Reply to referee C. Frankenberg

Dear Referee,

Below you will find detailed responses to your review of manuscript amt-2013-38, 'Retrieval of aerosol parameters from the oxygen A band in the presence of chlorophyll fluorescence'. The review helped to improve the manuscript and we would like to thank the referee for his effort and time.

Sincerely,

Bram Sanders (on behalf of the authors)

Note: page numbers in reviewer's comments refer to amtd manuscript, page numbers in responses refer to revised manuscript

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The manuscript "Retrieval of aerosol parameters from the oxygen A band in the presence of chlorophyll fluorescence" describes a sensitivity study of the potential to derive chlorophyll fluorescence as well as aerosol parameters using the oxygen band. The paper focuses on linear error analysis and precision estimates derived from the model Jacobians and prospective instrument specifications. As such, the topic of the study is interesting. However, I feel that the authors misinterpreted previous studies that have dealt with exactly the same topic and are being criticized here. There is already a big discussion about how to best perform fluorescence retrievals and this manuscript unfortunately adds more confusion than clarification by focusing on precision errors rather than accuracy (which is most important, esp. once you have millions and millions of data points from satellites with which you can, in principle, reduce the standard error to arbitrarily low values by averaging; accuracy errors, however, won't reduce by the factor 1/sqrt(n) but stay).

Reply: The intended focus of the manuscript is the effect of fluorescence on aerosol retrieval (hence the title). We have not made this clear enough, as we apparently have given the reviewers the impression that the manuscript was more directed towards fluorescence retrieval itself. Upon re-reading the manuscript we can understand why this happened. We have modified the manuscript throughout and now focus more explicitly on aerosol retrieval. In the revised manuscript, we refrain from any remarks concerning the optimal way to perform fluorescence retrievals (except a remark on computational efficiency on p.5,l.8-11).

Concerning the reviewer's comment on averaging: The goal of an O2 A aerosol retrieval would be to achieve a good single-retrieval precision. Fluorescence retrievals may be compiled into spatio-temporally averaged maps, but this is not desirable for retrieved aerosol parameters (e.g. when for aviation safety purposes).

On top of that, the underlying aerosol formulation is very simplistic and forward model error (the dominant source of error in these kind of retrievals) is entirely neglected. Precision estimates are derived from a very simple retrieval setup and the claims/accusations made in the paper are, in my mind, not substantiated. Given the cost of satellite missions, one should be very careful what to claim and acknowledge that specific forward model errors (e.g. different aerosol types, height distributions, fractional cloud cover, cirrus clouds and the list goes on) can bias the retrieval, both in fluorescence and aerosols. This has been shown in Frankenberg et al (Frankenberg, C., O'Dell, C., Guanter, L., and McDuffie, J.: Remote sensing of near-infrared chlorophyll fluorescence from space in scattering atmospheres: implications for its retrieval and interferences with atmospheric CO2 retrievals, Atmos. Meas. Tech., 5, 2081–2094, doi:10.5194/amt-5-2081-2012, 2012.) but the authors here strongly criticize this work and claim that our statements are erroneous and that chlorophyll fluorescence and aerosols can be retrieved alongside just based on the oxygen A-band even in the absence of Fraunhofer lines. This would indeed be wonderful and I would love to be proven wrong in that respect but I don't think that this particular study does a good job in that. We are happy to share simulated data to prove us wrong. Also, there are plenty of satellites out there that already provide data with which the claims by the authors could be easily corroborated. Without this exercise, however, the manuscript can't be published in its current form.

