BASCOE ASSIMILATION OF OZONE AND NITROGEN DIOXIDE OBSERVED BY MIPAS AND GOMOS: COMPARISON BETWEEN THE TWO SETS OF ANALYSES

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ABSTRACT

MIPAS (v4.61) and GOMOS (v6.0a) observations of O_3 and NO_2 have been assimilated separately by the Belgian Assimilation System of Chemical Observations from Envisat (BASCOE). In the first experiment, MIPAS observations have been assimilated from October 2002 to March 2004 (18 months) including also observations of HNO_3, N_2O, CH_4 and H_2O data. For the second experiment, which concerns GOMOS data, a reduced time period was considered, from mid–July to end of November 2003 (4.5 months) where only O_3 and NO_2 dark limb data are taken into account.

The agreement with respect to HALOE and POAM–III data is good. However, comparison between assimilated MIPAS ozone data and the BASCOE MIPAS analyses shows a significant bias of about +20% at 0.5 hPa. We find that this bias has to be attributed to MIPAS data (v4.61).

Key words: MIPAS; GOMOS; 4D-Var assimilation; BASCOE; ozone; nitrogen dioxide.

1. INTRODUCTION

The use of assimilation in satellites data validation is growing. Marchand et al. (2004) have assimilated GOMOS O_3 and NO_2 with a photochemical box model and compare NO_3 from GOMOS and the analyses. They found a good agreement (about 10%) which indicates that O_3, NO_2 and NO_3 GOMOS measurements are self consistent. Within the validation framework for MIPAS, Vigouroux et al. (2007) have compared MIPAS N2O and HNO3 with ground based FTIR measurements for 2003. They use a co-location criterion of 1,000 km around ground-based stations. In order to increase the number of co-locations, they also use MIPAS N_2O and HNO_3 analyses produced by BASCOE. This reduces the bias and standard deviation between FTIR and MIPAS.

The goals of this study are two–fold. First, we would like to evaluate the ability of the BASCOE system to assimilate GOMOS O_3 and NO_2, and MIPAS NO_2; BASCOE MIPAS O_3 has been validated by the ASSET O3 intercomparison project (Geer et al., 2006). Second, we would like to extract information from these analyses in order to contribute to the validation of GOMOS and MIPAS data.

The paper is organized as follows. Sections two, three and four describes, respectively, the BASCOE system, the data used in this study and the set–up of the assimilation experiments. Sections five and six discuss the results obtained by the O_3 and NO_2 analyses, respectively. The paper closes with conclusions.

2. BASCOE SYSTEM

The Belgian Assimilation System of Chemical Observations from ENVISAT (BASCOE, http://www.bascoe.oma.be) is a 4D-Var assimilation system descended from that described in Errera and Fonteyn (2001). A study of the 2003 Antarctic winter using one version of the BASCOE CTM has been discussed by Daerden et al. (2006).

The model includes 57 chemical species with a full description of stratospheric chemistry. All chemical species are advected using the Flux Form Semi Lagrangien scheme (FFSL) (Lin and Rood, 1996) with a time step of 1800 seconds and interact through 143 gas-phase reactions, 48 photolysis reactions and 9 heterogeneous reactions. The system of chemical differential equations is built using a Kinetic PreProcessor (Damian et al., 2002) and is integrated by a three-order Rosenbrock solver. The reaction rates and cross sections are all listed in the JPL 2003 compilation (Sander et al., 2003). Surface area density of Polar Stratospheric Clouds (PSC) and the loss of HNO_3 and H_2O by PSC sedimentation are calculated by a parameterization described in (Vigouroux et al., 2007). The CTM is driven by ECMWF operational analyses of winds and temperatures, and uses a subset of 37 of the ECMWF model levels, from the surface to 0.1 hPa, on a 5° longitude by 3.75° latitude grid. The model grid type is the so called Arakawa C type (Kalnay, 2003). In this configuration, wind field components are defined on the edges of the model grid points.

