Atmos. Meas. Tech. Discuss.,
doi:10.5194/amt-2019-384-AC2, 2020

Atmospheric Measurement Techniques
Discussions

Interactive comment on "Improved SIFTER v2 algorithm for long-term GOME-2A satellite retrievals of fluorescence with a correction for instrument degradation" *by* Erik van Schaik et al.

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Received and published: 15 June 2020

We thank the reviewer for this assessment and for his/her overall insightful and constructive review that has helped us to improve the manuscript. The reviewer's comment is in normal black font, our response is in blue font. In the accompanying revised manuscript the applied corrections are visible in the track changes.

1. What is the main achievement obtained through this study (it sounds more like a technical report)? 2. "Our results support the use of SIFTER v2 data to be used as an independent constraint on photosynthetic activity on regional to global scales". Where is this justified from the current paper?

1. The achievements of our work have been explained in the Abstract: we show a tangible improvement of the previous SIFTER (v1) algorithm presented in Sanders et al. [2016]. As a reminder, the improvements are (a) a spectral fitting approach that reproduces fluorescence in an end-to-end test (more about that below), (b) application of a principle component set based on 5-years worth of reference spectra, and (c) first-ever assessment of GOME-2A reflectance degradation, and a first attempt to correct for this.

2. The scope of this paper is not the use of our SIFTER v2 data to constrain patterns of photosynthetic activity, but rather to show the algorithm mechanics, necessary corrections for spatiotemporal biases, and to evaluate the product and its uncertainty against the NASA SIF retrievals. The fact that a pre-release of SIFTER v2 has already been used to constrain photosynthesis in the Amazon (Koren et al., 2018), and that this pre-release has now improved further (via the degradation correction) is in our view encouraging to users looking for new global proxies for carbon uptake.

While this study provides a well written overview of the improved algorithm for SIF retrievals, I am worried that it lacks original scientific content. The majority of the work is incremental in nature and reads, to the most part, like a well-written tech report. What I am missing are real scientific discussions on WHY these algorithm changes are important, why the omission of some absorption bands is so crucial (see later, this is a hot topic, it would be good to discuss this), etc. I just feel the authors need to a better job in outlining what is really part of their original work and what is not. Adding a more in-depth case study as to why the O_2 band is hurting the retrieval might help fill the gap in current originality. I don't want to be overly demanding but as nice as the paper reads at the moment, the authors have to be honest and clearly outline what is original vs. a reproduction of the most basic concepts of the Joiner and Koehler approaches. Without this, it would remain a tech report only and I would have to defer the publication decision to the editor.

We appreciate the reviewer's critical perspective, which moved us to analyse in more depth why excluding the O_2-A band from the spectral analysis for space-based approaches leads to a much better reproduction of the SIF signal in an end-to-end test. We believe that our postulated SIF 'air mass factor' is instructive in understanding how absorption of the SIF signal by O_2 between the Earth and GOME-2 distorts the relative depth of the Fraunhofer lines within the absorption band compared to the relative depth of the lines in the full transmission part of the spectral window (~740-758 nm). This opens up new avenues to further optimize the spectral fitting window in future studies. We now also discuss in more detail why we think the latitude-dependent bias is negative in the northern hemisphere, and positive in the southern hemisphere, also suggesting next steps, such as dynamically fitting the GOME-2A slit function in the non-linear least squares regression.

Please find a few more detailed comments below.

SIFTER needs to be explained in abstract already.

We now explain the abbreviation SIFTER in the abstract.

P2 Line 4: 19% released as heat: This sounds oddly specific. In fact the heat quenching is highly variable, make this clear.

We have now modified the sentence without making reference to seemingly exact percentages: *"Most of the solar energy that a plant receives is used for photosynthesis, but part is released as heat and between 1-2% is re-emitted as fluorescence at longer wavelengths [Baker and Oxborough, 2004]."*

P2 Line 9: SIF doesn't know about the CO_2 concentration (at least not directly). See Rev1.

Point taken. We removed this part of the sentence. The photochemical yield is influenced by the rate of CO_2 fixation by plants, and this rate is not directly related to the ambient CO_2 concentration.

P2 Line 31: KNMI needs to be explained in the first instance (not everyone knows it).

We have now added that the abbreviation refers to Royal Netherlands Meteorological Institute.

P6-7: Lines 23++: Are any of these steps new? Which ones are identical to Joiner et al.? Which ones are identical to SIFTER 1? Which ones come from this paper?

Section 2.2 provides the basic information for the SIFTER algorithm, and in Section 2.3 we have now included more motivation and highlight the delta's between the SIFTER v1 and the NASA algorithm.