Reply: We have now included in our retrieval simulations model errors in the single scattering albedo, surface pressure and temperature profile (see p.12-13). Furthermore, we have added calibration errors to the measurement error covariance matrix (next to the noise error). Finally, surface albedo and fluorescence emission in retrieval are described by a second-order polynomial (although we expect based on the literature that a linear wavelength dependence captures most of the spectral variation across the relatively small fit window). Effects of model errors on retrieval are investigated by including model parameters in the state vector with appropriate a priori errors. Thus, reported precision levels are estimates of the sum of retrieval errors due to measurement errors and smoothing errors but also model parameter errors. This approach takes into account that errors in retrieval parameters and forward model parameters may be correlated. We then take these precision values to represent realistic precision levels. Model errors in the aerosol phase function and the presence of more than one scattering layer are also discussed (p.16,l.17-28). We believe that we have covered the most important retrieval uncertainties.

We think that our results are in agreement with the results presented in Frankenberg et al. (2012) that show a reduction in XCO2 and AOT biases if fluorescence is included in the fit (stated on p.18,l.22-l.26 of the manuscript). However, if one is interested in fluorescence retrieval itself, a Fraunhofer line retrieval is indeed preferred (p.5,l.8-l.11 of the manuscript). These claims were already made in the initial amtd manuscript. In the revised manuscript we now refrain from any remarks criticizing (literal) statements made in Frankenberg et al. (2012), see also responses below.

We feel that the use of real data is beyond the scope of the present paper and that the retrieval simulations already provide interesting and valuable results.

I will go into more detail in the following:

Page 3186, lines 1-3: What we say in the paper is that aerosol and fluorescence parameters are not linearly independent and thus difficult to disentangle. It may still be true that both can be fitted but strong cross-correlations will occur (which we should try to avoid). On top of that, forward model errors (given that we can't model all aerosol possibilities) will bias both retrievals, fluorescence and aerosols. This won't happen using just Fraunhofer lines.

Reply: It is our experience that in an O2 A aerosol retrieval, errors in retrieved parameters (i.e. not only fluorescence) can be strongly correlated while it may still be possible to retrieve those parameters. The referee agrees on this point, but we had a different understanding from Frankenberg et al. (2011).

We prefer not to go into this any further because we fear to be entering a semantic discussion here. We have removed any remarks in which we criticize (literal) statements made in Frankenberg et al. (2011) and Frankenberg et al. (2012). Instead, in the revised manuscript we take the results presented in these papers as they are.

As mentioned above, the focus of our manuscript is the effect of fluorescence on aerosol retrieval, not the other way around. Aerosol (height) retrieval can of course best be done using the O2 A band, not just with Fraunhofer lines.

Figure 2: At the continuum level (around 772-775nm), the Fs derivative seems to be systematically higher than the other two. Do you know why that is (I assume because the solar irradiance is not flat)? I am wondering what added information this apparent slope (between the continuum at 755 and 774nm) provides for the Fs retrievals. It would be good to fit a slope to the albedo term as well to ensure that no information is provided by this effect (which mustn't be the case!). When you used a flat irradiance spectrum, was it just without Fraunhofer lines or entirely flat (so that the Jacobians in that particular case should be pretty similar and no difference in slope should be apparent between the albedo derivative and the Fs derivative. This could be crucial, so please check that.

Reply:
We used the HR solar reference spectrum for Fig. 2 in both the original and the revised manuscript. The Fs derivative being somewhat larger at the right side of the O2A band could indeed perhaps be due to the slight downward slope in the solar continuum.
In retrieval we now allow surface albedo and fluorescence emission to depend quadratically on wavelength. The supposed information contained in the slope of the solar continuum when fitting constant albedos and constant surface emission should thus be reduced, as is indeed appropriate for realistic retrieval simulations.
The simulations with the flat solar spectrum have been removed (see below).

Page 3186, line 15: You say that the shape is sufficiently different within the O2 Aband. This really only holds for tau. The albedo term and Fs is very similar and you also haven't shown the derivative of the height parameter. Also: If you would include the presence of thin high clouds, the story might also be different. You can still argue that in your particular case, they look different but I wouldn't generalize too much.

Reply: The reviewer is right. The statement is too strong at this point in the manuscript. Retrieval simulations should show whether spectral shapes are sufficiently different (stated on p.4,l.31-p.5,l.2). The statement has been removed. The derivative w.r.t. aerosol height has been added to the figure (see revised Fig. 2).

