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Atmospheric
Chemistry
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Discussions

Interactive comment on "Comparisons between ground-based FTIR and MIPAS N_2O and HNO_3 profiles before and after assimilation in BASCOE" *by* C. Vigouroux et al.

C. Vigouroux et al.

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The authors thank the referees for their helpful and constructive comments and questions. The manuscript has been clarified in many points. Therefore, the referees have contributed to a substantial improvement of the paper.

Referee #1

A. Major points

1) BASCOE

Referee: "The model BASCOE, including its assimilation 4DVAR scheme, is very rapidly presented"

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BASCOE descends from Errera and Fonteyn (2001, hereafter EF2001). Although several improvements have been done, there are many similarities between BASCOE and EF2001. A new appendix has been added to the manuscript. It describes the similarities and differences between BASCOE and EF2001.

Referee: "When considering the observations of MIPAS (H2O, NO2, O3, CH4, N2O and HNO3) are they (yes or no) correlated in the assimilation scheme?"

Yes, they are correlated since observed species interact through the chemical reactions explicitly modelled.

Referee: "If yes, how do HNO3 and N2O behave knowing that MIPAS HNO3 is biased because of spectroscopic parameter systematic error?"

There is a bias between FTIR and MIPAS HNO3 spectroscopic parameters. That does not mean that MIPAS is using the “wrong” ones. The spectroscopic parameters used by MIPAS are taken from more recent studies than the FTIR ones (see J.-M. Flaud et al., 2003a; this reference has been added to the manuscript).

On the other hand, we see a bias between MIPAS and BASCOE HNO3. The possibility that it could come from an incompatibility between the chemical scheme in BASCOE and a possible bias in one of the MIPAS assimilated species has been evocated in the old manuscript (p.46, l.18). Additional tests have been made in order to determine the origin of this bias. In the first one, HNO3 has been assimilated alone for a limited period of time in order to check if the other assimilated species could play a role in the HNO3 analyses. No difference was found between the two sets of analyses. An explanation of the bias was raised by the second test. For this one, HNO3 has been re-assimilated, again for a limited period of time, and sensitivity tests regarding the surface area density (SAD) of the sulphate aerosols were made. This has shown a significant impact on the HNO3 analyses. Therefore, we suggest that the HNO3 bias is related to the climatology of the SAD used to calculate the heterogeneous reaction on sulphate aerosols (see also last referee’s issue on BASCOE). The text has been changed in the revised manuscript.

Concerning the N2O behaviour in BASCOE possibly linked to the bias between BASCOE and MIPAS HNO3: a bias in HNO3 would not influence the N2O analyses because the time-scale of N2O (months to years) is much longer than the assimilation window (one day).

Referee: "What is the spin-up period of your run? Is it long enough?"

MIPAS has been assimilated from October 2002 to March 2004 (18 months). Thus, the spin-up period is 3 months, which is certainly long enough. Since the BASCOE spatial resolution is comparable to the MIPAS daily coverage, the necessary spin-up period should be less than 10 days.

Referee: "What are the horizontal and vertical correlation functions, if any?"

The question should be clarified. By "correlation functions", maybe it would mean off-diagonal term of the background covariance matrix B. In our study, the background matrix is diagonal. So, no correlation function is used to build the off-diagonal terms of the B matrix.

Referee: "Is the model error fixed or does it depend upon the considered molecule, or chemical family?"

Again, this question needs clarification. Theoretically, model error can be taken into account in the 4D-Var formalism by adding a term to the cost function (Ménard and Daley, 1996)[1]. However, model errors are difficult to estimate and only few case studies based on this approach have been reported (e.g. Zupanski, 1997)[2]. So, to answer this question, no model error is taken into account. However, maybe the question concerns the error of the background field (i.e. the field used to initialize the daily assimilation). In that case, the answer is that 20% error has been specified for every species in every model grid point (as mentioned in the manuscript).

1: Ménard, R., and Daley, R.: The application of Kalman smoother theory to the estimation of 4DVAR error statistics, Tellus, 48A, 221-237, 1996.

2: Zupanski, D.: A general weak constraint applicable to operational 4DVAR data assimilation systems, Mon. Wea. Rev., 125, 2274-2292, 1997.

Referee: "You also mention in the conclusion a "convergence criteria". Could you define it and explain why this parameter can play in the assimilation procedure?"

The convergence criteria are defined in EF2001. However, this sentence introduced information that is useless for this paper. Thus, this comment has been removed in the revised manuscript.