The SIFTER v2 algorithm has grown out of two years of collaboration (and exchange of ideas via email and on international meetings) between KNMI, Wageningen University, EUMETSAT and NASA-researchers. The product is thus partly independent, and partly reflects the best-practices consensus from a larger group of authors.

P7 –Lines 21-22: Maybe a copy&paste error? What does that sentence mean anyhow, I am not really sure (too vague).

This sentence should not have been there. We removed it.

P7 L30: Please make clear that the impact of transmission function is only of importance for the large spectral windows as needed for GOME-2.

We now state that accounting for spectrally varying transmission is relevant for the wide GOME-2 window.

P8-Lines6++: If I look at the list of changes made here, they really look rather incremental, fine-tuning some retrieval settings. The big question is whether this warrants publication in a peer reviewed journal as original work. You will have to justify this to some degree. (i.e. why is this more than an internal tech report?)

The list does not sum up the all the retrieval changes in this paper. Besides the narrower fitting window based on the sensitivity tests – including the exclusion of the O2-band as recommended by the reviewer – we now use a set of PCs based on a multi-year analysis of spectra over the Sahara rather than based on the last 12 months as was done before. We also implement a correction for degradation of the level-1 spectra over time, and show how this stabilizes the retrievals, which has not been done before.

P8-Line12: I think it is important to underline (again) that the exclusion of the O_2-A band actually helps the retrieval. This is the topic of a long-standing debate and the original algorithm included the O_2-A band under the assumption that it "helps" the retrieval. It would be good to elaborate more on that specific issue and show the community clearly why it harms the actual retrieval. This could be a valuable addition.

Thank you for bringing this up. This was exactly the motivation to do the sensitivity tests with DISAMAR, as described in the original manuscript (P8L9-13): "In SIFTER v1, a wide fitting window was selected (712-783 nm), which includes spectral features from the oxygen-A band (759-769 nm) and water vapour absorption (714-734 nm). These features potentially complicate the calculation of the transmittance terms with the principal component method. Here we investigate the possibility to reduce the number of PCs $f_k(\lambda)$ by selecting a narrower window that includes the strong fluorescence signature, but excludes the adjacent O_2-A and water vapour features."

We performed tests to highlight that exclusion of the O_2-A band improves the accuracy of the retrieval. In our end-to-end test, we specified fluorescence to be 4.0 mW m^{-2} nm^{-1} sr^{-1}, and then attempted to reproduce the signal from the DISAMAR TOA spectra for different retrieval scenarios and for three spectral windows, one excluding the O_2-A band, one excluding both the O_2-A band and much of the H_2O absorption, and one wide window (the original SIFTER v1 window). Table 1 below shows that the accuracy (bias) and uncertainty of the retrievals drastically improves by excluding the O_2-A band, and improves further by limiting the influence of H_2O.

Table 1. Results of tests to reproduce a SIF signal of 4.0 mW m^{-2} nm^{-1} sr^{-1} from an ensemble of 200 DISAMAR top-of-atmosphere spectra with different retrieval geometries, surface albedo values, and water vapour conditions.

	Window	Bias	Uncertainty
		(mW m^{-2} nm^{-1} sr^{-1})	(mW m^{-2} nm^{-1} sr^{-1})
Original window [Sanders et al., 2016]	712-783 nm	-0.47	0.53
Excluding O_2-A band	712-758 nm	-0.23	0.41
Including O_2-A band	734-783 nm	-0.49	0.57
Excluding O_2-A and H_2O (this work)	734-758 nm	0.00	0.39

Inclusion of the O_2-A band tends to lead to an underestimation of retrieved fluorescence. Proportionally similar underestimates occurs for different fluorescence signal strengths.

As to why including the O_2-A band harms the retrieval of SIF from space, we did an additional study into the sensitivity of top-of-atmosphere radiance to SIF at the surface, and included this in the revised manuscript in Section 3.2. We simulated TOA radiances for two ensembles: one without SIF and one with a SIF strength of 4.0 mW m^{-2} nm^{-1} sr^{-1} (at 737 nm). The DISAMAR radiative transfer model accounts for absorption by H_2O and O_2, and describes the effects of multiple scattering and a spectrally varying surface albedo. DISAMAR radiances have been convolved with the GOME-2 slit function (width $\sim$0.5 nm). The settings in DISAMAR were such that the ensemble average surface albedo, surface pressure, and viewing geometry were the same, so the essential difference between the two ensembles is in the presence of a SIF signal. No clouds or aerosols were included in the simulations.