Page 3186, line 27: If this is right (focus on aerosol parameters), the authors should reshuffle their claims and focus more on that aspect (for which the bias in aerosol parameters may indeed be not too malign). Only the claims regarding fluorescence are going way too far in my opinion while precision estimates of 0.01-0.02 also seem too good to be true (as they will be overshadowed by forward model errors which are not taken into account in this study at all). This should be discussed.

Reply: As mentioned above, the intended purpose of the manuscript is indeed investigating the effect of fluorescence on retrieval of aerosol parameters from the O2 A band. We have modified the manuscript throughout and more explicitly focus on retrieval of aerosol parameters. In addition, we have removed any remarks that (give the impression to) concern the optimal way to perform fluorescence retrieval.

Page 3188, line 26: I don't fully understand how you treat the finite resolution of the solar spectrum. If Figure 1 shows the simulations before convolution, the depths of the Fraunhofer lines seem to be way too small (Transmissions at high resolution are almost going down to 50% for some lines).

Reply: Initially, we subtracted the solar reference spectrum's FWHM from the FWHM of both the radiance and irradiance slit functions to provide a first-order correction for the solar spectrum's finite resolution. Later, we realized that this correction is questionable for convolution of the HR radiance, which is in turn the product of the truly high-resolution reflectance spectrum with the solar reference spectrum (FWHM 0.04). Therefore, we decided not to apply this correction altogether. The sentence concerning this correction should already have been removed in the initial submission. We have adjusted the text in the revision (p.7,l.6-8). All results presented so far, including the results reported in the initial submission, hold for the Chance & Kurucz (2010) spectrum with original FWHMs as referred to in Sect. 2.5.

The solar irradiance was given an offset so that the plot would not overlap with the reflectance plot. The offset has now been removed and we have also indicated the zero-level for clarity (see revised Fig.1A). Due to the finite

resolution of the Chance and Kurucz (2010) spectrum, the depth of Fraunhofer lines is somewhat underestimated, which we mention on p.7,l.6.

Page 3198, line 23:Why are you treating Fs as independent of wavelength? It changes dramatically within the fit window (as you also state earlier) and my hope was always that this may somehow actually provide some more information (which you ignore). For a better quantification, one would need to model that strong spectral slope (but then also fit a slope in the albedo term as otherwise the slope in continuum level radiance would provide most informations).

Reply: In retrieval we now allow both surface albedo and fluorescence emission to depend quadratically on wavelength.

Page 3190, lines 5-10: To really get an estimate of what can be expected under realistic scenarios, test cases should include different aerosols types (and height profiles) in the simulated radiances (and then still be fitted with your "average" aerosol type). This will provide accuracy estimates in the case of forward model errors (which is what we did in the 2012 AMT paper).

Reply: Effects of modelling errors in the single scattering albedo are now included in reported precision estimates. We also discuss modeling errors in the phase function and the presence of more than one scattering layer.

Also: You don't seem to fit for surface pressure while you might have to include it in order to see how independent it is. Surface pressure biases in met-fields can be 1-2hPa and if you have some pointing uncertainty in elevated areas, it will be even higher.

Reply: A priori uncertainties in surface pressures have now been included in the error analysis (p.12-13).

Page 3190, line 15: What happens if the temperature profile is a little bit off (between simulations and retrievals)?

Reply: A priori uncertainties in temperature profiles have now been included in the error analysis (p.12-13).

Page 3194, line 10-11: This is just not true and shows a conceptual misunderstanding of our study. Your study is full of a priori information. You assume that you perfectly know the aerosol type, its height profiles (basically a delta peak), the surface pressure, the atmospheric temperature profile, the absolute absence of clouds (no cirrus clouds, no fractional cloud cover etc). This is very stringent a priori information (basically a prior with zero uncertainty in the "Rodger's sense") and your conclusions are sound only in the condition that these assumptions are fully valid in reality (which is a rather strong assumption).