Referee: "When there is a bias between FTIR and BASCOE (e.g. for HNO3) is there a way to differentiate sources of the bias within BASCOE, namely is it due to the model, to the assimilation technique used, or to the satellite data?"

Yes, it could be possible to identify the source of the bias. First, when the background error is increased to 50%, a lower (but still present) bias is found between MIPAS and BASCOE for HNO3 (not shown). This set-up increases the weight of the observations in the final solution (EF2001). Second, satellite data could be biased and be incompatible with model chemistry. Assimilation of data from other instruments (if available) could partly solve the question. If a similar bias is found, one may believe that the model is biased. If no bias is found with respect to these extra data sets, one may believe that the former data set is biased. Third, one could test the model parameters that could influence the species for which a bias is found. In our case, a test of sensitivity to the climatology of sulphate aerosols produces a significant change in the HNO3 bias.

Nevertheless, this is an important point raised by the referee, that is still an open question in data assimilation in general.

2) FTIR

Referee: "Contrarily to N2O, the HNO3 averaging kernels do not peak... In that context, are FTIR vertical profiles very meaningful when comparing to MIPAS and could *that cause the systematic bias between FTIR and MIPAS?"*

Because of the low vertical resolution of the FTIR retrievals as compared to the MIPAS profiles, the main interest of the comparisons is in the partial column comparisons. Therefore we have added in the new manuscript figures of the considered partial columns averaging kernels, as well as the DOFS of the partial columns (additional columns in Table 2). As such, it will be easier to see that, even if the DOFS for N2O over the whole altitude range of the FTIR profiles is larger than that for HNO3, this is no more the case for the considered partial columns. At least one of the DOFS for N2O is situated in the troposphere, thus it is "lost" for the comparisons with MIPAS profiles that do not go down into the troposphere.

The partial column averaging kernels show that they peak in the right altitude range, therefore the partial columns can be compared without inducing any bias due to vertical resolution issues. There is no doubt about the fact that the bias is induced by the different spectroscopic databases.

The DOFS for the partial columns are larger than one. Therefore, we believe that it is still valuable to show profile comparisons. But we agree with the referee that, although the presentations have a high vertical resolution, the real information does not and thus these profile comparisons should not be over-interpreted.

Especially, as said in the previous manuscript, on p. 8356 (l. 3-8) and p. 8358 (l. 27-28) – p. 8359 (l. 1-3), the detailed shapes of the profile comparisons strongly depend on the individual FTIR averaging kernel shapes and thus on the FTIR retrieval parameters. To stress the point that one should focus on the partial columns comparisons, the comments on the N2O profile comparisons have been removed from the conclusions of the paper.

3) Transport vs. Chemistry

Referee: "What could you do to improve HNO3 assimilation? For instance, using a *full PSC microphysics instead of the PSC parameterization might probably improve the model output."*

Indeed, a better formalism to take into account the impact of PSC would improve BASCOE analyses. However, this will be only valid at the Poles when PSC are formed and the bias is present in all latitude bands. Globally, as mentioned above, improving the climatology of sulphate aerosols is expected to reduce the bias between MIPAS and BASCOE. By the way, as mentioned by Rood (2005), the problem of bias is perhaps the greatest challenge facing assimilation. This comment and the reference have been added to the manuscript.

4) Error

Referee: "Error on the mean should statistically decrease in sigma/sqrt(N),. . . , while there is no reasons for the standard deviation to decrease when considering more points in the coincident exercise."

Yes, you're right. But, in l. 25, p. 8375, we are talking about the error on the mean, not about the standard deviation. We think there has been a misunderstanding of the text by the referee.

We are not expecting that sigma would decrease when the number of coincidences will increase (we even expect that when using a stricter coincidence criteria, so less coincidences, the standard deviations would decrease for physical reasons!). So we look at sigma values when we want to discuss the scatter of the differences (so the" precision"), while we look at the bias (mean of the differences) when we want to discuss the "accuracy". The error on that bias is reduced when the number of coincidences increases because it is equal to sigma/sqrt(N). In the manuscript, we have multiplied sigma/sqrt(N) by 3, in order to be in the 99% confidence limits when we talk about the "significance" of the bias.

We hope the point is clarified now. We think there is no need to modify the manuscript itself.

