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Atmospheric
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Techniques
Discussions

Interactive comment on "Linearisation of the effects of spectral shift and stretch in DOAS analysis" *by* S. Beirle et al.

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Reply to Reviewer 1

We thank the reviewer for the thorough and constructive comments. Below we repeat the original review in blue and reply to it point by point.

Reviewer Comment: The paper describes an important further development of the DOAS technique, which may have significant impact on the data processing for future satellite missions. The paper is well written, with eye for detail. As a consequence I have, apart from a few minor details, only two points.

1. At several places in the paper it is mentioned that using the B-shift (on I_0) instead of the A-shift (on I) has the advantage that the derivative has only to be calculated once, with consequences for processing time. A bigger disadvantage of using the Ashift seems to me that it needs knowledge of the high-resolution radiance spectrum to calculate the derivative (according to eq. B3). While a solar high-resolution spectrum is readily available, generating a high-resolution Radiance spectrum invokes much more effort. This is because the radiance measurement itself (on lower resolution) cannot be used. Instead the SCD of the strong absorbers need to be known/estimated from the measured spectrum, and high-resolution cross-sections must be applied to a highresolution I_0 to obtain the radiances. Please consider this, e.g. in Section 3.3 and/or 5.3. Is the same issue not affecting the zenith-sky reference spectra for ground-based DOAS?

Authors' reply: We have actually calculated all derivatives (I' and I_0') on the spectrometer's grid and resolution. But as the reviewer points out, I_0' should, strictly speaking, be derived from the solar reference on high spectral resolution, as, mathematically, the derivative does not commute with the convolution by the instrument spectral response function (ISRF).
We have investigated this effect by comparing the derivative of the solar reference (taken from Chance and Kurucz, 2010) on spectrometer resolution (as in the paper) with the derivative of the high-resolution solar reference, convolved with the ISRF afterwards. The results are shown in the Figure below. Both derivatives are very similar, and their difference has high-frequent random structure, i.e. shows no potential interference with any trace gas absorption.
The difference is less then 0.1 W/m^2/nm/nm peak-to-peak, i.e. less than 4% of the peak-to-peak difference of the derivative itself, and is thus negligible. (For comparison: the respective difference of the derivatives according to Eqs. B1 and B2 is 0.4 W/m^2/nm/nm peak-to-peak. I.e., the numerical calculation of the derivative is more critical).
In the revised paper, we added the following paragraph to Appendix B:

"Strictly speaking, the derivative of I_0 would have to be calculated from the high-resolution solar reference, convolved with the instrument spectral response function afterwards. However, here we calculate all derivatives (for A_{Shift} and B_{Shift}) on the spectrometer's grid and resolution (FWHM 0.55 nm). This approximation does not affect our results; the introduced errors are small compared to other effects (e.g. the appropriate discrete derivative method)."

Reviewer Comment: 2. The paper concentrates on NO2, which is a medium strong absorber. The paper mentions that the method is less advantageous for strong absorbers. From the errors shown in the paper I have some doubt that the method would be applicable for weak absorbers such as BrO or Formaldehyde. In this case, NO2 may be the only tracegas for coming TROPOMI/Sentinel missions where the new method would give a processing speed advantage, which makes the new method much less interesting to be implemented in Level 2 processing. Have any prelimanary studies for weaker trace gases been performed? What are the expectations of the authors? Any hint to this in the paper would be valuable.

Authors' reply: We fully agree with the reviewer that our study has to be substantiated by an application of the linearisation scheme to more challenging trace gases. In the revised manuscript, we now also investigate the proposed linearisation for real satellite measurements for two routine retrievals at MPI-C Mainz, i.e. NO_2 and BrO.
The results for NO_2 are similar to those of the synthetic spectra. The results for BrO clearly demonstrate that the linearisation scheme works as well for minor trace gases, and substantiates the discussion of A_{Shift} versus B_{Shift} as well as the pre-shift in section 5, which were rather abstract in the AMTD paper. In the revised manuscript, the results of the NO_2/BrO fits for real satellite measurements are added in the new section 4.2, and the discussion is updated accordingly.

Reviewer Comment: Minor points:
page 8373 line 19 instrument function -> instrument spectral response function
p.8373 line 20 "[instrument spectral response function] can be determined during the calibration". Probably "calibration" in this sentence is meant as done in the framework of the WinDOAS software. But this does not determine the instrument spectral response function (ISRF). At most some parameters which characterise the ISRF (e.g.FWHM) may be fitted. But its shape (or its parametrisation) must still be known beforehand. As it is written, this part of the sentence is both untrue and unnecessary. Please remove.

