Comments to Author

Title of the manuscript: New methods for retrieval of chlorophyll red fluorescence from hyper-spectral satellite instruments: simulations and application to GOME-2 and SCIAMACHY
Authors: J. Joiner, Y. Yoshida, L. Guanter, and E. M. Middleton.

General Comments:

This is a timely paper which discusses the methods for the retrieval of chlorophyll red fluorescence from satellite-borne spectrometer data. In general it can contribute to the rapidly growing amount of publications in this field. Especially as it is connected closely to the work of Wolanin et al. (2015) who recently published first spectrometer retrievals of red Solar Induced Fluorescence (SIF) over land and ocean. Even though rather recently such similar studies have been published I feel that the results of this paper can anyway be very helpful for the community in absence of feasible validation sources. As long as such sources do not exist I am convinced that this paper can provide useful research information and data for future intercomparisons. Especially because some of the approaches taken here appear to be sufficiently different compared to the previous work of Wolanin et al. (2015) and provide novel research.

However, I was surprised that this manuscript is considered to be suitable for a journal focusing on <u>atmospheric measurement techniques</u> (nomen est omen). Only marginal relation to such atmospheric measurement techniques can be found except that the devices used for the retrieval algorithms were designed to measure atmospheric parameters. As two related papers led by the first author[1] and two papers as a co-author[2] have already been published in AMT it is only fair to publish this one as well. Accordingly its acceptance by the editors for a peer-review is comprehensible. Especially, as content and quality of the manuscript is, after revision, certainly worth to publish. However, as long as scientific journals are published in a themed fashion, readers continue to select them according to their foci. Thus, for the future I recommend to the editorial board of this journal (of which the first author is a member of) to either (1) reject such manuscripts and recommend a more appropriate one; (2) extend the topical focus of AMT (thus changing the title) or (3) probably create a new journal having an appropriate focus under the umbrella of "Copernicus Publications."

Coming to the **scientific general comments:**

1) I see one general shortcoming of the presented study which is related to the justification of several decisive settings. I found many places in the manuscript on hand where scientific reasoning is missing. Wherever I have found such unexplained decisions/settings I have asked for justification (see "Detailed Comments").

2) In general I think that the introduction of the O_2 - γ absorption band provides a potential *constrain* (probably a more appropriate term than "anchor") to the O_2 - B absorption used for the red SIF retrieval. However, for the sake of trace-ability (and if required also of reproducibility) the reader needs more information how precisely this has been done! In this respect and most others I cannot agree more with anonymous referee #1. I am not satisfied with the answer given to 1. referee as it mainly broaches the wording instead of explaining the underlying principle of how the use of O_2 - γ is beneficial.

3) The same general criticism is related to zero-offset correction (Sect. 4.4.4): Here the reader seemingly receives guidance but the instructions remain vague. Of particular importance (see further comments) is the necessity that principle components (PCs) are not affected by the zero-offset effect.

4) ~~Another general, though less critical, aspect is the fact, that the maps (or their color scales) should show units wherever applicable.~~ ← satisfying solution already proposed to referee #1

5) All comparisons of your results are qualitative. I admit that a quantitative comparison might be difficult with datasets of other non-institutional groups (for example Wolanin et al., 2015). However, at least the comparison of your nFLH retrievals and MODIS is feasible on a quantitative level. If there are no important technical obstacles please provide such quantitative comparison (by means of histogram or scatter-plot analysis).

6) ~~Please discuss the potential impact of Vibrational Raman Scattering (VRS). You are only indicating this in Sect. 6.5.~~ ← satisfying answer already given to referee #1

7) To my understanding, when introducing the O_2 - γ band to constrain the O_2 - B retrieval an important goal was to ensure that the impact of SIF shall be reduced to the latter, as the O_2 - γ is (correctly) assumed to be free of impact from SIF. However, no information is given how large the impact of the zero-offset and Rotational Raman Scattering (RRS) on the O_2 - γ band is expected. This is of importance, as the effects of both aspects cannot be discriminated spectrally from the effect of SIF (at moderate spectral resolutions).

8) Several times rather definite conclusions about the ability of the presented algorithms are given. I feel that these conclusions are coming too early, as most of the findings are coming from **qualitative** comparisons with others and visual inspections of monthly maps. I agree, that the proposed approaches seem to have promising potential, but announcing that "Our approach offers noise reduction" based on these comparisons and bearing in mind that the above mentioned open issues are not yet solved you should refrain from such statements (see further comments).