5) Winter-Spring disagreements

a) BASCOE / MIPAS

Referee: “In addition to the difficulties of tracking the vortex with the model considering its own resolution, how is the vertical descent actually represented in the model, and could that be another possible reason for explaining the systematic bias since it is known that models have great difficulties to reproduce the actual degree of vertical descent”.

Note: here, and whenever it is not specified, the figures numbering refers to the old manuscript.

A HNO3 bias between BASCOE and MIPAS is present in all latitude bands; see Fig.4 and, as an example, Fig.9 for Jungfraujoch. Indeed, it is larger at Arrival Heights for our set of comparisons (Table 5, Statistics 1 – Statistics 3), but it doesn’t seem from Fig.4 that the bias is worse in this latitude band. Thus, we cannot conclude that the difficulty of reproducing the vertical descent could induce a systematic bias. This is confirmed by the fact that for N2O, which is also concerned by the vertical descent, no bias between BASCOE and MIPAS is observed during winter-spring period at the pole, in troposphere and lower stratosphere (see Fig.4; also confirmed by comparing Statistics 1 and 3 in the whole period (Table 3) and in reduced winter-spring period (not shown)).

However, the standard deviation is worse at the South Pole during winter-spring, for both molecules (Tables 3 and 5, and Fig.4). This is partly due to the spatial resolution of BASCOE. Maybe, the vertical descent could also have an impact on the standard deviation. This has to be checked in further work.

Referee: “And for HNO3, what about denoxification/denitrification in the model? This *also might produce biases?*

As said above, in term of “bias”, it is not so clear from Fig.4 that the data assimilation for HNO3 in the winter-spring period at the poles is worse than for mid-latitude bands. The evolution of HNO3 in the South Pole polar vortex compares very well with MIPAS. This indicates that the parameterization of denoxification/denitrification is correctly set-up for data assimilation.

b) FTIR / MIPAS

Referee: “In winter-spring season, the comparisons between FTIR and MIPAS are poor. This is probably due to the presence of the vortex.”

"Why not also using a criterium based upon Potential Vorticity values for comparing within/outside/vicinity of the vortex? This should also reduce the bias.

We have envisaged this option, but finally decided to simply exclude the winter-spring season, also because we know that BASCOE is less reliable in that season. We believe that it would anyhow not change the final conclusions. We think that there would be no impact on the biases because PV differences between the compared data should cause a random effect, not a systematic one; therefore in the statistics they only impact the standard deviations, not the systematic bias between the data sets on a statistical basis.

Nevertheless, we have made some tests in support of the present discussion. We have added a PV criterion at Arrival Heights: at 450 K, the PV differences should not be more than 15%. This is the criterion that was suggested for the coordinated MIPAS validation work (Special Issue on MIPAS validation, to appear later). The results were the following: for N2O, Statistics 1 is slightly better (-5 ± 9 % for 232 coincidences, instead of -5 ± 10 % for 271 coincidences), and Statistics 2 remains the same (-8 ± 9%). The 24 coincidences at ± 400 km are all fulfilling the PV criteria. If we use a stricter PV criterion (2.5%), we obtain for Statistics 1: -6 ± 7 % for 53 coincidences.

Thus, the bias is confirmed, and adding a strict PV criterion has a positive impact on the standard deviations. One could notice that this additional collocation criterion is not sufficient to reach the standard deviation obtained by eliminating the winter-spring time period (5%). We suspect that in winter-spring, even if we limit the comparisons to those satisfying the PV criteria at the nominal locations of the MIPAS and FTIR observations, the compared airmasses still suffer from a too large variability within the horizontal extent of the airmasses (the so-called smearing or horizontal smoothing effect), that degrades the agreement.

This conclusion is even more evident when we look at HNO3. Using a strict PV criterion of maximum 2.5% PV difference, we obtain for Statistics 1: +15±17% for 80 coincidences instead of (+19±23%) for 318 coincidences, thus, a well-reduced standard deviation. Still the standard deviation is high when compared to that observed for the reduced time-period (9%). The bias is indeed reduced, in case of HNO3, but not significantly considering its error (3*sigma/sqrt(N)).

In conclusion, we would say that the approach adopted in the paper to eliminate winter-spring from the time period for comparisons at high latitudes gives a more satisfactory result than only adding a PV gradient criterion, as far as the standard deviation of the comparisons is concerned.

We have added a short notice concerning this point in the manuscript, in a new subsection (5.3.1).

6) Spectroscopy issues

Referee: "Why not showing the MIPAS-FTIR results directly considering the same spectroscopic parameters? Is this linear regarding the retrievals?"