Reply: We fully agree with the reviewer. We have been doing many retrieval simulations in preparation for O2 A band aerosol height retrieval with Sentinel-5 Precursor. We had the knowledge gained from these simulations in mind when

discussing the role of fluorescence in aerosol retrieval in the present manuscript. It was our intention to keep the story clear and to the point by only discussing -in our opinion- essential aspects. However, we now realize that in doing so the story appears oversimplified to the reader.

As explained above, we now provide more realistic precision estimates (including modeling errors in single scattering albedo, surface pressure and temperature profile, and calibration errors).

Page 3197, line 8: To really differentiate the information from the A-band and the Fraunhofer lines, you would have to run two cases: One (which you did) by flattening the irradiance spectrum and one, where you turn off oxygen lines. Ideally, you zero out both to ensure that your Fs retrieval will break down in that case as it won't be distinguishable from albedo changes.

Reply: Indeed, but we intend to retrieve aerosol parameters. Turning off oxygen lines precludes retrieval of aerosol height. The conclusion concerning the contributions of filling-in of FH and O2 lines stated in the original manuscript therefore only holds when assuming that the two signals are uncorrelated (mentioned on p.3200, l.13-16 of the amtd manuscript).

However, as reviewer Guanter remarks, the discussion of the relative contributions of the two mechanisms might not be that relevant for the purposes of the present manuscript. We have now replaced these retrieval simulations with simulations investigating the dependence of retrieval precision on the a priori error in the fluorescence emission. This is perhaps more relevant for O2 A aerosol retrieval: a pre-retrieval of fluorescence using FH-lines can be used to provide an a priori value for O2 A aerosol retrieval.

Page 3198, lines 14++: The authors state (in a very direct way) that we basically disproved ourselves by making apparently contradictory statements in our 2012 paper. First of all, if I find such contradictions (which apparently no one writes on purpose), I would advise just directly asking the respective authors what they actually meant instead of citing entire sentences in a rather condescending way. Here is what the sentence meant in a nutshell: "using the potentially added information contained in the O2 absorption structures seems to do more harm than good for the fluorescence retrieval because interferences are introduced". ! It means that the inclusion of Fs in the full retrieval can in principle (theory) improve the Fs retrieval but in reality won't because there are forward model errors that (even in the absence of instrument noise!) bias the fluorescence retrievals because we don't include the right aerosol types and height profiles in the retrieval model. Please compare the errors in Fs retrievals in Figure 8 and 11 (on our 2012 paper) and say that the errors (all of which are systematic, i.e. accuracy errors because we used noise-free data) in Figure 8 are smaller. By including Fs in the full-physics O2-A band fit for our XCO2 retrievals, we still improve the XCO2 retrievals, however. This is because we get rid of the apparent bias that may depend on true Fs (which is very critical as it can co-vary with CO2 fluxes). Note that we really focused on pure accuracy errors as we used noise-free retrievals. The Fs precision may have been improved but the accuracy using the O2 band deteriorated. This is all we

wanted to say, maybe we could have phrased it more clearly as such a misinterpretation is unfortunate and can certainly happen to other people too if you saw it that way.

Reply: We did not mean to be condescending in any way and if we made that impression, we apologize for it. Since the papers are published (no discussion papers), we have to take them at face value. We cited sentences from the papers (Frankenberg et al., 2011, 2012) to point out exactly where we thought to be disagreeing. We felt that this was an objective approach, because the reader could then compare the arguments and form her/his own opinion.

We have now removed the citations and, as mentioned above, focus on the results themselves presented in these papers. As already pointed out, much of the confusion arises because it was apparently not clear enough that we focus on aerosol retrieval. Thus, the relevant comparison for us is between figure 5 and figure 8 of Frankenberg et al. (2012) and not between figure 8 and figure 11.