Detailed Comments:

Page 1

line 8:

You state:

"Our approach offers noise reductions ..."

I suggest to remove this sentence, as substantiation is based on visual inspection, which can come also to other conclusions (see comments below).

line 10:

anchor → constrain (?)

biases due to … → biases most likely due to …

line 18:

I do not understand the connection: soil moisture and what? Furthermore, soil moisture is mentioned only here in the abstract and is not subject of discussion any more

1 Joiner et al. (2012) – <u>doi:10.5194/amt-5-809-2012</u> and Joiner et al. (2013) – <u>doi:10.5194/amt-6-2803-2013</u>.
2 Koehler et al. (2015) – <u>doi:10.5194/amt-8-2589-2015</u> and Guanter et al. (2015) – <u>doi:10.5194/amt-8-1337-2015</u>.

Page 2

line 29:

Add Khosravi et al. (2015)

line 47:

Many different terms have been used in this manuscript for retrievals utilizing solar Fraunhofer lines. It would be helpful to introduce a common term/description (or even abbreviation) for solar Fraunhofer line based retrievals used throughout the paper.

line 48:

Add Koehler et al. (2015), Wolanin et al. (2015) and Khosravi et al. (2015)

line 50:

Why is "surface reflectance" not listed in the enumeration?

Page 3

line 58:

Please use the full information available about the ESA report.

line 9:

biochemstry → biochemistry

line 12:

quantaties → quantities

line 14:

use oxygen → use of oxygen

line 14cont.:

Is no impact of SIF on cloud top height retrievals using $O_2 - A$ expected? If not, it should be added as this retrieval was one of the first exploiting the $O_2 - A$ in such a way and has been proposed by Yamamoto and Wark already in the early 60ies and applied by Kuze and Chance first time to satellite spectrometer data.

line 25:

remove "straightforward".
Even though I am sure I have undestood what you mean by "straightforward" approach, interested readers without specialized knowledge will (at this point) have difficulties why this approach is more straightforward than the $O_2 - B/A$ retrievals.

Page 4

line 28:

effects of → instrumental effects such as

line 34:

a single month → two months

line 35:

You state:
"While promising, the monthly averages appear to be noisy, and a significant offset between GOME-2 and SCIAMACHY red SIF magnitudes was shown."
- Obviously the GOME-2 results over ocean in Wolanin et al. (2015) show a similar pattern as the ones from SCIAMACHY (Fig. 9/page 253 compared to Fig. 13/page 256) but the scale seems to be different and compared to your results (Fig. 15/page 40) they are in fact more noisy and do not appear to be on a mature level.
- When looking into the land or ocean results based on SCIAMACHY in Wolanin et al. (2015) (maps in Fig. 14/page 257) these values are not showing particularly noisy or patchy features. You are repeating this statement in section 6.5 where you explain in more detail:
  "Results from GOME-2 and SCIAMACHY, using the full wavelength range between 660 and 713 nm, are less noisy than those obtained by Wolanin et al. (2015) with a smaller fitting window that includes only solar Fraunhofer lines."
  Your result for SCIAMACHY seems to me not (yet) conclusive, as you are also mentioning in section 6.5:
  "SCIAMACHY, which alternated between limb and nadir mode observations, is gridded at a resolution of 1° so as not to show too many gaps between grid boxes."
  As your SCIAMACHY land or ocean results show similar "unsmooth" features as shown in Wolanin et al. (2015) poorer statistics (in terms of less pixels per gridcell compared to GOME-2) is another very conceivable possibility.
To summarize, either remove your statement or adapt it in a way to that GOME-2 and SCIAMACHY results for land and ocean are individually judged.

line 41:

the sentence is more easily understood when you would bold-face the word "nearby".

line 44:

anchor → constrain (?)

line 50:

For the sake of completeness: PCA-based approaches in remote sensing have been used earlier to retrieve aquatic parameters from satellite borne instrumentation (Bracher et al., 2009).

Page 5

line 60:

Again you assert that the results of Wolanin et al (2015) are of poor quality. As mentioned above, you should explain better what you mean or remove the sentences. In fact, Wolanin et al.'s results for GOME-2 are debatable but the SCIAMACHY results seem to have the similar quality as those shown in your manuscript. To be more precise: The results of your Fraunhofer line retrieval leads to very similar global features while the $O_2 - B$ band retrievals appear to be smoother. But several issues of the latter are not well explained (see below), so that the quality of these results seem to be promising but remain worth discussing.

line 68:

"GOME-2 and SCIAMACHY measurements. Application of our approach leads to unprecedented precision and

accuracy for red SIF data sets that span more than a decade."
Please remove this sentence and as you cannot prove this quantitatively.

