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Atmospheric Chemistry and Physics Discussions

Interactive comment on "HOCl chemistry in the Antarctic stratospheric vortex 2002, as observed with the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS)" *by* T. von Clarmann et al.

T. von Clarmann et al.

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Replies to the reviews

The authors would like to thank both reviewers for their helpful comments.

Reply to the review by M. von Hobe:

PSC occurrence (Page 18970, line 23; Figure 1):... It is good to include a figure showing the presence of PSCs...

We agree that information on PSC existence throughout the entire relevant episode is necessary. We will replace Figure 1 by a figure which shows time series of MIPAS PSC observations in all relevant altitudes.

Vortex evolution and position:..
We will include figures showing PV maps for 1000 K and 475 K and will include symbols representing the locations of the MIPAS daytime and nighttime measurements. These figures will provide the user with information of the development of the vortex, illumination and MIPAS sampling.

Evolution of Cl species in heterogeneous chemistry regime:...
The discussion of vortex inhomogeneities will be extended and the Grooß et al. paper will be referenced.

Page 18970, line 14: The last sentence of the introduction...
A sentence on this will be added at the end of the introduction.

2. Page 18971, line 25: Please specify what you mean by "similar".
The criterion will be better defined in the revised version.

3. Page 18972: For the present study, why do you not simply use the diagnostic KASIMA model ...
The use of a pure CTM is not favorable for this study as the available ECMWF (re-)analyses for September/October 2002 are not realistic in terms of long-term transport (see also: Monge-Sanz, B. M., M. P. Chipperfield, A. J. Simmons, and S. M. Uppala (2007), Mean age of air and transport in a CTM: Comparison of different ECMWF analyses, Geophys. Res. Lett., 34, L04801, doi:10.1029/ 2006GL028515)

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and thus a nudging procedure is more appropriate.

... for all altitudes?
We use the measurement grid for the analyses in order to support a more meaningful intercomparison of measured and modeled data. For this purpose the modeled data had to be smoothed by the MIPAS averaging kernels, and the representation on the measurement grid is the natural choice then. Given the coarse MIPAS HOCl altitudes resolution, comparison on a finer altitude grid would not provide much additional information.

4. Page 18973, line 7 + page 18976, line 9 + page 18980, line 6: What is the reason for not using Sander et al., 2006 (as opposed to 2003) in all model runs?
As said in the paper, we use (aside from species measured by MIPAS and HCl) multi-annual model runs for initialization. These are based on Sander 2003 and cannot easily be reproduced on the basis of Sander 2006 reaction rates. We are afraid that switching the reaction constants after initialization might lead to oscillations of the calculated chemical state. For the chlorine species, which are in the focus of this study, the recommended data did not change between the 2003 and 2006 versions. In addition, as we use an online photolysis scheme in KASIMA, the preparation of the temperature dependence of the absorption spectra and quantum yields has to be done very carefully and will be done for the next JPL recommendation which will be released in 2009. Thus, we decided not to change the rate constants only from Sander 2003 to Sander 2006 as we hesitage to merge the data sets.

5. Figure 2 Some of the panels are very busy...
These figures will be changed as suggested.

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Reply to the review by S. Chabrillat

The process of selection of the observations...
The selection criterion will be better specified. See also reply to minor issue 2 of the review by Marc von Hobe.

There is no figure to report the geographical and temporal distribution of the selected observations...
Such a figure will be added to the final version. See also reply to major issue 2 to the review by Marc von Hobe.

While the manuscript mentions repeatedly the irregular spatial sampling ...
The main impact of irregular sampling is that the mean values of measured data might not be representative for the vortex as a whole. The standard error of the mean might underestimate the representativeness component of the error. This aspect will be discussed in the revised version with all necessary statistical formalism.
In order to avoid problems due to irregular sampling, we draw our quantitative conclusions only from the differences between measurements and matching output of model calculations. Due to the matching sampling between measurements and model output under consideration, there is in first order no effect due to irregular sampling. We do not quantitatively discuss day-to-day differences, because these would indeed be affected by the sampling problem. We had stated this in the text of the original manuscript but we will try to better clarify this issue for the final version.

