Atmos. Meas. Tech. Discuss., 8, C5092–C5104, 2016
www.atmos-meas-tech-discuss.net/8/C5092/2016/

Atmospheric Measurement Techniques Discussions
Open Access

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8, C5092–C5104, 2016

Interactive comment on "Stratospheric CH_4 and CO_2 profiles derived from SCIAMACHY solar occultation measurements" *by* S. Noël et al.

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Received and published: 22 January 2016

We thank the referee for the detailed comments and will consider them 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.

General comments:

The manuscript is a good introduction to the new SCIAMACHY retrieved data sets. It's great to see new data sets of CH4 and CO2 from an atmospheric limb sounder, as these are rare. The paper is fairly well written. There's a bit of concern with some *of the uncertainty characterization and the choice of coincidence criteria. The lack of correlative CO2 comparisons is also an issue, especially when there is an ACE CO2 data set (as referenced in the paper). Other than these issues, there are just a few minor issues and technical corrections that are needed.*

The mentioned issues are covered by the specific comments below.

Answers to specific issues:

1. *If the majority of ACE profiles are within 1 hour, why not make that the coincidence criteria (as opposed to 6 h) and have it consistent with HALOE? Even if that were to halve the number of coincident profiles, 650 pairs would still be statistically significant. Similarly, a 9 h criteria, yielding 25,000 coincident pairs with MIPAS, isn't necessary. Tightening up the criteria to something closer to the HALOE 1 h criteria will lead to more reliable comparison statistics while in no way sacrificing statistical significance.*

   Unfortunately, it is not possible to use the same coincidence criteria for all instruments. The coincidence criteria have been optimised for each instrument combination to achieve not only a sufficient number of coincidences but also a good coverage over time.

   For the comparisons with the occultation instruments (ACE-FTS, HALOE) the important criterium is the maximum time offset. This is because as long as always sunset data are used for the comparison, the temporal mismatch between the different solar occultation data sets is always small (because local time of the measurements is the same). This is why we also have a small temporal mismatch with ACE-FTS; in fact, the maximum time difference in this case is 1.2 h, and only 37 combinations (of about 1300) have a difference larger than 1 hour, and removing these would have no impact on the validation results.

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For ACE-FTS we used a maximum spatial distance of 500 km, because this gives a reasonable number and temporal distribution of collocations. Using 500 km also for HALOE would remove data from 2002 and 2005 (leaving only about 130 collocations), therefore we chose a maximum distance of 800 km.

The situation is different for MIPAS, which measures in limb mode while looking into a different direction as SCIAMACHY, so there is always a temporal mismatch of several hours. If we would use the 1 h criterium also for MIPAS, there would be no collocations with SCIAMACHY at all. Therefore it is required to have a larger temporal distance, we chose 9 h, which gives in combination with a maximum spatial distance of 800 km an almost complete coverage of coincidences over all seasons. We also checked a maximum distance of 500 km for MIPAS and smaller time offsets, but in these cases some months are no longer covered. Therefore we decided to stay with 9 h/800 km.

We will clarify the reasons for the different criteria in the revised version.

Updated text in ACE-FTS section:

For the comparison with SCIAMACHY, we take about 1300 collocated ACE-FTS V3.5 data between 2004 and 2012 based on a maximum spatial distance of 500 km. The maximum temporal distance of these data is usually below 1 h (maximum distance 1.2 h). This is because both ACE-FTS and SCIAMACHY measure in solar occultation geometry and only sunset data are used, which automatically results in a similar measurement time for collocated data.

Updated text in HALOE section:

Because the HALOE time series ends in August 2005, there are only few collocations with SCIAMACHY. To achieve a suitable number and temporal distribution of collocations, we chose a maximum spatial distance of 800 km, which results in about 300 collocations. We only use HALOE sunset

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data, therefore the temporal mismatch to SCIAMACHY is here also very low ($<$ 1 h).