Data assimilation is done using 4D-Var (Talagrand and Courtier, 1987). Its technical implementation, including how the adjoint is built and how the minimization is

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achieved, is discussed in Errera and Fonteyn (2001) and Vigouroux et al. (2007).

3. OBSERVATIONS

Four sets of data are used in this study: MIPAS and GOMOS data are assimilated while independent data sets from HALOE and POAM–III are used for a posteriori analyses evaluation. For this latter purpose, HALOE and POAM–III will be monitored by BASCOE. In this procedure, BASCOE will look for any observations of these two instruments at each model time step. If any profile is found, the BASCOE state is interpolated spatially to the data location and saved into a file. Using this method, the maximum time shift between data and model values is 15 minutes. This is an important detail especially for NO_2 evaluation, considering the diurnal cycle of this species.

Assimilated observations from MIPAS, onbord ENVISAT, are O_3, HNO_3, H_2O, NO_2, N_2O and CH_4. Usually there are around 1000 MIPAS profiles available per day. Each species are assimilated together without any distinction of day or night data. Eighteen months of data have been assimilated from Oct. 2002 to Nov. 2003 (version 4.61) and from Dec. 2003 to Mar. 2004 (version 4.62[1]). Both ozone (v4.61 and v4.62) and nitrogen dioxide (v4.61) have been validated for scientific applications. Between 1 to 50 hPa, the ozone bias with correlative data is lower than 10%; it increases to 25% at 100 hPa; and at pressures below 1 hPa, the number of correlative data is too small to derive quantitative conclusions (Cortesi et al., 2007). In the lower and middle stratosphere (below 45 km), the accuracy and precision of MIPAS NO_2 is about 10–20% and 5–15%, respectively (Wetzel et al., 2007).

GOMOS, onboard ENVISAT, is a stellar occultation instrument that retrieves vertical distribution of O_3, NO_2, NO_3, OClO, BrO, air number density and aerosol extinction vertical profiles. In dark limb mode, GOMOS provides around 200 profiles per day. Only O_3 and NO_2 (version 6.0f) have been assimilated, from mid–July to end of November. Intercomparison of ozone with correlative observations has shown a good agreement, with biases in the range [2.5, 7.5]% between 14 to 64 km (Meijer et al., 2004). In a first attempt at comparing GOMOS NO_2 and ACE-FTS correlative data, Fussen et al. (2005) found considerable differences between both data sets. This is in contradiction with results obtained by Marchand et al. (2004). Recent progress fortunately shows a better agreement between GOMOS and ACE, with biases lower than $\pm 10\%$ between 22 and 42 km (Didier Fussen, personal communication).

HALOE uses solar occultation to derive atmospheric constituent profiles of including O_3, NO and NO_2. About 15 sunset and sunrise occultations (30 altogether) are made every day. Each occultation mode covers a thin latitude band (a few degrees) during that time and global coverage is obtained in about one month. Version 19 of HALOE is used to validate our analyses. Intercomparison of ozone with correlative data shows good agreement usually within the instrumental errors between 0.03 to 100 hPa. Between 1 and 30 hPa, HALOE typically agrees within 5% (Brühl et al., 1996). The NO_2 measurements show mean differences with correlative measurements of about 10 to 15% over the middle stratosphere. The NO differences are similar in the middle stratosphere but sometimes show a negative bias (as much as 35%) between 30 and 60 km with some correlative measurements (Gordley et al., 1996). In this study, analyses of NO_x (NO+NO_2) will be compared to HALOE NO_x. This is done in order to reduce a possible large error at the terminator due to a maximum time shift of 15 minutes between analyses and observations.