For 3 reasons: First, this validation work has been initiated before the HITRAN 2004 database was available. Thus, all the FTIR retrievals have been made using the HITRAN 2000 (+updates) database. Usually a “jump” to a new spectroscopic database is made carefully by the users: they often wait for a validation of the new spectroscopic parameters. Second, by the end of this work, new FTIR retrievals have been made using the HITRAN 2004 database: these results will be part of another publication by Blom et al., to appear later in a Special Issue of ACP on MIPAS validation. Note that the HNO3 spectroscopy in HITRAN 2004 is not exactly the same as that in the MIPAS database used for the MIPAS v4.61 products (Flaud et al., 2006), but the HNO3 line intensities are nearly equivalent. Third, the HNO3 line intensities are still under debate. New improvements have already been included in the MIPAS database (Flaud et al, 2006). This reference has been added in the manuscript.

As the main change between both spectroscopic databases is a scaling factor in HNO3 line intensities, the effect is expected to be essentially linear: a difference of 14% between the HNO3 retrieved profiles (Raspollini et al., 2006; reference added to he manuscript). This has been confirmed by the new paper in progress, regarding partial columns and profiles comparisons. But, as pointed out by Referee 2, there are also some additional new lines (hot bands) in HITRAN 2004, and also the spectroscopic parameters of interfering species have changed in some cases (e.g., for OCS). These changes can have some impact on the FTIR retrievals (at least reducing the residuals), but the main effect, according to the more recent analyses mentioned above, seems to be the bias of 14% indeed. So we believe that our estimation of the effect of the spectroscopic data changes, as presented in the paper, is valid.

Remark: In the original manuscript, the bias was mentioned to be 13%. But, in the revised manuscript, we prefer to use the bias of 14% mentioned by Raspollini et al. (2006). It is also closer to what has been observed in the work in progress for Blom et al., Special Issue MIPAS validation paper.

7) Smearing effect

Referee: ”Could you quantify the “smearing effect”? And what could be done to reduce this effect?”

Indeed it would be interesting to quantify the “smearing effect”, also called the “horizontal smoothing”, as it appears to be a major source of high standard deviations of the comparisons. We see that in case of very high spatial variability (such as for HNO3 in polar winter) the spatial and temporal coincidence criteria alone cannot explain the too high standard deviations. Adding a PV criterion doesn’t solve the problem because this only ensures that the airmasses at the nominal retrieval location are well collocated (as would do a stricter spatial collocation). The problem of “horizontal smoothing” is inherent of the measurements and the retrievals themselves; it is due to the fact that we are dealing with *integrated* measurements. To introduce this smearing effect more clearly in the paper, we have added a subsection (5.3.1) in the manuscript. We call it now “horizontal smoothing” since this is the terminology used by von Clarmann (2006), which is a reference added in the new manuscript.

Our colleagues J. C. Lambert and C. De Clercq are working on a model to estimate the error due to the “horizontal smoothing” in the case of limb infrared emission spectra (De Clercq et al, 2006[3]). They participate to the Special Issue of ACP about MIPAS validation where they present a quantitative estimate of the impact of the smearing effect on partial column comparisons, for O3 (Cortesi et al., in preparation) and for temperature (Ridolfi et al, in preparation). They found a good correlation between the obtained horizontal smoothing error and the standard deviations of the comparisons. Preliminary results for N2O and HNO3 have also indicated a reasonable agreement. As their calculation of the smearing effect is using results from BASCOE to evaluate the target gas spatial variability, we have preferred not to use their results explicitly in this paper. The use of an independent model would provide a good test.

3: De Clercq, C. and Lambert, J.-C.: A forward model of limb infrared emission spectra in two-dimensional atmosphere, Proceedings of the First Conference on Atmospheric Science, Frascati 8-12 May 2006, ESA Special Publication SP-628, 2006.

One can reduce the horizontal smoothing effect by using a two-dimensional retrieval technique instead of the one-dimensional one used to obtain the ESA MIPAS Level

2 products. Different teams are working on that problem, for example at IMK-FZK, Karlsruhe, for the MIPAS/IMK products.

8) Arrival Heights

Referee: ”Comparisons considering FTIR in Arrival Heights are systematically poor compared to all other stations. Could you comment? Could that be a problem of measurements, of modelling, of assimilation, of coincidence criteria?”

