentration could be contested. As the authors themselves point out,

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there are numerous factors influencing the relationship between in vivo absorption and pigment concentration which will affect the result.

A: We now made clearer in the discussion that the PhytoDOAS approach is quite different to the other approaches, because the discrimination of cyanobacteria and diatoms is classified by their characteristic absorption spectrum within the fitting wavelength window. The text in the discussion was changed to the following:"In contrast, the PhytoDOAS method exploits the information of the whole spectrum within the fitting wavelength window and discriminates cyanobacteria and diatoms by their characteristic absorption spectrum. Cyanobacteria and diatoms are quantified without assuming empirical relationships as chosen for other PFT methods. It is therefore possible to detect changes in the global distribution of these PFTs biomass which have not been foreseen. PhytoDOAS uses in its retrieval in-situ absorption spectra measurements from natural samples chosen to be representative for a certain group. Absorption spectra chosen to be representative for a certain group might also change the marker pigments in their quantity due to pigment packaging but probably not in their quality which is determining the differential signature. For the diatom-like spectrum the fitting to this spectrum might be influenced in parts by the absorption of prymensiophytes and dinoflagellates. Further adjustments of the fitting wavelengths window are necessary to overcome this issue to allow quantification of these groups. By taking into account the details of the fitting wavelength window, PhytoDOAS enables a reliable atmospheric correction which in other ocean colour retrievals is a significant source of error in the chl-a algorithm. In addition, PhytoDOAS simultaneously yields the depth to which the radiation penetrates. The PFT biomass derived is a depth-integrated mean over this depth. In comparison the other PFT methods, besides Uitz et al. (2006), give estimates for the surface water only without knowledge as to how much the chl-a conc. from deeper layers influences the estimate. The limitations to our method are the rather coarse resolution of SCIAMACHY pixels with at best 30 km to 30 km and a global coverage, which is poorer than of other ocean color sensors such as SeaWiFS, MERIS or MODIS. But, as stated by Aiken et al. (2007) phytoplankton distributions

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may be geographically distributed over 50 to 100 km and these structures persist over a few days."

13. Fig. 3 R1: the spectral range given for the fitted cyanobacteria spectrum in the top panel differs from that in Fig. 2. Please explain.

A: We changed now the range of Fig. 2 to the exact wavelength range where PhytoDOAS was performed, which is also illustrated in Fig. 3.

Technical corrections 1. Abstract, line 20 R1: Avoid using acronyms without definition, i.e., NOBM.

A: This was changed

2. Introduction, p. 4561, line 2 R1: "As IS well known"

A: This was changed.

3. Introduction, p. 4561, lines 25-26 R1: suggested word substitution: "diagnostic" for "specific".

A: This was changed.

4. Introduction, p. 4562, line 8 R1: "It PARTIALLY explains"

A:This was changed.

5. Introduction, p. 4563, line 7 R1: "THE Aiken et al. (2007) APPROACH WAS applied"; also in line 16 - "different phytoplankton communities WITH respect"

A: Both were changed.

6. Introduction, p. 4563, line 27 R1: "slant columns" and "absorbers" should be clearly defined.

A: This was changed to "The differential signal of each molecular absorbers within a considered wavelength window is used to retrieve slant columns of the absorbers along

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the optical path from the satellite observations of solar backscattered electromagnetic radiation."

7. Results, p. 4570, line 12 R1: spelling of "eigenvector"

A: This was changed.

8. Results, p. 4571, line 27 and elsewhere R1: NOBM "Model" is redundant.

A: This was cut accordingly.

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