POAM–III[2] is also a solar occultation photometer instrument which measures the chemical stratospheric constituents O_3 and NO_2 in the polar regions (Lucke et al., 1999). Here we use POAM version 4 data. POAM measures at most 15 profiles per day in each hemisphere. The latitude at which the profiles are taken varies slowly throughout the year, but remains in the polar regions. In Antarctic winter periods, the latitude varies smoothly between about 65°S (winter solstice) and about 87°S (equinox). On average, POAM O_3 profiles agree to within 5% with respect to correlative data from 13 to 60 km (Randall et al., 2003). On the other hand, comparison of POAM and HALOE has shows a good agreement, within 6% from 20 to 33 km and increasing up to 12% at 40 km (Randall et al., 2002).

4. SET–UP OF EXPERIMENTS

MIPAS assimilation is done with a background standard deviation set to 20% of the background volume mixing ratio, for each species. The GOMOS assimilation has a slightly different set–up. During day 1 (14–Jul–2003) to 5, we perform a free model run initialized by MIPAS analysis. The assimilation then starts with the background standard deviation set to 50% for 5 days of analyses. From then, the background standard deviation is reduced to 20%.

MIPAS and GOMOS data provided by ESA only include with their instrumental error. At the time we started to assimilate MIPAS (in 2002 for the NRT), the total errors (including the retrieval errors) were not available[3]. We then add a representativeness error of 8.5% to each observed species. This set–up is used for this study.

For such a long assimilation period as to one used in this study, data filtering has to be applied to avoid outlier observations entering the system. This is even more true when the assimilated data come from a research instrument. Observations are thus subjected to an Optimal Interpolation Quality Check (OIQC). This procedure compares the background field with the observations during

[1] Analyses using this later version will not be used in this study

[2] For brevity, we will drop the "III" in the following part of the paper

[3] The description of the MIPAS v4.61 errors can be found at http://www.atm.ox.ac.uk/group/mipas/err/

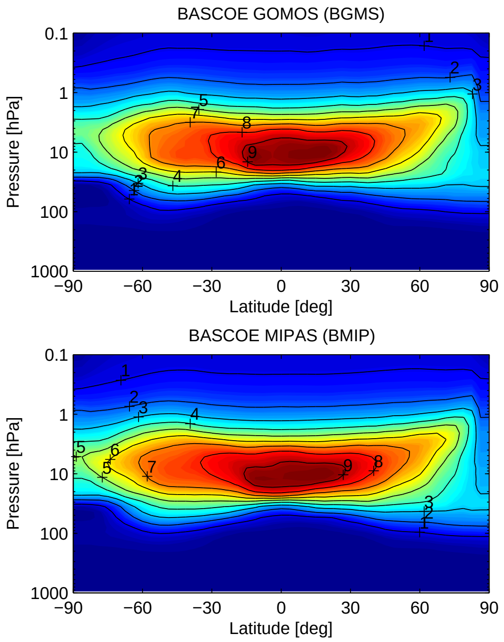

Figure 1. Zonal mean of ozone (ppmv) on Sep. 30, 2003, at 12UT from GOMOS (top) and MIPAS analyses (bottom).

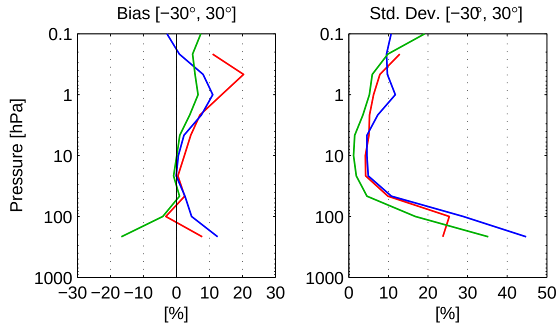

Figure 2. Bias and standard deviations for ozone between MIPAS and BMIP (red line), GOMOS and BGMS (blue line), and HALOE and BHAL (green line). Results obtained from BMIP and BGMS are an average over three months (Sep. to Nov. 2003) while results obtained from BHAL are an average over 19 days.

the first model integration. If the departure between the data and the background is greater than 3 times the background error, the data are rejected. We will see later on the implications this has on the analyses.

In the following sections, BASCOE MIPAS analyses and BASCOE GOMOS analyses will be denoted by, respectively, BMIP and BGMS.

