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Interactive comment on "Stratospheric CH₄ and CO₂ profiles derived from SCIAMACHY solar occultation measurements" *by* S. Noël et al.

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We thank the referee for the overall positive judgement and will consider the comments in the revised version of the paper. In the following, the original reviewer comments are given in *italics*, our answer in normal font and the proposed updated text for the revised version of the manuscript in **bold** font.

Answers to main comments:

1. It is mentioned in the manuscript that CO2 is also retrieved from ACE-FTS. It would have been very interesting addition to compare SCIAMACHY CO2 profiles with real observations in addition to the comparison with CarbonTracker model, C5083

even with a limited coverage. By doing that the discrepancy due to different atmosphere (pressure, temperature) would be reduced. Would there be a possibility to add this?

We thank the referee for this suggestion. We have contacted the providers for ACE-FTS CO_2 and will include a comparison with our results in the revised version of the paper. This will however be limited to the altitude range where both products overlap, i.e. about 17–24 km.

2. Vertical resolution of the profiles. The vertical resolution of the instruments in the stratosphere should be discussed, now only SCIAMACHY resolution is mentioned. How are the (potentially) different resolutions taken into account in the comparisons?

The vertical resolution of the data products from the instruments used in the CH₄ comparisons is quite similar:

- · ACE-FTS: about 4 km.
- MIPAS: about 2.5-7 km.
- · HALOE: about 2.5 km.
- · SCIAMACHY: about 4.3 km.

This is why we did not consider these explicitly in the comparisons (e.g. by application of averaging kernels). This approach is consistent with the one used in Laeng et al. (2015), who state that the inclusion of averaging kernels in similar comparisons has an effect of only about 2%.

CO₂ data are compared with the CarbonTracker model, which is given at certain altitude levels, there is no information on vertical resolution.

For clarification, we will mention the values for the vertical resolution of the different instruments in the manuscript (section 5.2):

The SCIAMACHY methane data have been compared with results from ACE-FTS, HALOE and MIPAS. The vertical resolution of these data products is quite similar (ACE-FTS about 4 km, MIPAS about 2.5–7 km, HALOE about 2.5 km). This is why we did not consider differences in vertical resolution explicitly in the comparisons (e.g. by application of averaging kernels). This approach is consistent with the one used in Laeng et al. (2015), who state that the inclusion of averaging kernels in similar comparisons has an effect of only about 2%.

Answers to minor comments:

1. *P-11469 L -23: Methodology to retrieve the altitude (Bramstedt): as this is quite important, it would be nice to have few more words about the methodology: what is it based on?*

In short words, the method by Bramstedt uses scans over the sun to determine the position of the solar centre which is then compared to the astronomical position. From this we get an individual pointing correction for each solar occultation measurement which does not depend on the attitude information of the satellite.

We will mention this in the manuscript:

For the solar occultation data we make use of the method developed by Bramstedt et al. (2012), which determines the precise pointing from scans over the solar disk to determine the position of the solar centre which is then compared to the astronomical position. From this we get an individual pointing correction for each solar occultation measurement which does not depend on the attitude information of the satellite.

2. P-11469 L-17: The sentence is unclear. Also, it seems that CO2 profile data available from ACE-FTS. Hast this data been compared with SCIAMACHY CO2

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presented here? To me it sounds very interesting addition to the model comparison.

For clarification, we will reformulate/extent this sentence as follows:

For example, ACE-FTS usually uses CO_2 to determine pressure and temperature profiles and thus the altitude grid of the measurements, but still CO_2 data in the altitude range between 5 and 25 km (Foucher et al., 2009, 2011; Sioris et al., 2014) and in the mesosphere and lower thermosphere (Beagley et al., 2010; Emmert et al., 2012) can be derived. For this purpose, N₂ instead of CO_2 absorption is taken at lower stratospheric altitudes, whereas at mesospheric/thermospheric altitudes the geometrical pointing information is used.

A comparison with lower stratospheric CO_2 data from ACE-FTS will be included in the revised version, see above.

3. P-11471 L-18: Intuitively it would be better to use all data and not a subset of the measurements. Therefore, I suggest to add more discussion why it is important to select a subset of the measurements for the analysis.

Indeed it would be best to use all measurements, but because of the scan over the sun there are many measurements which only see a small part of the sun which results in a small signal / high noise. Including these data would increase artificial oscillations due to the onion peeling method.

We will reformulate/extent this section as follows:

During a scan over the sun the measured signal varies strongly, because only a small horizontal stripe of the sun (with varying area) is seen during one readout. Furthermore, the different scans over the sun overlap in altitude. In order to avoid large fluctuations with altitude caused by too noisy data, we select a subset of SCIAMACHY occultation data to be used in the retrieval. The basic idea for this selection is to preferably use the data with the highest signal in one scan and to avoid large fluctuations with altitude.

4. Section 3: How are the aerosols treated in the retrieval?

Aerosol effects are spectrally broadband and covered by the fitted polynomial P_j . We will mention this in the text:

As typical for DOAS-type retrievals, broadband absorption features (e.g. from aerosols) and uncertainties in the radiometric calibration are handled via a low-order (in the present case second order) polynomial P_i .