Updated text in MIPAS section:

For the selection of collocated data from MIPAS we used the same maximum spatial distance of 800 km as for HALOE, but the maximum temporal distance was chosen to be 9 h, taking into account that MIPAS performed about 72 (in HR) and 96 (in RR) limb measurements per orbit at varying local times, whereas there was only one SCIAMACHY solar occultation measurement per orbit at local sunset. Because of the different viewing geometries it is not possible to restrict the maximum temporal offset to about 1 h (as for ACE-FTS and HALOE), as this would result in no collocations with MIPAS. With the chosen criteria, we usually get several MIPAS measurements which match with one SCIAMACHY measurement, from which we selected the (spatially) closest one. This results in more than 25 000 collocations between August 2002 and April 2012, which essentially cover all seasons.

2. *As noted in the manuscript, ACE does have a CO2 product. Even if it doesn't have the same altitude range as the SCIAMACHY data it does have overlap in the lower altitude range. It would be extremely beneficial to include comparisons with ACE in the overlapping altitude range.*

   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.

3. *Smoothing the data would only reduce the error if the error was purely random. There will absolutely be systematic uncertainties in the derived scaling factors, and smoothing the profile does not reduce these errors. If you are going to claim that smoothing improves your error estimates, then there needs to be a more rigorous analysis of the breakdown of the altitude dependent systematic and ran-*

dom errors in the retrieval, and show how these are both affected by the smoothing and how they contribute to the total estimated uncertainty.

As explained in section 4.1, the error of the products is estimated from the fit residuals and thus has both random and systematic contributions which cannot clearly be separated. The smoothing of the profiles (see section 4.2) is then used as a kind of regularisation procedure after the retrieval. The main purpose of this is not to reduce the error of the products, but to reduce (systematic) artificial oscillations caused by the onion peeling method.

The smoothing therefore affects both random and systematic errors. As written in the text, the reduction of the error by the factor $\sqrt{4.3}$ is indeed only an estimate assuming uncorrelated (random) data, but as long as the systematic errors are not fully understood (best example is the unexpected vertical oscillations in the resulting profiles which we cannot reproduce with model data) this is the best we can currently do.

We will update the text in section 4.2 accordingly:

Since boxcar smoothing is similar to averaging, the error of the retrieved scaling factors is reduced after smoothing by a factor of $\sqrt{4.3}$. This assumes that the error is random and the underlying data are uncorrelated, which is in fact a conservative estimate since – as explained above – adjacent altitudes are typically anti-correlated. Considering also the broadband error correction described in the previous section, this is a reasonable estimate.

4. *As the saturation and temperature scale factor values can be relatively large, there needs to be some further analysis and discussion on what uncertainties there are in the pre-calculated scale factors and how these contribute to the overall uncertainty in the derived profiles.*

To clarify this, we will change the end of section 4.3 as follows:

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The effective corrections to be applied are therefore usually quite small, typically not larger than a few percent. The correction factors are derived from radiative transfer calculations and are therefore in principle as accurate as these calculations. The main uncertainties arise from (1) their calculation via scaled profiles and (2) the later interpolation of the data base. Using scaled profiles is a valid approximation, considering that the vertical resolution is about 4.3 km, which is essentially determined by the vertical smoothing, and that most information is derived from altitudes close the tangent height. The interpolation error is quite small (typically below 0.1%) and could be further reduced by extension of the data base. Overall, the contribution of the uncertainties of the correction factors to the error of the derived profiles is considered to be very small.

5. *A number of times pressure/temperature differences between data sets has been cited as a source of uncertainty. It should be fairly straight forward to quantify the error in the SCIAMACHY VMRs due to p/T uncertainties and include this in the total error.*

   We do not refer to the expected accuracy of ECMWF p/T data here, which is quite high (e.g. accuracy of temperature profiles of about 1 K, well below 1%). The impact of this on the estimated error of SCIAMACHY profile could indeed be calculated quite straight forward, but it should be low compared to other error sources and is therefore neglected.

   What we are concerned about are unknown systematic effects of the ECMWF model data or how we use them in our retrieval (e.g. different altitude grids, interpolations, ...) – these errors cannot be quantified (because they are unknown), but maybe we could reduce their impact on the VMRs if we e.g. also retrieve p and T from SCIAMACHY data (see conclusions).

