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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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Specific Comments

A: We thank Anonymous Reviewer 1 for his/her positive review and his/her critical comments. In the following, we answer each comment and highlight where we made changes in the manuscript.The comments by Reviewer 1 are introduced with "R1" and our reply to this comments are introduced with "A:".

Critique in general comments: R1: Validation of the methodology is preliminary. Number of in situ data used in the validation is simply not sufficient (5 points), especially when the authors oppose regional approaches (L18-20, pp4562) and their interest is the global scale. In addition, a more sophisticated strategy for validation campaign

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is required when the satellite data with such a low resolutions are used; I am not impressed with validation result where the authors used match-up data taken in a 12-hour and 180km window.

A: We now explained this in the discussion section: 'Comparisons of our results so far are still preliminary as a thourough validation is difficult to perform at this stage. In-situ measurements are quite sparse in general, and they only provide punctual data points instead of an integral over the large surface footprint of an ocean color sensor (˜1-9 km2 and for SCIAMACHY $>$30 km2). Nevertheless, these first comparison to in-situ data indicate that the range of SCIAMACHY phytoplankton group chl-a concentrations are reasonable and plausible. Since the NOBM simulations combine global ocean colour biomass data with global data sets on nutrient distributions, sea surface temperature and current conditions (Gregg et al. 2003) to calculate various PFTs, it certainly is not the tool to validate PFTs satellite retrievals. However, it does provide information on the global performance of the SCIAMACHY PhytoDOAS retrieval.'

R1: Presentation of this potentially-good work is not necessarily excellent. Critical information (e.g. a protocol to determine phytoplankton reference spectra, sensitivity of the reference spectra to the DOAS outputs, and reliability of ground truth data used for validation, protocol of validation exercise etc.) is missing, while redundant words/sentences are scattered here and there. Because the main part of this paper is about the DOAS methodology, sufficient (but concise) explanations of the methodology are required so that somebody other than the authors can also replicate the same/similar results presented in this paper. Unfortunately this requirement is not met. I believe that both of the authors and readers benefit from some kind of revision as to the presentation of the paper before final publication.

A: We now added a lot of information on the method as pointed out under response to specific comments to section 2.2, 2.3, 3.2 and to reviewer #2 specific comments 6.-10.

Specific Comments Introduction L21-25, 4561: R1: Please clarify that you are talking

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about the Chla-specific absorption coefficient of phytoplankton (aph*=aph/Chla) rather than the absorption coefficient of phytoplankton (aph), since it affects interpretations of your statement.

A: This was changed accordingly 'Many field measurements have confirmed that the spectra of specific phytoplankton absorption differ in magnitude which shows that they are independent of chl-a'

L25-27, 4561: R1: Please add reference(s) to support this statement, since classification of phytoplankton by bio-marker pigments do have anomaly.

A: We add the reference of Jeffrey and Vesk (1997)

L6-11, 4562: R1: Please add reference(s) which indeed shows that global satellite Chla algorithm is actually distorted by the packaging effects of phytoplankton absorption. In the paper, references cited are not meant to support your statement about the packaging effects as a cause of the algorithm error.

A: We actually now removed this part from the introduction (by restructuring it). But a references which support the statement are the following: 'This varying specific absorption dependent on pigment-packaging and pigment composition significantly influences the chl-a retrieval by empirical ocean color algorithms (Arrigo et al. 1998, Dierssen and Smith 2000, Bracher 1999).'

2. Instrument and methods 2.1 Satellite sensor SCIMACHY and principles of retrieval technique DOAS R1: Almost entire paragraph was copied from the previous publication (Vountas et al, 2007). I am not familiar with publication policy of BG regarding copy right and duplicated publication, but this is definitely not a good exercise, even if you were a co-author in the previous publication. This kind of presentation should be avoided. I will leave a judgement about this to the Editor.