5. P-11476 L-20: Non-linear least squares fit is used here. It would be good to write down the actual retrieval problem. It remains unclear for me if the noise in the data is taken into account in the fit. Also, which methodology is used for solving the non- linear problem. Does the method provide error propagation from the data to the end products, (also related to sec 4.1).

The fit function is given in Eq. (1). We use a Levenberg-Marquardt algorithm. The noise of the data is not considered in the fit, because as explained in the text we do not directly use the measured data in the fit but interpolated spectra. However, because we select the high signal data, see above, measurement noise is usually low and for one tangent altitude quite constant over the spectral fit interval, so the impact on the fit results should be low.

We will mention this in the text:

A non-linear least squares fit (Levenberg-Marquardt algorithm) is used to determine from Eq. (1) for each tangent altitude the shift and squeeze parameters, the coefficients of P_j and the corresponding $a_{j,k}$. The noise of the measurement data is not considered in the fit.

6. *P-11477 L-27: pre-calculated data. Some clarification to explain a bit more what the pre-calculated data actually is would be nice. What variables are taken into C5087*

account? Also, it is somewhat unclear to me if the oscillations that are seen in the profiles may be related to the discretization of the pre-computed tables.

"Pre-calculated data" refers to the data base containing transmittances and weighting functions for reference conditions. These are computed at the retrieval altitude grid (to which the measurements are interpolated) and at a higher spectral sampling than the measurements (about 6 points per spectral resolution) such that an interpolation to the measurement spectral grid is uncritical. It is therefore unlikely that the discretisation of the tables is the reason for the oscillations.

We will change the text accordingly:

Furthermore, no individual radiative transfer model calculations are required during the retrieval, because a pre-calculated data base can be used for the weighting functions and the reference transmittances. This data base has been calculated on a high spectral sampling grid which is then interpolated in the retrieval to the wavelength grid of the measured spectra.

7. P-11476 L-24: refraction. Would be good here to clarify with few words more what is meant by the refractive effects here.

We will reformulate this as follows:

With this we account for effects due to refraction and the vertical smearing of the signal by the instrument field of view. Because of refraction the light path through the atmosphere is no longer a straight line but bended such that also atmospheric layers from below the tangent altitude affect the measured signal.

8. *P-11479 L-8: It seems that the error is estimated from the residual and not using error propagation – is there a reason why this approach is chosen? Which "covariance matrix" is refereed here?* Currently, the error of the measured spectra is not used in the fit (see above), therefore error propagation is not possible and we estimate the error from the fit residuals. The mentioned covariance matrix is also determined during the fit.

Clarification in the text:

The error for $a_{j,k}$ is the fit error, which is derived from the covariance matrix of the fit parameters obtained in the fit and scaled with the RMS of the fit residual.

9. *P-11479 L-13: I would appreciate a bit more explanation on how the empirical correction was estimated/justified. Was this based on simulations?*

The error propagation has been performed based on measurement results, not simulated data. We took the error obtained from the retrieval at one altitude and propagated it to the next lower altitude. This is then repeated for the lower altitudes (like onion peeling).

The new text will read:

This value has been derived by application of standard error propagation to about 10 000 retrievals on measurement data. In this context, the error obtained from the retrieval at one altitude has been propagated downwards in an onion peeling way.

10. Figures 8,9,10: panel top right. The axis of this figure could be changed to cover more interesting area, eg., something like -50% . . . 50%.

Reducing the x axis range to e.g. $\pm 50\%$ would result in a cut-off of the mean differences and error curves at upper altitudes. We think it is important to show that for CH₄ the relative errors become quite large at these altitudes, therefore we prefer to keep the current axis range.

11. Fig 9: Please, check the figure. At least in my printed version the shaded area is missing (figs 8,10 and 11 ok).

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The shaded area in Fig. 9 is there, it has a light grey colour. We will make this colour somewhat darker in the revised version.

12. *P-11489 L-27: I suggest adding clarification to the SCIAMACHY data used here: nadir observations?*

Yes, the total column data are from nadir measurements.

New text:

However, the ONPD CH_4 trends below 20 km of about 3 ppbv year⁻¹ are roughly in line with total column trends derived from nadir measurements.

13. P-11491 Speculations on future work. Have you considered, instead of performing full retrieval for all altitudes simultaneously which requires solving a large problem, applying two step approach used e.g. in GOMOS stellar occultation retrievals: solve first horizontally integrated densities one-by-one using non-linear least squares fitting and then perform linear profile retrieval using regularization (with smoothness requirement). If this sounds interesting, you might have a look on e.g. Kyrola et al, Retrieval of atmospheric parameters from GOMOS data, ACP, 2010.

Indeed, a GOMOS-like algorithm may also be an alternative to look at. We will include this in the text and add the corresponding reference:

Especially for CO_2 , another option to be followed in the future is the application of alternative retrieval algorithms. Possible candidates for this would be a two step approach used e.g. in GOMOS stellar occultation retrievals (Kyrölä et al., 2010) or the use of a full optimal estimation based retrieval, including online radiative transfer calculations, to the SCIAMACHY solar occultation data (see e.g. Bramstedt et al., 2009). Especially the latter kind of retrieval is computationally much more expensive, but vertical oscillations can be better handled via appropriate regularisation, and the retrieval

is less sensitive to non-linear effects arising from e.g. saturation or varying temperature and pressure.

Interactive comment on Atmos. Meas. Tech. Discuss., 8, 11467, 2015.

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