Response to Referee 1

The authors thank the reviewer for the careful reading of the paper and address all comments below shown in bold which are constructive and helpful for improving the manuscript.

Reviewers specific comments:

1. You mentioned in the introduction, that the photon path in the atmosphere is modulated strongly by aerosol and clouds and this fact makes the retrieval in the O2-A and B absorption bands so complicated (s.a. Frankenberg et al. 2011). How do you correct the O2 absorption in the O2-B band retrieval for different atmospheric conditions, mainly aerosol and partly clouded pixel? The O2-Gamma retrieval is used to estimate the actual spectral structure of the O2-B band. But aerosols are affecting both bands?

Here, we added in the introduction "Both bands are affected by clouds and aerosol, in a related and predictable way. As will be shown below, principal component analyses of cloudy observations over ocean show that a large fraction of the spectral variability in both bands (>99.96%) is described by just two modes, one dominated by O_2 absorption and the other by H_2O absorption. Therefore, the fluorescence-free O_2 gamma-band can be used to estimate the amount of absorption in the fluorescence-contaminated O_2 B-band under all-sky conditions. Reflectance in the continuum surrounding both bands is very similar for cloudy conditions. Over land, there are small differences in continuum reflectance surrounding the two bands that may produce small errors (see e.g., Fig. 1) when using the O_2 gamma-band to estimate B-band absorption. However, fluorescence also produces filling-in of solar Fraunhofer features shown in Fig. 1 both inside and outside the O_2 B-band. This provides additional information to disentangle the spectral signature of absorption from fluorescence within O_2 B-band and thus uses this band to reduce noise in retrievals of the very small red fluorescence signal."

2. What do you mean with "O2-Gamma band can be used as an anchor to estimate the spectral structure of the O2-B band"? Please describe more in detail.

We have removed this wording (the use of the word "anchor") where it occurred in multiple places within the manuscript (abstract, introduction, body, and conclusions). For example, in the body of the paper, we revised to "The purpose of the PCA is to relate the absorption in the O_2 gamma- and B-bands in the absence of fluorescent

emissions. Then, in the retrieval step the O_2 gamma-band is used to disentangle the spectral structure of absorption and fluorescence within the O_2 B-band." We hope that this is more clear. Also, please refer to the response to question (1).

3. I am confused with the wavelength regions you used. In Section 4 you describe the spectral fitting window for the O2-B band is 682-698nm.
And in Section 4.3 and Section 6 the fitting window is 682-692nm.

Please also see answer to comment (5) below. We revised sections 4 and 4.3 to state that we use "two different fitting windows between 682 and 698 nm." We changed Table 1 so that the majority of the results are now shown for the 682--692 nm fitting window (the window used for GOME-2 results in Section 6) and 682-698 nm is used only to demonstrate noise reduction and increased bias in simulation mode with the use of a larger fitting window.

Further in Section 4.2 and in Fig. 2 the wavelength range for the PCs are 680-713nm. Why this extend to 713nm for the PCs and isn't that problematic?

We added "Note that we use a slightly larger O_2 B-band window for the PCA as compared with the retrieval. The larger PCA window is needed to fit the continuum so that atmospheric transmittance may be accurately computed. The leading principal components are related to atmospheric absorption from oxygen and water vapor as well as instrumental effects such as wavelength shifts that span this full wavelength range. Testing with simulation data confirms that using a larger fitting window for the PCA as compared with the retrieval does not present problems. In other words, we are able to use smaller fitting windows for SIF retrievals that are contained within the larger one used for the PCA."

4. I think Figure 4. is unnecessary. It is a normal behaviour for all spectrometer that SNR increase with measured intensity. The ranges can be described in the text with one sentence.

Since the referee feels that this figure is unnecessary, we have removed it and describe the range in the revised text as suggested.

5. Why did you not include the fit window of 682-692nm, which you finally use in the satellite data retrieval, into the sensitivity Section 5 and Table 1. Also in Figure 6 the relation of true SIF to retrieved SIF for the fit window of 682-692 would be of more interest.

We have modified Section 5, Fig. 6, and Table 1 to use the fitting window of 682-692 nm in the simulations in place of results shown for 682-689 nm as suggested. None of the conclusions have changed.

6. No spectral fit results of real satellite data are shown? Can you show at least examples of the satellite measurement and the fit result?