A: We apologize for doing so therefore we rewrote the paragraph to change the wording, added relevant information and deleted unnecessary information.

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R1: There is no description about radiometric accuracy (e.g. for spectral response) of SCIAMACHY over the ocean. How accurate are SCIMACHY data? How do the SCIAMACHY data compare to the well-calibrated sensor like SeaWiFS? Since sensitivity test of the DOAS method is not presented in this paper, the authors need to present a justification of the use of SCIAMACHY data in oceanic applications in some way.

A: We added this information which shows SCIAMACHY is well calibrated and has a good signal-to-noise ratio: 'The signal-to-noise ratio of SCIAMACHY at 340 to 500 nm is above 2000 (Bovensmann et al., 1999) in each spectral bin of 0.2 to 0.4 nm width. This is more sensitive considering the value of 1650 for the broadband wavebands in similar spectral regions of the well calibrated MERIS ocean color sensor (Bezy et al., 2000). The draw back of the high spectral resolution is a rather large pixel size for the phytoplankton information retrieved in our study with an ocean surface scene being 30 km by 30 km at best. Thus for the present high spectral resolution observations of the ocean color are limiting its application to the open ocean and necessitates analyses over longer time periods than conventional ocean color sensors. The radiometric accuracy of SCIAMACHY was specified prior to flight for the reflectance with 2-4% (Bovensmann et al., 1999). These values were confirmed by comparisons with MERIS and AATSR measurements (Kokhanovsky et al., 2008) for the newest level-1 data processor version 6.0 which was used in this study. However, for our study only the relative calibration quality is relevant because we use the DOAS method which is only sensitive to differential structures (more details given in 2.2).'

2.2 The retrieval technique: differential optical absorption spectroscopy (DOAS) R1: Re-consider terminology *Earthshine radiance*.

A: This is probably a scientific community dependent terminology (it is totally correct within the atmospheric science community to speak of earthshine spectra), so we changed it to 'solar backscattered radiance'

R1: This section is meant to explain the DOAS method itself before specific descrip-

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tions of the method applied to phytoplankton classification. But it actually does not help reader understand the rest of your paper (especially to understand Section 2.2.1 and 2.2.2; one of the key sections of this paper), because descriptions in Section 2.2.1 and 2.2.2 assume that readers are familiar with Vountas et al., 2007 and this section does not explain Vountas et al 2007 at all. Please provide a brief review of Vountas et al 2007.

A: We provide a brief review now of DOAS used in satellite retrievals from Burrows et al. (in 2.2) while we give a more explicit explanation of the phytoplankton group retrieval in 2.2.1 and 2.2.2 as wished from both reviewers.

R1: Description about atmospheric sensing is irrelevant here. For example, readers of this paper will not care about the achievement of 30km x 60km spatial resolution by SCIAMACHY for derivation of atmospheric trace gases.

A: We cut now this information from this section.

R1: It seems that some sentences in this paragraph are copied again from the previous publication by Vountas et al. 2007 (but with a slight modification).

A: We changed now the entire paragraph.

2.2.1 Retrieval of differential absorption by certain phytoplankton groups L2, pp.4566: R1: You are writing about the methodology for phytoplankton classification in this section, so this sentence is irrelevant. If you still want to include such a sentence, it may fit in Section 2.2 rather than here.

A: We cut the sentence.

L3-6, pp4566: R1: The objective of this paper is already given in Introduction, so these sentences are redundant. In this section, you are assuming that readers are familiar with Vountas et al 2007 (indeed, this paper heavily depends on Vountas et al 2007 which is cited throughout this paper). However, since Section 2.2 does not explain Vountas et al 2007 at all, one would not be able to understand all details written in the

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rest of this section. Please re-write Section 2.2 so that readers can understand the rest of the paper. If readers do not understand this section, they cannot re-produce the same result you present in this paper; if no body else but only you can produce results shown in this paper, your science does not appeal any value to others.