The DISAMAR simulations show that the presence of a SIF signal leads to a small addition of radiance across the spectrum. The surplus radiance closely follows the magnitude and spectral shape of the fluorescence source spectrum between 740-758 nm, but is weaker between 734-740 nm and 759-766 nm, where water vapour and oxygen partly absorb the SIF signal travelling from the Earth's surface towards the sensor (upper panel of the new Figure 3 in the revised manuscript, included here below). The sensitivity of the radiances to changes in the 'state' thus shows a strong spectral dependence. Put simply, within the O_2-A band transmission is low and only half of the SIF signal makes it to the sensor. But between 740 nm and 758 nm (and also for 768-783 nm), transmission is high and almost all SIF photons reach the sensor.

The SIF AMFs calculated from the DISAMAR model between 742 and 758 nm are indeed close to 1 (Figure 1 below revised Figure 3), demonstrating the good sensitivity to fluorescence in this spectral range for our ensemble. Between 734-742 nm the AMF has values close to 0.9, and within the O_2-A absorption band the AMF drops to values of $\sim$0.5.

This explains why a spectral fit with a wide spectral window that includes the O_2-A band will not reproduce but rather underestimate the SIF signal prescribed in the simulations. The spectral fitting procedure attempts to match all spectral features within the window. For the wide window this comprises the in-filling of the Fraunhofer lines in spectral regions where sensitivity to SIF is close to 1, but also the SIF in-filling of the O_2-A band, where sensitivity to SIF drops to 0.5. The single, 'window mean' retrieved SIF value then becomes a trade-off between partial SIF in-filling within the O_2-A band and complete in-filling outside the absorption bands. The result is a compromise, a structural underestimate of SIF. The lower panel shows the diagnosis: much larger average spectral residuals (model minus observation) for the 734-783 nm window in grey, especially around the Fraunhofer features, than in the 734-758 nm window (in black).

The above explanation and Figure 3 has now been included in the manuscript (Section 3.2).

P13-Lines 25 and around: Again, you are converging to a similar fitting window as Joiner et al did for a long time already. The only thing new is that you provide some more tests (of which I'm sure Joiner did as well).

See above. We now provide more insight in Section 3.2 into the reasons why excluding the O_2-A band leads to a more accurate SIF retrieval. As said before, the other new

elements of our retrieval are the PCs based on a multi-year analysis of spectra over the Sahara rather than based on the last 12 months, and the correction for degradation of the GOME-2A level-1 spectra over time.

Page 15, lines 4++ Temperature can have a profound effect on water vapour absorptions (due to a wide range of lower state energies), just using the Sahara might underrepresent this change in spectroscopy.

This is exactly one of the reasons why we take the ensemble of all 2007-2012 spectra recorded over the Sahara to base our PCs on. PCs based on such a 6-year period comprise relatively high water vapour absorptions compared to a reference PC set based on the last 12 months only. Still, we acknowledge that the variability of H_2O in the reference spectra is likely too low for the variability encountered in GOME-2A spectra over moist tropical forests. Our AMF analysis above suggests that this could be prevented for future improvements by narrowing down the spectral window even further to 740-758 nm, but this should be the focus of future work, as now discussed at the end of Section 3.2.

P18 L1++ Why should the bias depend on latitude at all (and not, say Air Mass Factor alone)? 1 degree also sounds really fine. What I am missing in most discussions is the lack of mechanistic motivation for certain choices. Why is the latitude dependent bias not symmetric? Why do you assume it is there in the first place?

The issue was also raised by ref1. The GOME-2A slit function is known to change significantly over time because of temperature changes [Munro et al., 2016]. Changes in the shape of the slit function are known to have caused highly structured spectral responses and thereby problems with the fitting of HCHO, O_3, and NO_2 in the UV-Vis part of the GOME-2A spectra (e.g. De Smedt et al. [2012], Miles et al. [2015], Azam and Richter [2015], Beirle et al. 2017]). These changes occur along an orbit (thus with latitude) and (we now include in the manuscript text) *"appear as an increase in the width of the slit function, with implications for the depth of the Fraunhofer structures:*

the wider the slit, the less deep the Fraunhofer lines. Shallower Fraunhofer lines may then be interpreted by the fitting algorithm to have been caused by fluorescence, which explains the positive fluorescence bias in the southern hemisphere (Figure 4). Conversely, sharper and deeper Fraunhofer lines (relative to the width of the lines over the Sahara), may well be interpreted as caused by negative fluorescence, explaining the negative bias for latitudes north of the Sahara."