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Answers to minor issues:

1. *Abstract: Just needs a few more details about the actual retrieval. E.g. Spectral band, CO2 altitude range, etc. Also the discussion of trends could be more specific and give the values/altitudes/significance.*

   The abstract will be updated accordingly:

   Stratospheric profiles of methane (CH_4) and carbon dioxide (CO_2) have been derived from solar occultation measurements of the SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY). The retrieval is performed using a method called "Onion Peeling DOAS" (ONPD) which combines an onion peeling approach with a weighting function DOAS (Differential Optical Absorption Spectroscopy) fit in the spectral region between 1559 and 1671 nm. By use of updated pointing information and optimisation of the data selection and of the retrieval approach the altitude range for reasonable CH_4 could be broadened from 20 to 40 km to about 17 to 45 km. Furthermore, the quality of the derived CO_2 has been assessed such that now the first stratospheric profiles (17–45 km) of CO_2 from SCIAMACHY are available. Comparisons with independent data sets yield an estimated accuracy of the new SCIAMACHY stratospheric profiles of about 5–10 % for CH_4 and 2–3 % for CO_2. The accuracy of the products is currently mainly restricted by the appearance of unexpected vertical oscillations in the derived profiles which need further investigation. Using the improved ONPD retrieval, CH_4 and CO_2 stratospheric data sets covering the whole SCIAMACHY time series (August 2002–April 2012) and the latitudinal range between about 50 and 70°N have been derived. Based on these time series, CH_4 and CO_2 trends between 2003 and 2001 have been estimated. CH_4 trends above about 20 km are not significantly different from zero, the trend at 17 km is about 3 ppbv year^{-1}. The derived CO_2 trends

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show a general decrease with altitude with values of about 1.9 ppmv year^{-1} at 21 km and about 1.3 ppmv year^{-1} at 39 km. These results are in reasonable agreement with total column trends for these gases. This shows that the new SCIAMACHY data sets can provide valuable information about the stratosphere.

2. *SCIAMACHY data section: should state/describe what the absorption features are being observed*

   We will update the relevant part of this section as follows:

   In this study we use SCIAMACHY radiance spectra measured in solar occultation mode taken from the current Level 1 data set, i.e. V7.04, consolidation degree "W". SCIAMACHY measures from the UV (about 214 nm) to the SWIR (about 2386 nm). We use here the spectral interval between 1559 and 1671 nm in which mainly CO_2 and CH_4 absorb.

3. *HALOE data section: It should be noted that the HALOE validation reference was using v17 data, not v19.*

   Good point, will be mentioned:

   The precision of HALOE CH4 profiles is in the order of 7%; the total uncertainty including systematic errors is about 15% (Park et al., 1996, based on v17 HALOE data).

4. *11470 lines 10-13: I don't think these lines are necessary*

   We think these lines are necessary, because the SCIAMACHY data set is available via the GHG-CCI web site. This information will be added:

   In the context of the ESA Greenhouse Gas Climate Change Initiative (GHG-CCI), the SCIAMACHY CH_4 and CO_2 profile retrieval has been further improved. The data set used in the present manuscript (V4.5.2) is part of the

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Climate Research Data Package (CRDP) generated in the context of this project and available via the GHG-CCI web site (www.esa-ghg-cci.org).

5. *11471 lines 9-14: If this altitude region isn't considered, there isn't much need for this discussion.* This is mentioned, because the previous product version used a higher tangent altitude as reference and therefore could only use state 49 data. As this is one of the improvements of the new version we prefer to keep this part, but add some clarification:

   Above 100 km, two different measurement configurations (so-called "states") were used: For state 47 (executed for typically two orbits per day) the measurement ends with pointing to the solar center; for state 49 (executed during the other orbits) the scan over the sun is continued until almost 300 km. In contrast to the algorithm of Noël et al. (2011) the analysis described here uses only data below the 100 km tangent altitude and therefore is applicable to both measurement states.

6. *11471 lines 26-28: The way this is worded makes it sound like you are only using one reference spectrum rather than two.*

   The text will be updated to clarify this:

   The upward reference spectrum is obtained by selecting for one upward scan around this altitude the spectrum which has the highest signal outside the absorption (i.e. at the lower edge of the fit window at about 1560 nm). The same is done for a corresponding downward scan to determine the downward reference spectrum.