As requested, we have added examples of satellite spectra and the fit (see below) with appropriate text: "Figure 6 shows a sample spectral fit for an observation over the southeast US. Improvements in the fit are visible only when the spectral range is reduced to limit the y-axis range. The reflectance residuals show that reductions over the entire spectral range are subtle owing to the small values of red SIF; the overall reduction in the RMS of the residuals is approximately 7%. A relatively high signal-to-noise is necessary to retrieve the small red SIF signal." And "Figure 16 shows a sample spectrum and fit off the Mexican coast. Improvement in the fit can be seen to result from fitting the broad spectral feature of SIF emission, particularly at wavelengths 660–685 nm. The overall reduction in RMS of the reflectance residual is about 30%"
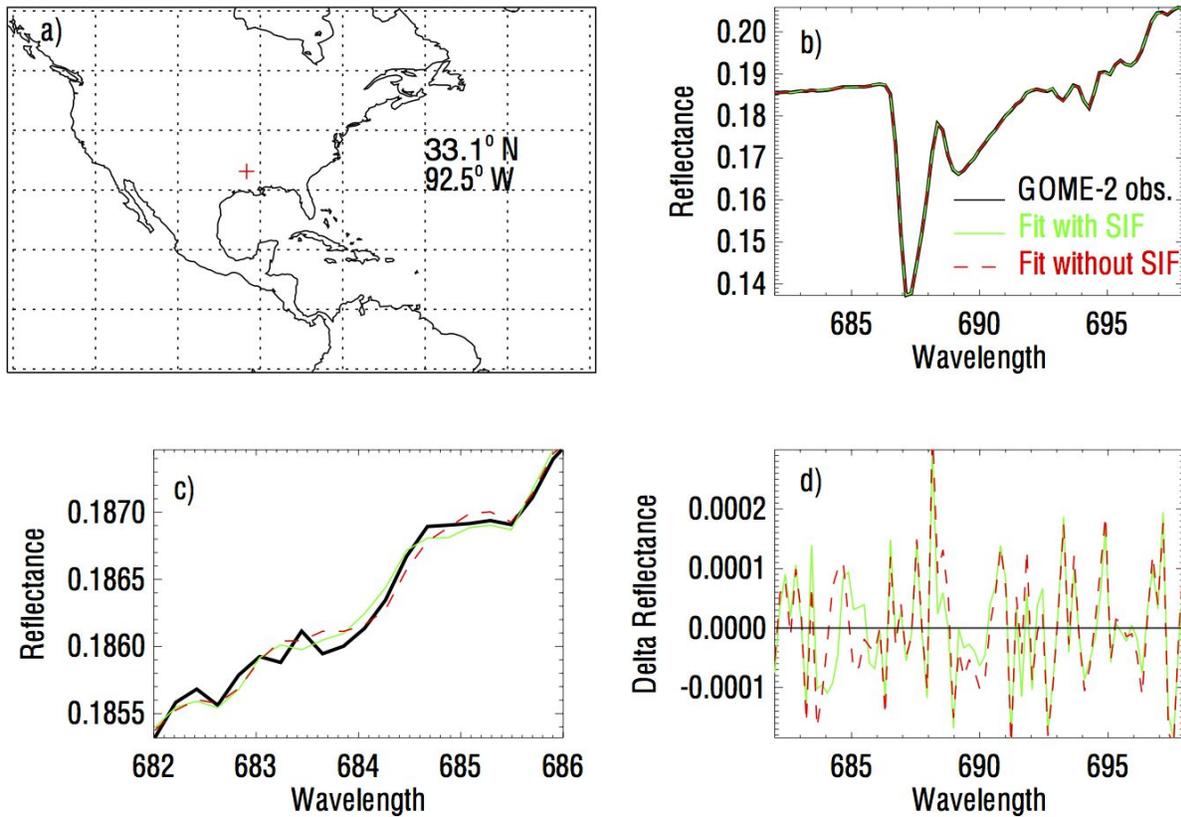
Figure 6. A sample GOME-2 spectrum on 01 July 2012 at location specified in (a), spectral fits with and without SIF in (b) and (c), and residual spectra in (d). The retrieved SIF at 682 nm was 2.25 mW/m^2/nm/sr. RMS of the residual spectrum is 9.35e-5 when SIF is fit and 1.01e-4 when SIF is not fit.
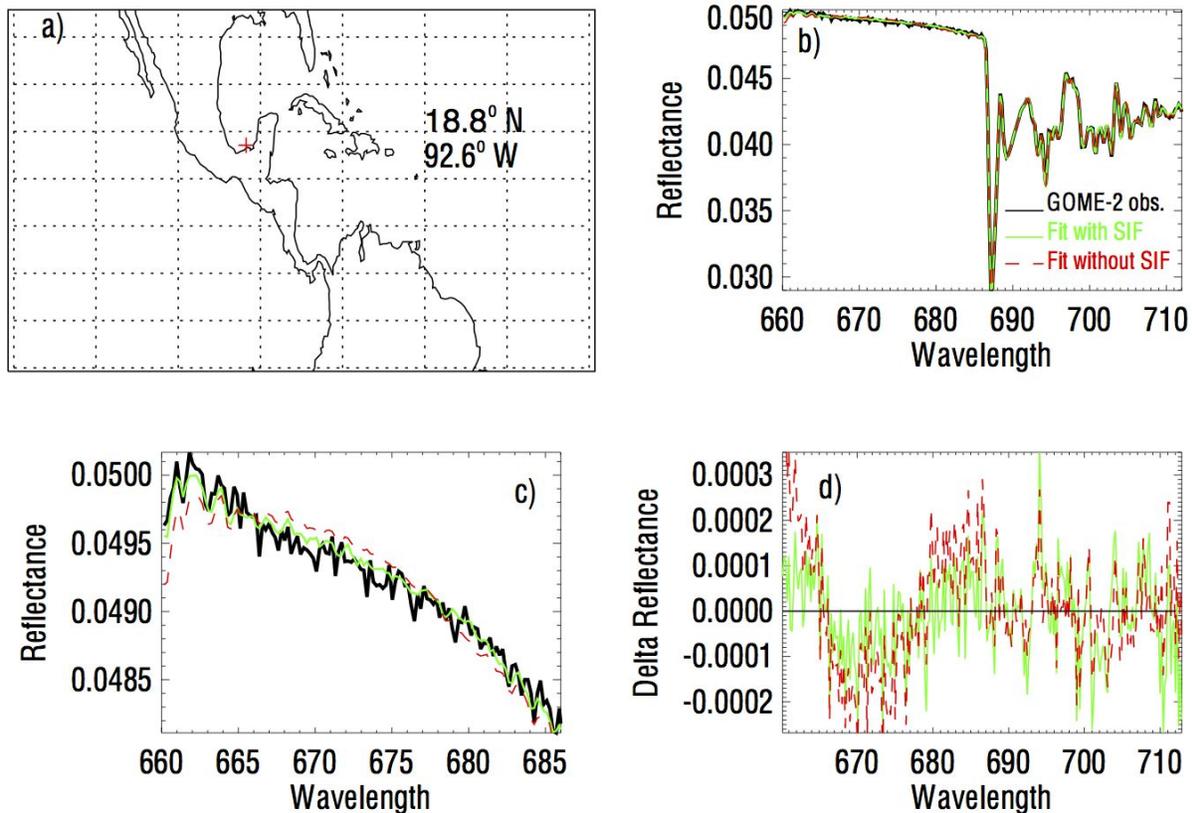
Figure 16: Similar to Fig. 6 but showing a GOME-2 observation on 01 July 2012 and spectral fits for an ocean pixel with retrieved FLH of 0.57mW/m^2/nm/sr. RMS of the residual spectrum is 1.04e-4 when SIF is fit and 1.35e-4 when SIF is not fit.