Page 6
line 101:

Which solar spectrum have you used (please give reference).
line 103:

Guanter et al. (2010) and Vasilkov et al. (2013) discuss thoroughly spectral features in the O_2 - A/B bands or nearby. None of them discuss the effect of RRS on the O_2 - γ band. Please give information why you think that RRS is negligble.
line 1cont.:

As already recommended by referee #1, please explain how mathematically and technically the O_2 - γ band absorption is taken into account. Your answer to the referee is already leading to a better explanation. However, it is still not completely clear to me how precisely the O_2 - γ band information is used in the O_2 - B retrieval.
line 9:

the selection of the spectral window for ocean SIF is not justified. Why exactly this window? Or you relying on previous works or defined it based on own findings? (and if so, how?)

Page 7
line 16:

I doubt that the effects of aerosol scattering can certainly be ignored but I suppose you are taking it into account through the PCs(?)
Eq (1):

This relation has been derived phenomenologically in Joiner et al. (2013). It is not strictly valid in case of Bidirectional Reflectance Distribution Function (BRDF) like reflectance behavior. It would be helpful if the authors discuss the implications on the retrieval results.
Eq (2):

You also **model** transmittances for later analyses (not only use the PCA for application to experimental data only). In such a case the canopy-to-satellite transmittance that you create using radiative transfer must be created using the correct lower boundary condition. Can you please elaborate (not needed in the manuscript).
Eq (3):

Such a relation would lead to unitless SIF. Your answer to referee #1 is not sufficient, as a (formal) substitution of Eq (3) into Eq (1) is not leading (overall) to the right units. A sentence like "SIF ...is given in radiance units" is not correcting the formal mistake. The simple introduction of a factor having the right units would help.

Page 8
line 43:

I clearly see a need in emphasizing advantages of a developed method/methodology from the author's perspective but from the perspective of the reader I prefer a better balanced discussion. Please add a discussion of the disadvantage as well (the danger of: improper selection of the underlying multivariate dataset or loss of interpretability of the individual orthonormal PC etc.)

line 52:

I suppose, that the polynomial fits produce "envelope" polynomials(?)
line 62:

PCA in → PCA is
line 64:

anchor → constrain (?)
line 69:

and well as → as well as
these window → these windows

Page 9
line 82:

Eqs. (1-???)
line 86:

As this is rather general information it would be good for the reader to have a decent reference (Rodgers?)
line 100:

"good fits": this needs further explanation: what are "good" fits? The assessment of goodness might differ to mine or any other reader.
line 2:

Please check: GOME-2 measures the solar irradiance once per day, SCIAMACHY does it once per orbit.
line 5:

I suppose "cloudy data" and the removal of "biases" refer to subsections 4.4.2 and 4.4.1, respectively. If so, please refer to the section. If not, what kind of "biases" are you referring to in this line? Zero-offset biases?
Page 10
line 12:

Joiner et al. (2013) and Koehler et al. (2015) → Joiner et al. (2013), Koehler et al. (2015) and Khosravi et al. (2015)
line 31cont.:
   • I have checked the reference "Joiner et al. (2013)" to which the reader is guided in order to understand more about the "effective cloud fraction" used here. From there the reader is directed to Joiner et al. (2012) which is discussing SCIAMACHY cloud fractions, but provided that the analysis is done near 866 nm? Please make it more convenient for the reader to have everything on hand, for both GOME-2 and SCIAMACHY.
   • Furthermore, specify the used thresholds (if different from the one given here), and if differing from the original manuscripts (Joiner et al., 2012/2013), please provide reasons why.

- One interesting finding of Koehler et al. (2015) was that the retrievals of far-red SIF are not significantly "suffering" from cloud cover. They stated:
  "On this basis, a cloud fraction threshold of 0.5 is a reasonable compromise between the loss of measurements and changes in the SIF average. "
  Please explain why SIF retrievals are only shown for $f_c < 0.3$.
- You eliminate solar zenith angles (SZA) > 70°. Which is consistent with your statements in Joiner et al. (2013) but why is this threshold different from the one used for the PCA (see page 8/line 48). As far as I could figure out this is in line with your approach from 2013 but was not explained there as well.