7. *11473 line 16: is 800 km a typo? It says this is the same as the ACE criteria, but the ACE criteria was previously stated to be 500 km.*

   The ACE-FTS criterium is indeed 500 km, but we use 800 km for HALOE to get a reasonable number of coincidences. The number is actually the same as for

MIPAS.

The corresponding text in the instrument sections has been updated, see above.

8. *Error correction section: what is being used as the covariance matrix?*

   The mentioned covariance matrix is 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 obtained in the fit and scaled with the RMS of the fit residual.

9. *When comparing with ACE profiles, it should be noted that the ACE error bars represent the retrieval statistical fitting error, which are not necessarily representative of the precision (or the accuracy or the total uncertainty).*

   This information will be included in section 5.1:

   The ACE-FTS error bars represent the retrieval statistical fitting error.

10. *11480 line 4: It might not be accurate to say that most optimal estimation algorithm make use of regularization*

    We changed “most” to “many”:

    In contrast to e.g. many optimal estimation type retrievals, the ONPD method does not include a regularisation.

11. *Comparisons with MIPAS: In order to be more accurate, the agreement is not “almost perfect”, the systematic differences are near zero.*

    Agreed, will be changed:

    As can be seen from this plot, the systematic differences between SCIAMACHY and MIPAS are near zero above 25 km.

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12. *Figure 1 caption: last sentence is more discussion that belongs in the main text than information about the plot.*

    Agreed, the sentence will be changed. Updated caption:

    Illustration of the solar scan strategy. The orange/yellow area indicates the size of the refracted/geometrical sun. The black curve shows the scan as function of time, relative to the time where the geometrical sun reaches 17.2 km (which is the sun-fixed event used in mission planning for this measurement). The white dots indicate (as an example for one upward scan) the position of individual readouts. The corresponding reference readout for an upward scan is also shown.

13. *Figure 3 caption needs to be more specific.*

    The caption will be updated as follows:

    Example for a fit. Top: normalised measured spectrum (red line) and fitted spectrum (green line) at 25 km tangent altitude. Bottom: resulting residual, i.e. relative difference between measurement and fit.

14. *Figure 12: Latitude units should indicate that it's Northern hemisphere (e.g., $^\circ$N).*

    Will be changed in the plot.

Technical issues:

1. *All references to "manuscript" should be "study"*

    Will be done.

2. *11468 line 8: "extended to" should be something like "broadened from ?? – ?? to 17–45 km".*

    Covered by updated abstract, see above.

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3. *11470 line 5: "to CH4 retrieval" should be "CH4 retrievals"*

   Will be changed.

4. *Line 6: unclear what "at that time" refers to*

   It refers to the previous study. The text will be reformulated:

   However, in this previous study, not much attention was paid to the quality of the derived CO_2 profiles.

5. *Line 24: "most recent" should be deleted*

   The text will be reformulated (see above).

6. *11471 line 6: "already" should be deleted*

   Will be done.

7. *Line 19: is signal to noise meant by "signal"?*

   No, we really mean "signal" here, as this is what is used in the selection method, but of course highest signal in this case also implies high signal to noise.

8. *Line 25: "scan" should be "scans"*

   Will be changed.

9. *11774 line 7: "in" should be "on"*

   Will be changed.

10. *11775 line 1: ONPD has already been defined*

    Agreed, updated text:

    The ONPD algorithm is essentially based on a weighting function DOAS fit (see e.g. Perner and Platt, 1979; Burrows et al., 1999; Coldewey-Egbers et

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al., 2005) in combination with an onion peeling approach (see e.g. Russell and Drayson, 1972).

11. *Line 17:"in solar occultation" isn't necessary*

    Will be removed.

12. *11776 line 3: "radiative transfer calculations using" could be better as "using the radiative transfer model"*

    Will be changed.

13. *11782 line 12: "as can be seen from this figure" is not needed*

    Will be removed.

14. *11786 line 13: delete "also"*

    Will be removed.

15. *11791 line 12: "in" should be "on"*

    Will be changed.

16. *Figure 2 caption: last sentence is not necessary*

    Will be removed.

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