Is the model output (fig. 38211;-6) interpolated to the location of the observations prior to averaging...
The model output was first interpolated to the measurement locations and then

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averaged. In the revised version, we will better describe this procedure.

- What is the strength of the nudging towards ECMWF analyses...
The nudging of temperature towards ECMWF analysis prevents the model calculations from diverging from the true atmospheric state. As opposed to a free-running purely prognostic model calculations, the nudging constrains the dynamics towards the true atmospheric state, and the resulting fields are considered better valid than a purely prognostic model run. However, the use of a pure CTM is not favorable either (see reply to the review by von Hobe for details). We think that nudging is an appropriate compromise between the two extremes 'free running GCCM' and 'CTM'. The weight of ERA-40 data is 100% up to 18 km and 0% above 1 hPa. The relaxation term used in between will be referenced in the revised paper, where their validity has been demonstrated.

The large model underestimation of lower stratospheric HOCl and ClO is attributed...
A description and critical discussion of the PSC scheme in KASIMA will be added. However, since PSCs often occur at sub-synoptic scales, particularly when triggered by orographic wave activity as in this particular year, it is not astonishing that modeling of PSCs sometimes fails. The model resolution of about 2.8 degrees KASIMA is only able to resolve synoptic scale PSC fields and not such small scale structures.

Specific comments Abstract, p. 18968, lines 68211;9: this sentence is too long...
This sentence will be split.

- Abstract, p. 18968, line 20: the words "comparison with a model run...
This sentence will be rewritten.

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- Introduction, p. 18969, reactions (R8) and (R9): since these are heterogeneous reactions...
This information will be included as suggested.

- Introduction, p. 18969, line 14: "there do not exist...
Not clear what's wrong here.

- MIPAS measurements, p. 18971, lines 25-26: 8220;For definition of the vortex edge...
This information will be included.

...I recommend plotting maps of the vortex edge at 1000K and 475K...
Such plots will be provided.

The first time series plots (figure 3) should also include the number of MIPAS profiles used per day...
We consider this redundant, because the newly included figures include this information, and since the number of observations has already gone into the estimated standard errors in the time series figures.

- MIPAS measurements, p. 18972, line 7: "HOCl, ClO and ClONO2 mean values ... ".This should also include HNO4.
This will be corrected.

- Model calculations, p. 18972, line 17: "A horizontal resolution of T21...
We have used T42. T21 is a typo which will be corrected for the revised version. T42

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resolution is pretty standard for this type of global modeling studies.

- Model calculations, p. 18973: ... description about the parameterization (or micro-physical modelling?) used for the abundance of PSCs...
This information will be included (including relevant references).

- Model calculations, p. 18973, line 7: the chemical rate constants use an outdated version...
We do not expect major changes in the results presented here. More details on this issue are discussed in our reply to reviewer Marc von Hobe.

The dates chosen for the reinitialisation (beginning of the observation period) ...
The choice for the reinitialization date indeed is driven by the availability of MIPAS measurements. What we aim at is to see the short term divergence of the model results from the observations. Comparison of free-running and re-initialized model results did not show any suspicious features which might hint at specific re-initialization related problems.

+ Finally, the effect of this reinitialisation does not appear on several time series plots...
The procedure of reinitialisation will be discussed in more detail in the revised paper. There are two explanations for the apparent contradiction between MIPAS and KASIMA on September 18, where one might expect equal mixing ratios from MIPAS and KASIMA:

1. The resampling is performend on a pressure grid, while the output data are shown on a potential temperature grid. Due to different temperature profiles in KASIMA and the MIPAS data set, this implies a shift in the vertical. $ClONO_2$ with its pronounced vertical vmr gradient is particularly sensitive to this.

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2. The data shown in the papers for September 18 are those resulting after one timestep of the model. Since total KASIMA ClO_x of the model is conserved (ClO is the only ClO_x component seen by MIPAS), the application of the family concept immediately redistributes the ClO_x components.

We will carefully investigate the impact of these issues on the model results and our conclusions and will include the findings in the revised version.

- Figure 2 is quite difficult to read...
This figure will be simplified as suggested.

- Figures 3 and 5: it is difficult to see the difference between the two model simulations...
We prefer not to change the colour coding between the figures, because this might lead to confusion. Instead we add information to the figure caption on which are the higher and which are the lower values. This should remove all related ambiguity.