Page 11 and Page 12
line 40:

Why "particularly for GOME-2 measurements"? and not for SCIAMACHY? Is this based on own findings our on Wolanin et al. (2015) or/and Koehler et al. (2015)? Both are explicitly mentioning the problems of the SAA for GOME-2 retrievals.

line 53:

"Khler et al. (2015) found that GOME-2 and SCIAMACHY far-red SIF retrievals exhibited biases, ..."
Koehler et al. (2015) showed that the bias for GOME-2 can almost be a factor of two to three larger than for SCIAMACHY (see Fig. 17/ page 2604). For the effect on SCIAMACHY results they state:
"Nevertheless, a slight offset of about 0.1 mW m−2 sr−1 nm−1 is introduced in latitudes above 40° N."
- According to your maps in Fig. 10 the adjustment for SCIAMACHY is neither simple nor following a simple latitudinal dependence.
- While you were writing the article, you were obviously not aware that Khosravi et al. (2015) provided a thorough analysis of the zero-offset for SCIAMACHY far-red SIF retrievals. In their Fig. 2/page 7 they show that the difference between the retrievals for SIF for vegetated and non-vegetated regions can be in the range of a factor of two.

To summarize: please add a more comprehensive discussion on what has been done in the field of zero-offset correction so far and the main findings.

line 64cont./section 4.4.4:

The description of your developed zero-offset correction scheme is not clear. Please revise this section by taking into account the following questions:
- "SIF retrievals over ocean" - The whole oceans or only selected parts?
- What is a "clear sky solar irradiance?"
- Why is $SIF/\cos(\theta)$ a valid approximation?
- How do you define the continuum radiance and
- why do you think is the dependence on θ_0 and continuum radiance yield the intended result? And how exactly are you relating both to the regression?
- How do you exactly "apply the derived coefficients?"
- Why have you introduced latitude bins at these particular positions?

Please provide also illustration of your regression coefficients or similar.

line 86/Page 12:

You state: " We also have not added barren land.."
As long as there are no illustrations of the dependence of the zero-offset on "continuum radiance" and θ_0 it is hard to decide whether ignoring barren land has no impact on the quality of your regression coefficients. Background: I tend to doubt that clouds can represent land spectral features.

line 94cont.:

For those having experience in the field of sensitivity studies the terms "true" and "retrieved" might be clear. For interested third parties it might not be obvious. Please add a short explanation.

line 97/Section 5:
- According to your response to referee #1 you seem to have already fixed the wavelength range selection already. This was indeed important. Thank you for that.
  However, using the fourth order polynomial for the synthetic data set while for real data (according to 4.3) you fit a third order polynomial makes me doubt that the surface treatment in the radiative transfer is representative.
- I appreciate very much the depth and thoroughness of the sensitivity study but I am clearly missing an important dependence analysis for zero-offset adaption. I do understand that it is most likely an instrumental spectral feature but even without precise knowledge it is possible to assess its impact. Please add, or justify why this is not needed.
- Scenario "Line 6" is not discussed. Please add discussion or remove scenario.

Page 13
line 9:

Eq. ?? → correct reference.

Page 15
line 74-76:

Makes more sense as part of the introduction of Section 5.

line 80:

You state:
"This implies that reasonable red SIF retrievals should be obtained using our new approach with existing instruments (provided they behave as expected) ..."
Bearing in mind that your findings are based on self-consistent theoretical data analyses (end-to-end simulations) it is clearly too early to state that. The sensitivity study gives you at best guidance rules. Please keep in mind, that you excluded aspects like zero-offset correction, RRS (especially in the O₂ - γ bands) or VRS. Please remove this sentence or weaken the statement.

line 6:

The selection of this wavelength range is not explained/justified. This is unfortunate as a rather thorough sensitivity

study has obviously not been used to support a wavelength window change from either Wolanin et al. (2015) or the window used in the sensitivity study (682 – 686.7 nm). Please justify!

Page 17
line 60-61:

I recommend to mention individual sensitivities of your algorithm(s) on the factors. Currently the list can be perceived as completely disconnected to your retrievals. For instance, the solar Fraunhofer line retrieval might be more/less affected by poor SNR values than the O_2 - B retrievals.

Page 18
line 79:

Please mention explicitly that this leads actually to a better spatial coverage.

line 89:

there are some some … → there are some

line 90cont.:

I cannot follow this argument. Koehler et al. (2015) show clearly stronger biases for GOME-2 than for SCIAMACHY while you are showing the opposite. Also the latitudinal dependence shown here is obviously more complex in case of SCIAMACHY than for GOME-2. Please explain in more detail or remove related sentences.

line 96cont./Section 6.4:

Please give reasons for the selection of these boxes. Furthermore explain why you have decided to use a 3°x3° box.