5. OZONE RESULTS

Figure 1 shows the ozone zonal mean at noon on Sep. 30, 2003 from BMIP and BGMS. Qualitatively, the agreement is excellent: the ozone maximum is very similar and both panels exhibit the same structure. This indicates a good agreement between ozone data from both instruments.

We found that, most of the time, the assimilated observations minus analyses statistics (OmA) are insignificantly biased for both BMIP and BGMS analyses (not shown). Only MIPAS-BMIP statistics show a significant bias up to 20% at 0.5 hPa (more details will be given below). Standart deviations are generaly lower than 10% in the middle stratosphere and increase to 20% at 100 hPa and above 1 hPa. This is within the observational error range (taking into account the representativeness error) and validate the set-up of the assimilation experiments.

Figure 3 shows the bias and standard deviations between both analyses with respect to independent data HALOE and POAM for an average over three months (Sep. to Nov. 2003), five latitude bands and 13 pressure ranges (3 pressures per decade). Statistics from BMIP and BGMS are very similar which, again, indicates a good agreement between ozone data from GOMOS and MIPAS. Except during the South Pole ozone hole, biases are lower than $\pm 10\%$. Standard deviations are almost lower than 10% between 1 to 50 hPa and increase to 20% at the lid of the model (0.1 hPa). At the tropopause, biases decrease (lower than -50%) and the standard deviations increase (higher than 50%) probably due to (1) the lack of tropospheric chemistry/physics in the BASCOE CTM, (2) the higher variability of the observations (assimilated and independent) and (3) the growth of instrumental errors when looking around and below the tropopause. It has been shown during the oral presentation that the ozone hole evolutions from both analyses are in reasonable agreement with POAM observations. In general, BMIP and BGMS overestimate POAM ozone by only around 0.15 and 0.1 ppmv, respectively, during October 2003 between 70 and 150 hPa.

To conclude this section, we would like to come back to the bias between assimilated MIPAS data and BMIP around 0.5 hPa, mentioned earlier (see Figure 2). The +20% bias between MIPAS and BMIP around 0.5 hPa is much higher than the bias between GOMOS and BGMS. The latter one being maximum at 1 hPa with a value of +10% which is within the total error (instrumental and representativeness). This is not the case for MIPAS-BMIP comparison, with the MIPAS error being around 10%[3]. We must then realize that the ozone chemistry of the BASCOE CTM is in disagreement with ozone provided by MIPAS v4.61. In addition to GOMOS and MIPAS ozone data, BASCOE has assimilated HALOE from 18 November to 6 December when both sunset and sunrise observations covered the Tropics. The goal of this experiment (BHAL) was to evaluate how BASCOE CTM and HALOE ozone data compare. The results, shown on Figure 2, are excellent; the bias between HALOE and BHAL is below [0, +7]% between 0.1 and 100 hPa. Therefore, we suggest a positive significant bias in MIPAS v4.61 around 0.5 hPa.

