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Interactive comment on “Retrieval of aerosol parameters from the oxygen A band in the presence of chlorophyll fluorescence” by A. F. J. Sanders and J. F. de Haan

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This manuscript describes linear retrieval error estimation of aerosol parameters and chlorophyll fluorescence within the oxygen A-band using simulated data. The paper is clearly written, contains original material, and the topic is timely and appropriate for AMTD. The paper could be accepted for publication after revision, if it is properly placed within the context and scope of previous and current works, with all caveats and simplifications fully and carefully explained including implications for a full retrieval algorithm with real satellite data. This simulation study would be more realistic and meaningful if other parameters are included in the state vector that affect absorption in

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the oxygen A-band as described below.

Major points:

Dr. C. Frankenberg has already written a thorough review. Since he has made many of the same comments that I would have made, I will expand on a few points. Our group has also conducted a full retrieval exercise using simulated data in and around the O₂ A-band, and we have also retrieved fluorescence with the GOME-2 instrument using this spectral region. Please see the following reference that went on line shortly after this paper:

Joiner, J., Guanter, L., Lindstrot, R., Voigt, M., Vasilkov, A. P., Middleton, E. M., Huemmrich, K. F., Yoshida, Y., and Frankenberg, C.: Global monitoring of terrestrial chlorophyll fluorescence from moderate spectral resolution near-infrared satellite measurements: methodology, simulations, and application to GOME-2, *Atmos. Meas. Tech. Discuss.*, 6, 3883-3930, doi:10.5194/amtd-6-3883-2013, 2013.

In our work, we used a simulated data set consisting of 230,400 different scenarios. We did not assume that the surface pressure was known, nor did we assume that we had a single, perfectly known atmospheric temperature profile. As Dr. Frankenberg states, these variables need to be included in a retrieval that uses the O₂ A-band. The statement on L 20 of p. 3194 would apply only to a minimum set of fit parameters within a simplified simulation environment. In a realistic scenario, these other variables need also to be considered (in addition to other aerosol parameters mentioned in Dr. Frankenberg's review). In our simulations, the fluorescence and surface reflectance also had realistic spectral variations. When all of these parameters and conditions are included, a physically-based non-linear retrieval algorithm becomes quite difficult and in practice extremely problematic to implement.

I am concerned about the statement on p. 3199, "We have noticed in our work on the O₂ A band that retrieval precision significantly deteriorates for very specific combinations of ..." parameters. This warrants further investigation. The spectral shape

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of the aerosol Jacobian varies quite a bit with all parameters, but particularly with surface albedo, aerosol optical thickness (AOT), and aerosol height. The shape of the AOT Jacobian shown in Fig. 2 should be explained. More insight can be obtained by examining the high spectral resolution Jacobian shown in Frankenberg et al. (2011a). There, one can see different behavior for saturated and unsaturated O₂ lines. I believe this effect is coming from enhanced absorption due to scattering between ground and aerosol layer. This will increase absorption in line wings or in unsaturated lines, but has no effect on saturated lines where the aerosol brightening effect will cause the Jacobian to have the opposite behavior. Our own simulations (not published) show that this enhanced absorption effect is not significant under all conditions. It decreases with AOT, aerosol layer height, and surface albedo. For example, In cases of low AOT, height, and/or surface albedo, the AOT Jacobian spectral shape will be more similar to those of surface albedo, surface pressure (not included as a state variable in the simulations here), and aerosol height. This may explain in part the mentioned instability under certain conditions and necessitates more analysis. Is there any evidence of the so-called critical surface albedo effect or is this speculation?

The paper also mentions the neglect of rotational-Raman scattering (RRS). Our calculations of RRS in the presence of aerosol show similar behavior (please note that the title of our RRS paper has changed since the publication of your manuscript); RRS has a complicated dependence on aerosol parameters and surface albedo for the same reasons discussed above regarding absorption. The effects of RRS are more costly to compute than radiances because they involve convolutions with RRS spectra.

Note also that the very low radiances within the O₂ A-band and large contrast with the continuum make O₂ A-band observations susceptible to biases due to instrumental effects such as non-linearity (e.g., seen in SCIAMACHY deep solar lines in the reference listed below and the GOSAT zero-level offset problem also discussed in several papers) as well as stray light contamination.

This O₂ A-band retrieval problem is extremely non-linear and also computationally

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costly if on-line radiative transfer calculations (including RRS) are required; a table lookup approach appears to be intractable for this problem. Discussion of these implementation details for a realistic physically-based retrieval algorithm would be appropriate in this work.

In short, due to all of these issues, we decided to implement and test a principal component analysis approach as described in our paper as opposed to a physically-based approach where one attempts to disentangle all of the parameters that have significantly correlated effects on radiances. Using thousands of observations for “training” with both simulated and actual satellite data (including cloud-contaminated pixels with real GOME-2 data, because cloud-contamination is a serious issue for any of the instruments mentioned in the paper), we are apparently able to model the O₂ A-band complexity with a reasonable number of principal components. However, in our simulations, we do not get particularly good fluorescence retrievals when using only the O₂ A-band wavelengths with a fitting window similar to the one used here. We get a much better fluorescence retrieval for similar spectral resolution using a fitting window of 715–747nm which is dominated by filling-in of solar Fraunhofer lines, although there is some filling-in of H₂O lines and H₂O absorption must be accounted for.

In more recent studies since our paper was submitted, we find that removing the A-band wavelengths from the fitting window results in not much if any decrease in retrieval noise with GOME-2 data. We compare better with GOSAT when the oxygen A-band wavelengths are removed from the fit (relatively small biases in the tropics are removed). We also tried to retrieve fluorescence with GOME-2 using just a small fitting window around the A-band similar to the one used in this paper. We obtained poor results (noisy retrievals as in the simulations and biased with respect to GOSAT).

I disagree with the statement on L28 of p. 3198 that “there is no reason... to determine fluorescence from spectral regions outside the O₂ A band.” If given the choice, based on our simulations and experience with GOME-2, we would choose regions outside the O₂ A-band over the O₂ A-band for fluorescence retrievals. I agree with Dr. Franken-

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berg that such statements in a published paper can be very dangerous if used to justify a particular choice of expensive space-based hardware. I also agree that it would be nice if we could use only the A-band for fluorescence retrievals since there are several available instruments with this band. That is why we did give it a try. But in the end, it did not work very well, at least with our principle component approach that apparently works well with radiances outside the O2 A-band.

We also looked at the effects of spectral resolution and found not much improvement using the O2 A-band region for fluorescence retrievals with higher spectral resolution, consistent with your results. However, when using the fitting window outside the O2 A-band, we got significantly better results at 0.3 nm spectral resolution as compared with 0.5 nm. Therefore, the effect of spectral resolution on fluorescence retrievals depends upon the fitting window used.

Minor points:

L8, P3196: The use of “fluorescence yield” is confusing. The fluorescence emission should depend on solar zenith angle, but not necessarily the fluorescence yield which is sometimes used synonymously with fluorescence (quantum) efficiency.

The following reference should also be used for GOSAT fluorescence retrievals:

Joiner, J., Yoshida, Y., Vasilkov, A. P., Middleton, E. M., Campbell, P. K. E., Yoshida, Y., Kuze, A., and Corp, L. A., 2012: Filling-in of near-infrared solar lines by terrestrial fluorescence and other geophysical effects: simulations and space-based observations from SCIAMACHY and GOSAT, *Atmos. Meas. Tech.*, 5, 809-829, doi:10.5194/amt-5-809-2012.

Interactive comment on *Atmos. Meas. Tech. Discuss.*, 6, 3181, 2013.

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