Authors' reply: In the revised manuscript, we changed this sentence to "The instrument spectral response function (ISRF) has to be known; if necessary, a parameterised (e.g. Gaussian) ISRF can be fitted during calibration by e.g. DOASIS or WinDOAS." In addition, we moved the last sentence of section 2.2 (page 8374 lines 1-2) to the top of the itemization, i.e. the reference to DOASIS and WinDOAS is now given before.

Reviewer Comment: p.8375 line 1 Why do cross-sections and pseudo-absorbers (like Ring) have to be Doppler-shifted when I_0 is shifted ? This doesn't make sense to me, as they are attached to the unshifted radiance spectrum. Please explain (is I_0 not actively shifted?) or reword.

Authors' reply: Our implementation of the DOAS algorithm for passive applications is described in section 2.2. We start with the solar reference spectrum measured by the detector itself. This is spectrally calibrated with a high-resolution solar spectrum (Chance and Kurucz). Thus, even if the irradiance is measured Doppler-shifted, our calibrated "I_0" has the correct wavelengths assigned to the detector pixels, and pseudo-absorbers like the Ring spectrum are calculated appropriately. But for the radiance measurements (without Doppler-shift), this wavelength-pixel allocation is not matching. I.e., I_0 and I are shifted with respect to each other. Now, each earth-shine spectrum could be shifted appropriately, which would be rather time consuming. Instead, we propose to pre-shift I_0 and all cross-sections/pseudo-absorbers consistently. As long

as undersampling is ruled out, this is mathematically equivalent and has the advantage, that it has to be only done once per orbit. Summarized, the pre-shift accounts for the different wavelength-pixel-allocations of I_0+cross-sections versus I.
In the revised manuscript, the proposed pre-shift is now explained and applied to actual satellite measurements in the new section 4.2. The discussion is revised accordingly.

Reviewer Comment: p.8384 line 14 “For the linear fit, the results [..] are identical” This must be wrong. In Table 3 the results differ by a factor of 10. Also on line 22 it is said that for the linear fit MATLAB performs better than DOAS. Please correct.

Authors’ reply: This is a misunderstanding: The statement in p.8384 line 14 refers to the fit results, i.e. NO_2 slant column densities. “Identical” refers to the comparison of SCDs from linear fits implemented with either MATLAB or DOASIS. In contrast, Table 3 refers to the differences in computation time. We clarified this in the revised manuscript by specifying the subject of comparison (either residue/SCD or computation time) in the respective section (4.1.3. in the revised manuscript).

Extensive figure caption:

Illustration of the effects of taking the derivative on detector grid. Top: Derivative of I_0 on detector resolution (blue), compared to the derivative of the hi-res sun spectrum, convolved to the detector resolution afterwards (red). Bottom: Difference of both derivatives.

Interactive comment on Atmos. Meas. Tech. Discuss., 5, 8369, 2012.

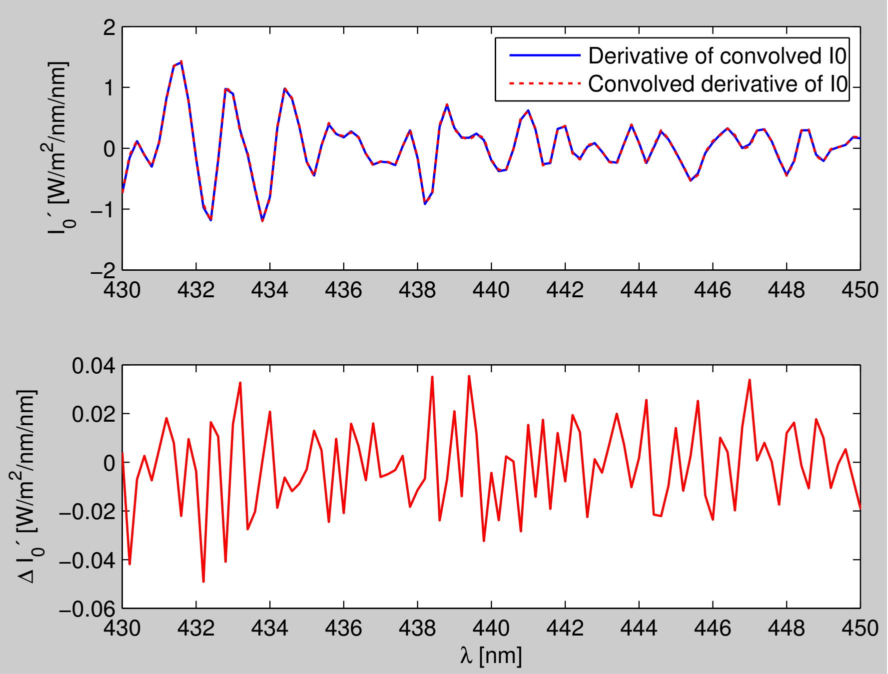

Fig. 1. Illustration of the effects of taking the derivative on detector grid.