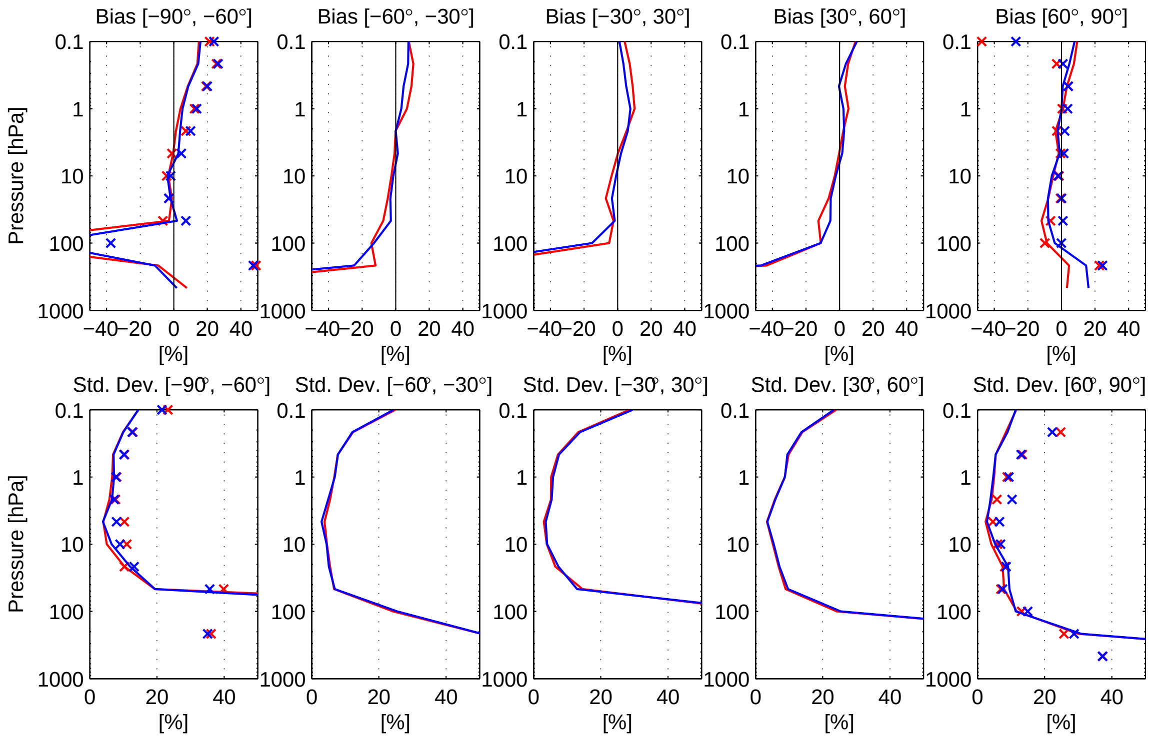

Figure 3. Bias and standard deviations for ozone between HALOE and BMIP (solid red line), HALOE and BGMS (solid blue line), POAM-III and BMIP (red cross), and POAM-III and BGMS (blue cross). This is an average over 3 months (Sep. to Nov. 2003).