7. I think Section 6.1, which refer to Fig.7, has to be revised carefully, because it is a crucial issue, that the fit of SIF nearly do not affect the fit residuals and do not yield to an improvement of the fit quality. The simulations show a complete different behaviour and also the residuals of the ocean fits show an improvement by including SIF in the algorithm. Please add some explanations, even if assumptions.

The reason that the simulations showed a different behavior is that we had included simulations with very high values of red SIF. Those values do not apparently exist in nature owing to reabsorption within leaves and canopies that may not have been accurately simulated. Therefore, we revised all simulation results (including the former Figs. 5, 6, and Table 1) to include only those scenarios with SIF at 685 nm < 1 mW/m^2/nm/sr, consistent with our retrievals using GOME-2 and SCIAMACHY. This

reduces the number of scenarios in the simulation data set to 15,544 - still a large number of scenarios. We have revised text Section 6.1 and other sections as appropriate. While numbers in Table 1 have changed somewhat, the major conclusions remain the same. The new Fig. 5 is now much more similar to Fig. 7 in that it shows only subtle reductions in residuals, primarily at 684 nm and 688-690 nm. These small reductions in residuals are never-the-less sufficient to estimate SIF and show the expected size of the signal in terms fractional radiance (or %); residual reductions are of the order of hundredths of a percent at any given wavelength. We added "RMS residuals are reduced on average 1% in the wavelength range 682-692 nm for the GOME-2 data used here and about 2% in the simulated data set."
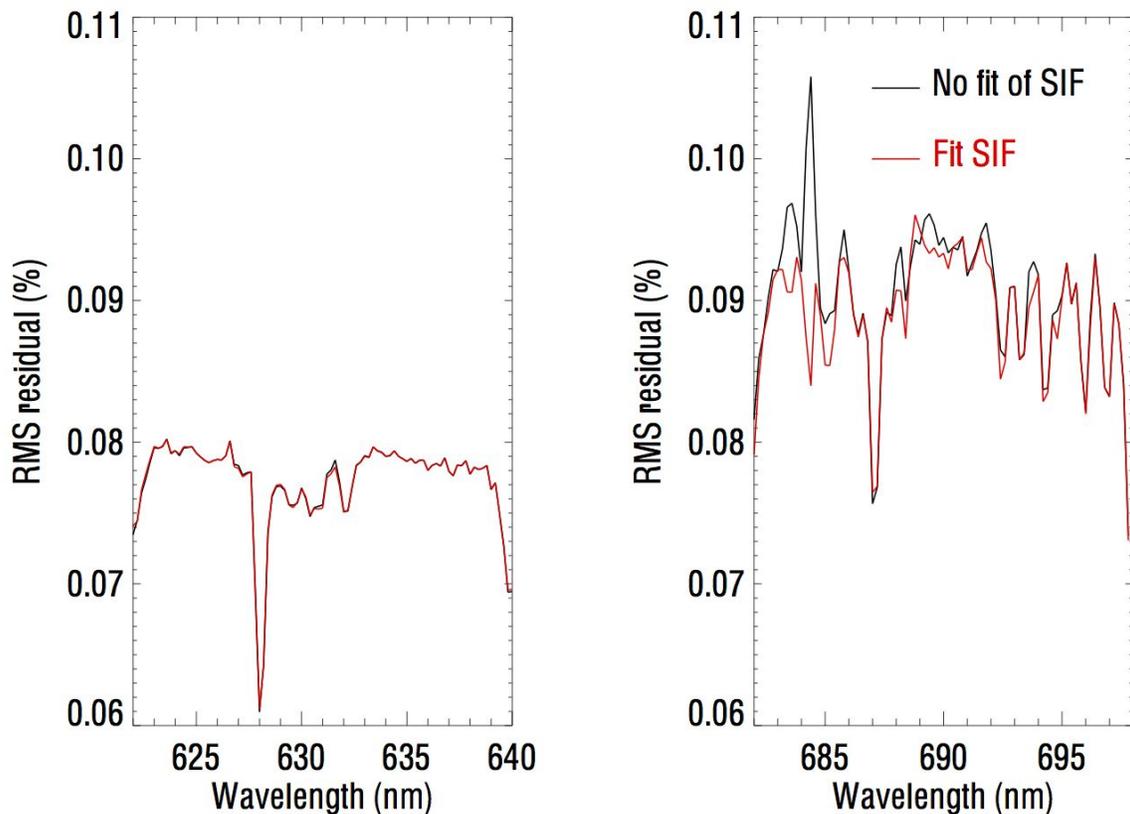
New Figure 5 showing smaller reductions in residuals when SIF is fitted in better agreement with Figure 7 generated with GOME-2 data.

8. In Bismarck et al. (2013) simulations of the Radiative transfer model (RTM) MOMO, which is also used in this study, show that the fraction of the vibrational Raman scattered radiation in the water-leaving radiance reaches values of over 25% in the visible and SWIR spectral region in totally clear seawater, and still values of several percent in moderately turbid waters. Also Wolanin et al. (2015)

showed by using the RTM SCIATRAN that the in-filling of Fraunhofer lines due to rotational Raman scattering is not negligible in this wavelength region and she correct her retrieval algorithm for this effect, whereas she mentioned that no correction for VRS is necessary. I recommended to clarify these inconsistencies by estimating the impact of these inelastic scattering processes to your fit windows by RTM simulations and investigate the errors in your approach due to these effects. Since the signal of the in-filling of the inelastic scattering processes are very small, it is important to estimate the deviations due to uncompensated processes.