A: We rewrote the whole section 2.2 to make it clearer.

L1-5, pp4567: R1: These lines are redundat since they do not help reader understand the rest of your paper.

A: As stated above, we rewrote the whole section to make it clearer, but actually these lines are necessary information to reproduce our method..

2.2.2 Retrieval of cyanobacteria and diatoms chl-a concentrations from SCIMACHY L7, pp4568: R1: Please re-consider the word, *earthshine radiation spectra*.

A: We changed that as pointed out above.

2.3 In-situ measurements of phytoplankton absorption and composition L13-16,pp4569: R1: The authors used CHEMTAX with the input matrix by Wright et al. (1996). How sensitive is the choice of the standard input matrix to the phytoplankton classification with your data?

A: Unfortunately, it was not stated in the BGD manuscript that actually two various matrixes where chosen as input matrixes according to the different origin of the water samples, since it has been realized, that this is a critical issue, when using the Chematax programme. The details are now stated in the text: 'The input matrixes for chosen according to typical ratios for a given oceanic region: for the southern ocean crusie (ANTXXI/3) the matrix was taken from Wright et al. (1996) and for the subtropical and tropical cruise (ANTXXIII/1) the input matrix was taken from Veldhuis and Kraay (2004).' The CHEMTAX programme is routinely used by the oceanographic community to assess changes in the taxonomic composition of natural phytoplankton assemblages using HPLC pigment data. The main advantage of this programme is to take into ac-

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count, that various marker pigments co-occur in different PFTs: e.g. fucoxanthin is besides in diatoms also present in phaeocystis and certain pelagophytes. When the diagnostic marker is used only for one group, this might result in overestimating the contribution of this single group, e.g. diatoms. Additional recent publications comparing CHEMTAX and microscopic data show in general a good agreement between these two approaches (e.g. Wulff, A., and S. A. Wangberg (2004), Spatial and vertical distribution of phytoplankton pigments in the eastern Atlantic sector of the Southern Ocean, Deep-Sea Res Pt Ii, 51, 2701-2713).

R1: The authors do not have microscopic data that give *true* phytoplankton classification, so their analysis is entirely relying on CHEMTAX. Please describe how much confident you are, as to your phytoplankton classification at ground data level.

A: The authors actually have colleagues which have microscopic data from the EIFEX cruise and from the cell counting it can be confirmed that the contribution of diatoms was 80 % for this sample (details in Smetacek et al., 2005). We now added this information in the manuscript: 'The pigment data analysed via CHEMTAX and verified by microscopic counts (Smetacek et al. 2005) indicate that the sample is dominated mainly by diatoms (˜79% of chl-a), the rest is mainly composed of Prymnesiophytes (˜ 17 %, mainly Phaeocystis), dinoflagellates (˜3%) and chlorophytes (˜1%).' Since this procedure and calculation would use another paragraph in this paper we did not include this additional information for this data point.

R1: Have you compared your classification to that by the diagnostic pigment analysis (Viddusi et al 2002 and Uitz et al 2006)? How similar/different will your result be, when the diagnostic pigment analysis is used to identify phytoplankton instead of CHEMTAX? Since there is no description about accuracy of CHEMTAX classification, the authors should compare their results with the diagnostic pigment analysis at least. These are very important points because validation of the DOAS will be useless if phytoplankton classification by ground data is not successful.

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A: The approach used by Viddusi et al. (2002) and Uitz et al. (2006) mainly focuses on the phytoplankton size classes, which would translate into: their microplankton would fall into our diatom range and their picoplankton would be our cyanobacteria. However, since this approach lumps together all various pigments e.g. divinyl chlorophyll a, the very specific diagnostic marker for prochlorophytes, together with the normal chlorophyll as well as marker pigments for diatoms and dinoflagellates etc., we think that this approach might serve as a valuable tool for certain questions but lacks the opportunity to identify PFTs in a more detailed way, which is the approach aimed for with our PhytoDOAS….