The problems have been mitigated in the trace gas algorithms by extending the fitting approach with dynamical fit parameters describing the width and shape of the slit function, with good results [Beirle et al., 2017]. Such an approach could also be attempted for GOME-2 SIF retrievals in the far-red part of the spectrum. These are limited by the reference spectra taken over the middle of the orbit, when the slit function has an intermediate width that is likely not representative for smaller widths north of 30°N, and the larger widths in the southern hemisphere.

P21, Figure 6: I don't understand what this figure is telling me. Why "should" the uncertainty depend on the SIF signal? What is being tested here? I am a bit lost. What would make sense is to plot the uncertainty against continuum level radiance, thus to the overall SNR of the spectrum. Absolute SIF will get noisier at higher signals (which can then lead to some correlations of SIF uncertainty and SIF signal as vegetation is very bright in the NIR). Here, however the single pixel sigma is used, which is so large that it is hard to see these effects.

Figure 6 (now Figure 7) shows that the uncertainty is not driven by the SIF signal itself, which is reassuring. This was already discussed in the text. Thanks for the suggestion to also show the uncertainty vs. reflectance level. We now do that in the new Figure 7(b).

Section 5.2: Wo what does this tell us? It is all purely descriptive. Sentences like "We find that both data products capture the seasonality of SIF, which suggests that actual fluorescence in response to photosynthesis is being measured" are rather vague. Is

the final key point of the paper that you managed to reproduce the Joiner retrievals?

Section 5.2 presents a quantitative intercomparison of SIFTER v2 against the NASA SIF product. Such intercomparisons are useful in assessing the mutual consistency of satellite retrievals, and to evaluate the SIF values and their uncertainties. A previous intercomparison of SIFTER [Sanders et al., 2016] and NASA showed large discrepancies, apparent as a suspicious 'fluorescence hole' over tropical forests in SIFTER against NASA, which was one of the drivers of the current study, which is the result of a longer collaboration between WUR, KNMI, NASA, and EUMETSAT. Section 5.2 clearly shows that this discrepancy is now gone. Moreover the comparison of the matched-up SIF pixels expressed as probability distribution of differences provides a welcome assessment of the combined statistical uncertainties from both products. That the combined uncertainties quantitatively match with their anticipated values based on the theoretical uncertainties further underlines that both SIF products and their estimated uncertainties make sense, despite the two algorithms being different in their PC-sets from different regions and time periods. We shortened the sentence that the reviewer finds vague to *"Both data products capture the seasonality of SIF."* The last word on retrieval quality is obviously with validation, which is underway for SIFTER, but beyond the scope of this study.

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Interactive comment on Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2019-384, 2020.

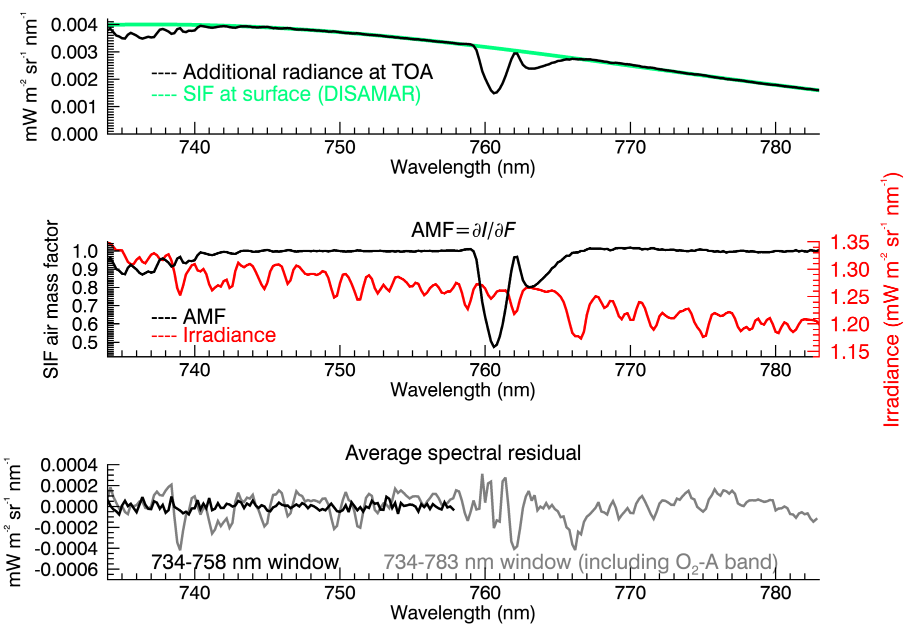

Fig. 1. Upper panel: Difference between ensemble average simulations of TOA radiances with and without a SIF signal at the surface (black line). Middle panel: SIF AMF as a function of wavelength.