We believe that there is not any obvious inconsistency between Bismark et al. (2013) and Wolanin et al. (2015). Bismark et al. show that at the wavelengths of interest to SIF retrievals, *the fraction of Raman scattered light in the water leaving irradiance* for a case of low turbidity with solar zenith angle of 54 degrees (near the maximum effect) is about 13-20%. The main effect is a smooth function of wavelength that will be removed in our retrieval. The remaining structure due to filling-in of solar and telluric features at the wavelengths of interest is a maximum of about 1% in the deepest part of O2 B-band *of the water leaving radiance* which at these wavelengths is very small (see for example Fig. 1 of Wolanin et al., 2015 that shows water leaving radiance values of <0.2 mW/m^2/nm/sr at 680 nm). This means that structure in spectra produced by VRS should be < 0.002 mW/m^2/nm/sr in the deepest part of O2 B-band which is very small as compared with the low frequency "continuum" signal of oceanic SIF. Bismark et al. simulations appear to be monochromatic, so effects will be even smaller at GOME-2/SCIAMACHY resolution. Note that Fig. 1 of Wolanin et al. (and in other works) shows that the oceanic SIF continuum signal can be clearly seen against the water leaving radiance continuum and is of the order of 0.5 mW/m^2/nm/sr at 680 nm. That is why MODIS and MERIS are able to detect the oceanic SIF by a simple radiance differential method in 3 channels. In the weak solar line feature at 684.5 nm used by Wolanin, the VRS effect should be very much smaller than that listed above for the deep part of the O2 B-band. Therefore, we do not see an obvious inconsistency in results and no reason to suspect any issues with Wolanin et al.'s or Bismark et al.'s calculations or conclusions. Bismark's conclusion is that if one is interested in *water leaving radiance* that VRS should be considered (depending on the application) as it can constitute a significant fraction. We therefore do not see a need to repeat the calculations and believe that errors in our retrieval approach (that relies primarily on the large scale continuum of oceanic SIF rather than the smaller filling-in signals, including those from SIF and RRS), due to VRS will be insignificant. We stand by our statement that "fitting the peak as well as both shoulders of the red SIF emission feature allows for a clean separation of its spectral structure with that of water leaving radiance,

atmospheric scattering and absorption, and Raman scattering in both the ocean and atmosphere." We added in reference to Figure 15 that "some of the remaining fine structure in the residuals may be due to residual filling-in from atmospheric rotational or oceanic vibrational Raman scattering or instrumental effects that we did not attempt to account for in this work."

9. Eq.(3) indicates that SIF is a dimensionless spectrum and not a single value? Please define SIF properly.

We added just after Eq. (3) that "SIF as a function of wavelength is given in radiance units." In section 4.3 describing the state vector of the retrievals, we revised to the state vector includes "either the peak value of the red fluorescence feature centered at ~683 nm or an averaged value of SIF over the SIF fitting window. For all results shown in the remainder of this paper, SIF refers to a single value that refers to either the peak value or an average over the fitting window as appropriate for the red or far-red emission features."

Minor issues:
- Label colorbars in global plots, what are the units of SIF etc.?

Instead of listing the units under each subplot, we listed the units in the first subcaption of each figure for the global plots.

- Some equation references are not set (only ?? is seen)
This seems to have been an issue with the last LaTeX compilation and wasn't caught. It has been fixed.

- Meanwhile a new paper (Khosravi et al., Front. Environ. Sci. 2015) about retrieval of fluorescence from SCIAMACHY data in the far-red spectral region data was published and should be also cited in the introduction to complete the overview of established retrievals.

Thank you for pointing out this new publication that was published just after our initial submission. It is now included in the references in the introduction. We have also added a few other recently published references (Damm et al., 2015; Rascher et al., 2015; Rossini et al., 2015; Walther et al., 2015; Wang et al., 2016).

- Title: New methods for the retrieval …

changed as suggested

- Page 2, line 26: ... over land include the MEdium …

fixed, thank you.

- Page 8, line 62: ... , a single PCA is performed …

fixed, thank you.

- Page 15, line 71: ... SIF is fitted, ...

changed as suggested