R1: How similar/different will your result be, when the diagnostic pigment analysis is used to identify phytoplankton instead of CHEMTAX?

A: As stated above and also included in the text, the CHEMATX approach rather decreases the relative contribution of a certain marker e.g. fucoxanthin by distributing the given concentration to all groups available and purchasing this pigment instead of overestimating a certain group.

R1: Since there is no description about accuracy of CHEMTAX classification, the authors should compare their results with the diagnostic pigment analysis at least. These are very important points because validation of the DOAS will be useless if phytoplankton classification by ground data is not successful. A: Also at this point, we share not the view of the reviewer, we now give in the text of section 2.3 the exact pigment composition of the two selected absorption spectra which indicate by themselves (without CHEMTAX or diagnostic pigment analysis) that one spectrum is composed of cyanobacteria only and the other one is diatom-like spectrum with a dominance of diatoms ˜80%.

L4-12, pp4570: R1: How representative are your reference spectra of diatoms/ cyanobacteria? This is an important point, because sensitivity of the DOAS to the reference spectra is not presented in this paper and there is no description for deter-

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mining the reference spectra in this paper (In Section 2.3 you only showed how the in situ absorption measurements were taken, but did not show how the reference spectra were determined from the measurements).

A: We now made clear in this section that we chose the 2 spectra based on their pigment composition primarily, then on the CHEMTAX taxonomic grouping and also out of a selection of over 200 spectra. In addition, these spectra show compared to culture absorption spectra show good agreement. We also added now in more detail how the selected spectra were selected and used as reference spectra within the PhytoDOAS retrieval in section 2.3: 'Fig. 1 shows the two representative absorption spectra of the two in-situ measured phytoplankton groups measured in the Atlantic Ocean. The spectra were chosen out of over 200 absorption spectra measured during the two Atlantic cruises. The selection was based on the samples absolute pigment composition determined with HPLC in addition to the taxonomical grouping by CHEMTAX. The spectra selected are in good agreement with absorption measurements on various pure diatom and cyanobacteria monocultures (by Johnsen et al., 1994; S. Gehnke and R. Röttgers, pers. comm.). Absorption measurements on natural samples were preferred to use as reference spectra for satellite retrievals because in cultures the pigment packaging, pigment composition and with it the overall absorption due to artificial light source and other nutrient conditions differ from natural samples of the same species.'

R1: Although Vountas et al. 2007 is also cited, I do not see any analysis to determine the reference spectra in Vountas et al 2007 (hence this citation is useless here).

A: Now we decided to not show anymore the absorption spectrum from Bracher and Tilzer (2001) which was used in Vountas et al. 2007, since it is not releveant for our paper here. Hence, we do not need the citation here anymore as suggested.

R1: Is there no ambiguity between differential aph* of diatoms/cyanobacteria and other phytoplankton (e.g. dinoflagellates and even nanoflagellates) in the spectral region of your interest ($<$ approx. 495 nm)?

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A: The diatom-like and cyanobacteria differential absorption spectra (Fig. 2) are not interfering because in the sense of orthogonality it is that the scalar product of the two spectra is equal zero. But sure the diatom-like spectrum has minimal contributions from prymnesiophytes and dinoflagellates. We wrote now in the text: '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. The correlation is described in the sense of orthogonality which means that the scalar product of the two spectra is not equal zero. Therefore, no separate liquid water fit was performed and liquid water absorption was included with fitting the month specific Eigenvector.'

R1: You discussed about the packaging effect in Introduction. When aph* for a specific phytoplankton varies due to the effect, does it not raise the potential ambiguity between aph* of two or more different phytoplankton?

A: The package effect is only changing the overall value of aph* but not the differential structure and is therefore not interfering with our retrieval results.

3. Results 3.1 Phytoplankton absorption of cyanobacteria and diatoms from SCIAMACHY L4-12, pp 4570: R1: I personally think that these descriptions fit better in Section 2 (Instrumentation and methods).