Considering MIPAS / FTIR comparisons:

The methodology used in the retrieval of the Arrival Heights HNO3 and N2O profiles is exactly the same as that of Lauder, but obviously, with differing instruments and site dependent input parameters, e.g., measurement Field Of View, a priori data, etc. The Arrival Heights Bruker (120M) spectrometer is calibrated to the same standard as that of both Bruker spectrometers at Lauder. The instrument, over the time frame of this comparison, was well calibrated and there were no anomalies in the instrument operation. Baseline issues were addressed in the quality control section of the data analysis. So, we can’t see any problem from the measurements side.

The spectroscopic parameters are the same and the retrieval code SFIT2 is used in both cases. At such latitudes as Arrival Heights, the a priori profile can differ dramatically from the actual profile. This could add a difficulty in the retrieval process and should be kept in mind. However, quality control of the data at the two sites is also the same.

So, the processing, retrieval and quality control side of the data processing are supposed to be as good at Arrival Heights as at Lauder.

The comparisons at Arrival Heights are worse mainly in term of standard deviations during winter-spring and that has been explained by the higher spatial variability of the airmasses coupled with the horizontal smoothing effect (see discussion above).

For N2O, looking at Statistics 1 in Tables 3 and 4, we see that the biases are significant at Arrival Heights and Wollongong compared to the other stations. The bias at Arrival Heights is still present in the reduced period, thus we think that it does not come from the collocation criteria. It should come from FTIR or MIPAS retrievals. We can notice that, for Wollongong and for Arrival Heights during the summer-autumn period, the FTIR and BASCOE comparisons show no bias. This could lead to the conclusion that FTIR retrievals are not causing the bias, but this should be confirmed by other correlative data.

Referee:” Could that be a problem of modelling, of assimilation?”

See previous comments on BASCOE.

B. Minor points

1) P. 8338: *Referee: "FTIR is not the only instrument tracking stratospheric HNO3 and N2O. There were already some ground-based microwave measurements of N2O and HNO3 performed by the Zafra’s team and instruments in Artic and Antarctic”.*

Indeed there were several ground-based microwave measurements performed in the past. According to our knowledge (NDACC Web pages), these measurements stopped in 1995, and therefore we haven’t considered them as being an “available ground-based source of data”. But, it is true that the sentence is misleading, so we have added in the manuscript that NDACC FTIR experiments are the only source of regularly available ground-based data during the considered period of MIPAS operations.

2) P. 8339: *Referee: "The latitudinal dependence of the lower limit in MIPAS retrievals is certainly related to the height of the tropopause. Could you comment on that?*

We have not seen a clear correlation between the lower limits of the MIPAS retrievals and the tropopause heights. Rather, the lower limit in MIPAS retrievals seems to be related to the presence of clouds, and the mean altitude of these clouds, which depends on latitude (Raspollini, 2006, Fig. 2): this comment and the reference have been added to the manuscript. For example, at Arrival Heights, the presence of PSCs makes that the MIPAS retrievals have quite a high lower limit, despite the low tropopause height.

3) P. 8346: *Referee: "I would use the term lowering instead of degradation"*

Following the second referee proposition, we will change “degradation” to “smoothing”.

4) Typo in Eq. 4.

Corrected.

5) P. 8350: *Referee: "Could you add references for baseline errors affecting N2O and HNO3 retrieval?"*

The baseline error is a particular contribution to the error due to the uncertainties in the spectral measurements. It refers to the uncertainty about the local 100% transmission level in the absorption spectra. We are not aware of any existing specific references.

6) P. 8340: *Referee: "Isn’t it “lower” instead of “greater”?"*

No, this is right. We reject scans for which the lowest valid MIPAS data point is at an altitude higher than 12 km for N2O and higher than 14 km for HNO3. The reason is that we want all the partial columns that go into the statistical data set for comparison at a given site to cover the same altitude range, and that we don’t want to use extrapolated (MIPAS) values in the calculations of the partial columns. If the lowest valid data point of a MIPAS scan is at 14 km, then we would have to use in the comparison some extrapolated values between 12 and 14 km.

The paragraph has been revised in the new manuscript for clarity.

See also answer to Referee 2.

7) P. 8338: *Referee: "I would write tropospheric “source” species and a stratospheric “source” species”.*

We have changed the manuscript to “tropospheric source species and stratospheric reservoir species”. HNO3 is a reservoir species in the stratosphere, not a source species.

Interactive comment on Atmos. Chem. Phys. Discuss., 6, 8335, 2006.

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