Bottomline: I really wish it was that easy to get accurate retrievals of Fs from just the A-band but you are not disproving us as you only focus on precision, not accuracy. We can share the model simulations from the 2012 paper and you can try your retrievals. There is also plenty of data out there from other satellites (GOSAT, SCIAMACHY, GOME-2, etc) and you can try to disprove us using real data. I would indeed love to be wrong but this simple study based on precision errors only doesn't show it. Our latest operational ACOS XCO2 retrieval from GOSAT also already includes the full Fs fit in the oxygen band but we advise not to use the Fs retrievals from this fit but the ones from the Fraunhofer line only fit (if you want to look at Fs). Looking at the precision error in our GOSAT Fs fit, they are on the order of 0.6-1.5 e11 photons s−1 cm−2 sr−1 nm−1. These are on the order of what you see (a little higher I would say) but GOSAT has a 0.02-0.03nm FWHM (and SNR are also approaching 500 in the combined P and S polarization). This may have to do with the fact that we use a more complex aerosol fit (though we even get aerosol information from the strong CO2 band, so including the CO2 bands should in turn help constrain aerosols in the O2 band). Again, we prefer to trade precision with accuracy and this is at the heart of the problem, actually for both, fluorescence and aerosols. If the focus of the paper is more on aerosols itself, the authors should also attempt to quantify systematic errors in those retrievals by having retrievals with inconsistencies between simulated radiances and the retrieval (which is what will happen in real life).

Reply: Issues raised here are now already dealt with in responses to previous comments.

Perhaps a final remark on accuracy errors to be absolutely clear about our approach: The effect of a forward model parameter error on the retrieved state is $\mathbf{G}_y\mathbf{K}_b(\mathbf{b}-\hat{\mathbf{b}})$ (Rodgers, 2000, Sect.3.2). The covariance of this accuracy error can be included in the a posteriori error by adding the model parameters to the state vector (with a priori errors equal to the variance of **b**). This is what we do. Hence, reported precision estimates include errors due to model parameter errors, as also explained above.

There are also citations missing regarding paper that already dealt with aerosol or cloud retrievals from the O2-A band: Sanghavi, S., Martonchik, J. V., Landgraf, J., and Platt, U.: Retrieval of aerosol optical depth and vertical distribution using O2 A- and B-band SCIAMACHY observations over Kanpur: a case study, Atmos. Meas. Tech. Discuss., 4, 6779-6809, doi:10.5194/amtd-4-6779-2011, 2011.

Kokhanovsky, A. and Rozanov, V.: The physical parameterization of the top-ofatmosphere reïnˇC´ ection function for a cloudy atmosphere-underlying surface system: the oxygen A-band case study, J. Quant. Spectrosc. Ra., 85, 35–55, 2004.

Kokhanovsky, A. and Rozanov, V.: The determination of dust cloud altitudes from a satellite using hyperspectral measurements in the gaseous absorption band, Int. J. Remote Sens., 31, 2729–2744, 2010.

van Diedenhoven, B., Hasekamp, O. P., and Aben, I.: Surface pressure retrieval from SCIAMACHY measurements in the O2 A Band: validation of the measurements and sensitivity on aerosols, Atmos. Chem. Phys., 5, 2109–2120, doi:10.5194/acp-5-2109-2005, 2005.

van Diedenhoven, B., Hasekamp, O. P., and Landgraf, J.: Retrieval of cloud parameters from satellite-based reïnˇC´ ectance measurements in the ultraviolet and the oxygen Aband, J. Geophys. Res., 112, D15208, doi:10.1029/2006JD008155, 2007.

Reply: We wanted to limit discussion of literature on O2 A band aerosol retrieval to (planned) operational algorithms. We have now included a paragraph in which we provide a more extensive discussion of O2A aerosol literature, including the references mentioned by the referee (p.2,l.13-p.3,l.7). We prefer to leave out Van Diedenhoven et al. (2007) as it discusses cloud retrieval, but if the reviewer insists we are happy to include this reference.