A: As requested, we moved this part now to the end of section 2.3

L13-15, pp4570: R1: This sentence is not easy to read because it is too long and there are too many “of”s. Please change the sentence.

A: We changed the sentence into two sentences: Fig. 3 shows examples of the differential optical depths of the SCIAMACHY spectral fits from the two considered phytoplankton groups. In addition, the results of the in-situ measured differential phytoplankton spectrum (from Fig. 2) scaled with the fit-factor are plotted.”

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L13 (pp4570) to L9(pp4571): R1: Are these lines absolutely necessary to draw the conclusions shown later? I can understand your later conclusion, without these (I personally think that Figs.6 and 7 shown later are sufficient).

A: We think it is necessary to show the results of this first step of PhytoDOAS retrieval in order to judge the quality of the retrieval.

3.2 Biomass of cyanobacteria and diatoms from SCIAMACHY L15-18, pp4571: R1: There are too many invalid pixels in the cyanobacteria distribution derived from the DOAS, and visual comparison with NOBM is not easy. Please change the figures in some way for easier comparison.

A: To make the visual presentation clearer we now changed Figs. 6 and 7 with also zoom-in on two regions each, so the NOBM and PhytoDOAS results can be better compared. The invalid pixels we did not plot in the publication, but we added Figs. 6a and 7a here at the end of our author response where also the invalid pixels are plotted (in white). In this plot one can recognise areas where no SCIAMACHY measurements were taken at clear sky and solar zenith angle $<60^{\circ}$.

R1: What is the basis to mention that the distribution of cyanobacteria retrieved from SCIAMACHY data agrees well with the calculations made by NOBM? Please add some kind of statistics to support the statement.

A: As stated in the point before this one, we now added for each global phytoplankton group map two zoom-ins in order to show the similarity in many parts of the map between NOBM and SCIAMACHY PhytoDOAS. We also added the text in the discussion 'Since the NOBM simulations combine global ocean colour biomass data with global data sets on nutrient distributions, sea surface temperature and current conditions (Gregg et al. 2003) to calculate various PFTs, it certainly is not the tool to validate PFTs satellite retrievals. However, it does provide information on the global performance of the SCIAMACHY PhytoDOAS retrieval.'

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L18-L24, pp4571: R1: Only 5 match-up data are used for the validation, and therefore there is no statistical significance in the result shown in Table 1. The authors should recognise it, but there is no discussion about it. Then what is the basis to mention *a reasonable agreement with a moderate underestimation*? How the error of -4% to -70% representative? I am not convinced with the validation result presented here, if the satellite and in situ data were matched up within a 12h-180 km window (especially for Diatoms). What is the basis to choose 12h & 180km? What is the protocol for your validation exercise? Please explain. Table 1: There are many SCIAMACHY [Chla] on the single day (but within 12h time window)? I suppose that some neighbouring pixels, rather than an exact matchedup pixel, are also used. But there is no explanation about the validation protocol as mentioned above. In any case, readers will have difficulty to understand how you validate your estimation by the DOAS. L25(pp4571)-L10(pp4572): The same comments above apply here, too. Table 2: The same comments apply here, too. It may be much easier for reader to evaluate your validation results, if the results are presented in a form of a usual scatter plot, rather than in two tables.