Page 19
line 3:

Why are you only focusing on GOME-2 now? Explain.

line 10cont.:

mean fields → means
Why more grid resolutions and why these values and no others?

line 25:

You state:
"This demonstrates the ability of the GOME-2 monthly red SIF at the box resolution to resolve signals of the order of +/-0.1 mw/m2 /nm/sr."
I think, that an important "ingredient" to reach such signal levels is not mentioned which is the deseasonalization/anomaly analysis. Please rephrase.

line 33:

I understood, that RRS is not that much of importance in this wavelength region (which has been well justified in other papers) but why is VRS not playing a role?

line 35:

Why is no further "zero-level offset adjustment" performed? On page 12/line 82 you showed such a correction. Why not here?

Page 20
line 40:

"GOME-2 provides superior ..." → "The reader is reminded that GOME-2 provides superior ..." (makes sense when applying proposed change Page 18/line 79).

line 45:

While this is true for GOME-2 this does not hold for SCIAMACHY. The results in Fig. 15/page 40 in this manuscript compared to Fig. 9/page 253 in Wolanin et al. (2015) are not directly comparable, as (1) the latter are shown for one year of data, while in this manuscript monthly data are shown and (2) the difference in color scales makes it impossible to compare reliably. A thorough quantitative comparison of both SCIAMACHY results could help. As long as you do not provide such a comparison please refrain from such statements or separate the qualitative comparison into two parts: one for GOME-2 and one for SCIAMACHY.

line 49:

You state that magnitude and patterns agree excellently. Please show this **quantitatively** and provide histogram of differences or a scatterplot.

line 62:

anchor → constrain (?)

line 68cont./Page 21:

You state:
"We demonstrate that use of the O2 γ- and B-bands can increase red SIF retrieval precision as compared with approaches that utilize a smaller fitting window confined to regions outside the O2 B-band where the SIF signal is obtained solely by filling in of solar Fraunhofer features."
As indicated before, assuming a better performance using additional spectral information suggests such an improvement. However, bearing in mind, that you have not yet elaborated on the impact of inelastic scattering (RRS and potentially VRS) and zero-offset :
- on the O_2 - γ "constrain"
- on the creation of PCs
I doubt the conclusiveness of the present study to allow such a statement.

Page 21
line 73:

Maybe I missed something but where in the manuscript can I find the analysis leading to the mentioned uncertainties? If this is not yet included please add or remove the statement.

Comment 6 of referee #1 and your answer

The results shown in Fig. 6 and 16 in your answer to referee #1 are very interesting and improving the reader's understanding.
I suggest to add "nm" to the annotation of the wavelength axis. Furthermore I recommend to remind the reader that "b)" is referring to the full (and "constrained") O_2 - B retrieval while "c)" shows the results for the solar Fraunhofer line retrieval. I suppose that "d)" is the residual for the full O_2 - B retrieval. Furthermore I'd like to reassure: the reflectances shown there are given as reflectances at top of atmosphere(?)

References:

Bracher, A., Vountas, M., Dinter, T., Burrows, J. P., Röttgers, R., and Peeken, I.: Quantitative observation of cyanobacteria and diatoms from space using PhytoDOAS on SCIAMACHY data, Biogeosciences, 6, 751-764, doi:10.5194/bg-6-751-2009, 2009

Wolanin, A, V.V. Rozanov, T. Dinter, S. Noël, M. Vountas, J.P. Burrows, A. Bracher, Global retrieval of marine and terrestrial chlorophyll fluorescence at its red peak using hyperspectral top of atmosphere radiance measurements: Feasibility study and first results, Remote Sensing of Environment, Volume 166, 1 September 2015, Pages 243-261, ISSN 0034-4257, doi:10.1016/j.rse.2015.05.018.

Khosravi N, Vountas M, Rozanov VV, Bracher A, Wolanin A and Burrows JP (2015) Retrieval of Terrestrial Plant Fluorescence Based on the In-Filling of Far-Red Fraunhofer Lines Using SCIAMACHY Observations. Front. Environ. Sci. 3:78. doi:10.3389/fenvs.2015.00078

Kuze, A. and Chance, K.V. (1994). Analysis of cloud top height and cloud coverage from satellites using the O_2 A and B bands. Journal of Geophysical Research 99: doi: 10.1029/94JD01152. issn: 0148-0227.