- Figures 4 and 6: the disagreement between observations and model is obscured by the different vertical scale...
It is not the main purpose of these figures to highlight the disagreement between measurements and model results. This can be evaluated using Figs. 3 and 5. Thus we think the different scale is acceptable in Figures 4 and 6. Adjustment of the scale would make the the fluctuations in the left panels of the figures virtually invisible. This is why we decided not to change the figures.

For figure 4 at least this is not necessary...
We show the total sum of inorganic chlorine in figure 4 in order to demonstrate that the modelled subsidence inside the vortex is homogeneous leading to a nearly constant

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sum.

- Gas phase chemistry regime, p. 18975, lines 218211;28: the significance of...
The plotted error bars are the standard errors of the mean under the assumption of random sampling: standard error = standard deviation/$sqrt(N)$ where N is the sample size. In the case of irregular non-random sampling, positive correlations between individual sample points would reduce the degrees of freedom of the sample, i.e. the division by $sqrt(N)$ underestimates the standard error. However, the quantitative assessment of the standard error of an irregular sample would require the mean correlation coefficients between the sample points, which are not obviously accessible in a robust way. We do not deny the existence of the observed feature, but we deny that it is representative for the entire vortex. Further, even if the true error bars do not overlap, this is no evidence of significance: Since we expect that 68% of the distribution are covered by the error bars, we expect that error bars have to overlap in only about 2 out of 3 comparison pairs. Error bars in the remaining 1 out of 3 comparison pairs may be non-overlapping without indicating significance. χ^2 analysis would give further insight into this but we do not see the point of inclusion of exaggerated statistics in a context which has no impact on our major conclusions. Particularly th non-availability of the correlation information would render further statistics questionable.

The second argument can not be verified due to the lack of plot...
While we certainly are willing to present the sampling information in the revised paper, and will present related figures, there is no obvious way to infer the significance or insignificance from this.

My personal guess is that this day-to-day variability is real...
If the spike is driven by local small-scale phenomena and thus not representative for the vortex as a whole, this is exactly what 'insignificant' means in the context of a

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time series which shall represent the entire vortex. We do not deny that it might have existed an area of elevated mixing ratios, but our data do not provide evidence that this elevation was representative for the vortex. Again: T21 was a typo, the T42 resolution has been used. This is fine enough for vortex dynamics on synoptic scales but not to study subsynoptic processes.

- Gas phase chemistry regime, p. 18976, lines 108211;13: "While around 20 September modeled [HCl] strongly increases...
See above.

Heterogeneous chemistry regime, p. 18977, line 6: "No substantial diurnal variation was observed here"...
Yes, exactly. Of course there's some fluctuation, but nothing systematic. The text will be changed to make clear that MIPAS does not observe the full diurnal cycle.

- Heterogeneous chemistry regime, p. 18978, lines 8-18: the whole paragraph is unclear and should be re-written with a focus on the cause of the absence of heterogeneous chemistry in the model simulation. Here are some further questions raised by the text:

This part of the text will be rewritten. For detailed discussion, see below.

+ "no PSCs appear in the model run during the observation period" - but do any PSCs appear in the model run? If yes, until what date?
This information will be included.

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Höpfner et al., 2004, observe PSCs until 21 September . . . . + "the part of HOCl also reproduced by the model must have been generated from previously heterogeneously generated ClO" - but both species are supposed to have been reinitialised to MIPAS observations on 17 and 18 September?
We draw our conclusion from the development after 18 September.

+ Line 15: the reinitialization date is now reported as 16 September?
This is incorrect. The correct initialization dates are 17/18 September. This will be corrected.

+ Line 16: the necessity for the reinitialization procedure must be moved to the model description.
Agreed; will be moved ahead.

- Heterogeneous chemistry regime, p. 18978, lines 18-20:... speculation that the quantitative understanding of ClO dimer chemistry is insufficient...
We agree that ClO dimer chemistry is not necessary to explain the differences but we think that this additional uncertainty should at least be mentioned.

Interactive comment on Atmos. Chem. Phys. Discuss., 8, 18967, 2008.

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