A: Now we made a scatter plot (Fig 8) to better visualise our results and added in the results section a broader explanation 'To further prove if SCIAMACHY cyanobacteria and diatom biomass data are in the right order of magnitude, the in-situ measurements of these phytoplankton groups chl-a conc. from the two Atlantic cruises described in Chapter 2.3 were searched for collocations with these data. The collocation criteria were that in-situ samples were taken within 12 hrs of the SCIAMACHY measurement and within the SCIAMACHY pixel or the next adjacent one (180 km). Mean values for SCIAMACHY pixels collocated to the same in-situ samples, and vice versa, were determined and are shown in Fig. 8. For the comparison of cyanobacteria and diatom biomass distributions only five match-ups each were determined. Compared to these collocated in-situ measurements and opposed to the comparisons with NOBM, SCIAMACHY PhytoDOAS underestimates the cyanobacteria chl-a conc. by 6% with a standard deviation of 44% and overestimates the diatom chl-a conc. by 15% with a standard deviation of 31%.' A 12 hr window is still appropriate for such compar-

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isons, the 180 km window is probably more questionable. We used the neighbouring pixels as well because of the time shift of up to 12 hrs and also neighbouring in-situ measurements to have a better match-up of point measurements with satellite measurements. If wished by the referee we can remove this comparison, since there are not enough collocations for comparisons. This paper is meant to demonstrate the potential of PhytoDOAS in discriminating two major phytoplankton groups, as pointed out now in the discussion, no validation just a verification can be performed at this stage. Also validation by in-situ measurements is always challenging as we pointed out in the text in the paragraph in the discussions: 'Comparisons of our results so far are still preliminary as a thorough validation is difficult to perform at this stage. In-situ measurements are quite sparse in general, and they only provide punctual data points instead of an integral over the large surface footprint of an ocean color sensor (˜1-9 km2 and for SCIAMACHY $>$30 km2). Nevertheless, these first comparison to in-situ data indicate that the range of SCIAMACHY phytoplankton group chl-a concentrations are reasonable and plausible.' As suggested, we changed the illustration of comparisons in Tables 1 & 2 into a scatterplot (now Fig. 8).

4 Discussions and conclusions R1: Description of this section is a mixture of summary, discussions, conclusions, outlook, and something else. It was not easy for me to pick up what was the main conclusion of this paper. Please re-organise this section. There are lots of irrelevant descriptions. For example, a role of diatoms on oceanic carbon cycling [(L24, pp4572 to L17 (pp4573)] as well as ecology of cyanobacteria (L20-29, pp 4573) have nothing to do with what was presented earlier in this paper (i.e. phytoplankton classification by the DOAS method using SCIAMACHY). These descriptions can easily be removed (Or be moved to Introduction).

A: We now completely rearranged the discussion to make it clearer and also added the discussion of comparisons to other PFT estimates from space.

L5-29, pp4574: R1: The authors point out that other published methods (for phytoplankton classification) are empirical based on the data taken in the past, and that

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unexpected changes in nature in the future will cause a bias in the classification by these methods. This is possibly true. However, the authors discuss that the DOAS is not an empirical method but an analytical method, and therefore free from such a risk of the bias. Unfortunately, this does not sound either logical or right to me, because the DOAS presented in this paper needs a spectral fitting to reference spectra empirically determined from measurements. The empirically assumed reference spectra can also have variability due to unexpected change in phytoplankton physiology (e.g. pigment composition) induced by climate variability for example. The DOAS cannot self-correct such a change in the reference spectra, even if a broader spectral region is used in the fitting. Thus the DOAS can also introduce a bias when the reference spectra determined empirically are not correct. In addition, Empirical Orthogonal Function analysis was used for some optimisation of the DOAS method presented here (if I understand this paper correctly), thus depending on data. In my opinion, the DOAS method presented here may involve more biological/physical mechanisms than other methods do, but it does not necessarily mean that the DOAS method is not empirical and is free from the problem which the other methods have.

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. Marker pigments for certain groups might change in their quantity due to pigment packaging and physiological state but probably not in their quality which is determining the differential signature. 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.

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

L2-L16, pp4575: R1: The whole paragraph is redundant here, because these discussions are not about what was presented in the earlier sections (Sections 2 and 3), although some sentences may fit to Introduction.

A: We now cut the paragraph and put some of the content (modelling) in a previous paragraph in the discussion where we thought it is appropriate.

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