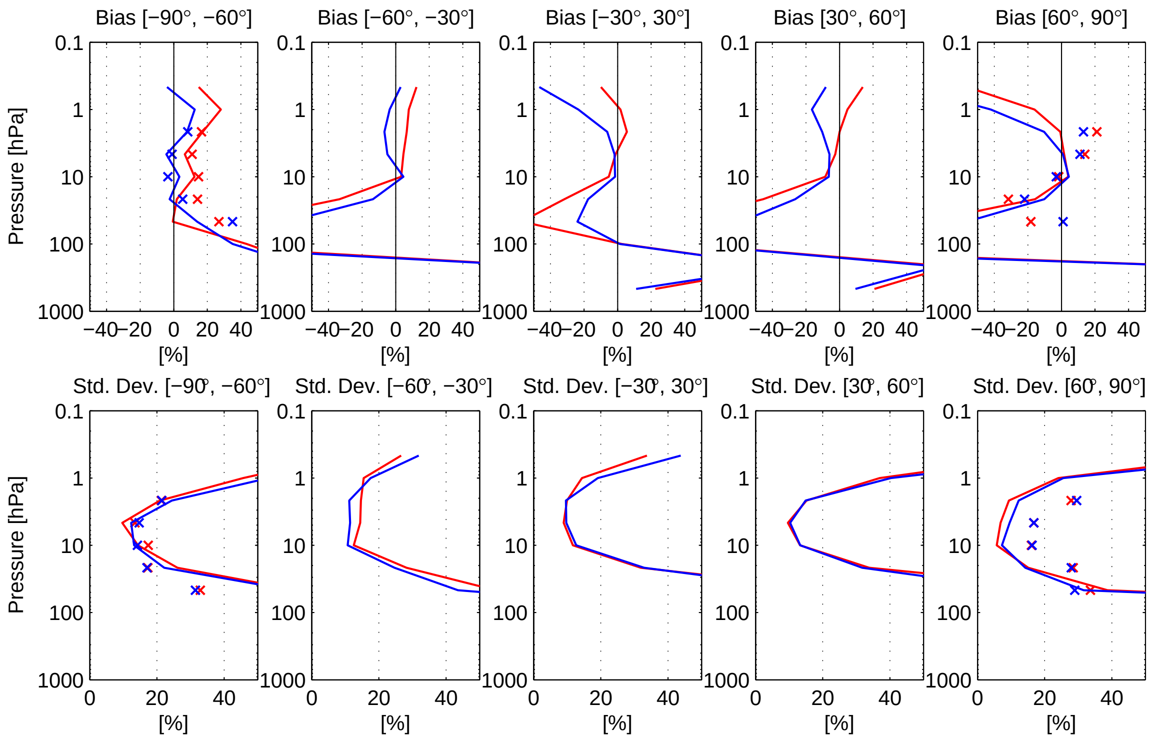

Figure 4. As Fig. 3 for NO_2 in the case of comparison with POAM-III and NO_x in the case of comparison with HALOE. For comparison with POAM-III, the average is done for the Oct. 2003 in order avoid period of stratospheric perturbation.

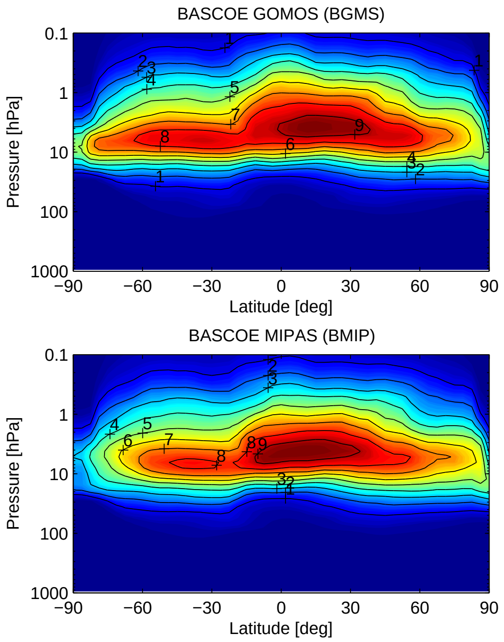

Figure 5. Zonal mean of the nitrogen dioxide (ppbv) on 30-Sep-2003 at 12UT from GOMOS and MIPAS analyses.

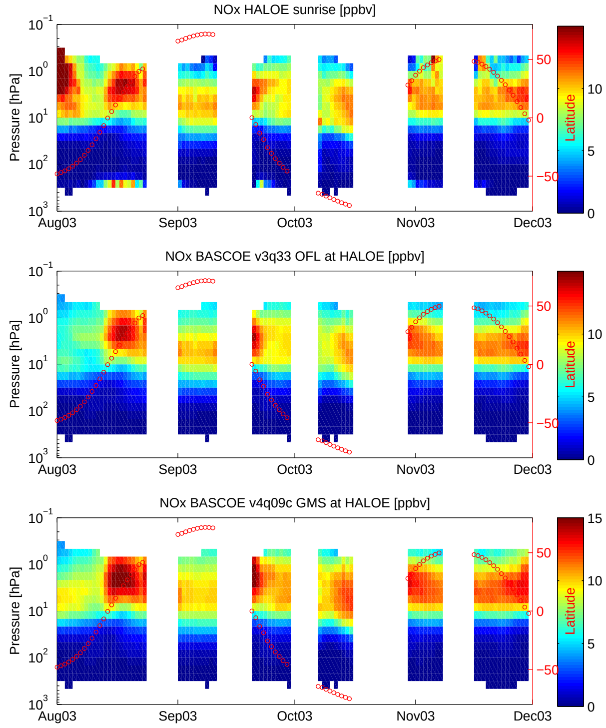

Figure 6. Top: time series of HALOE sunrise observations of NO_x *from August to November 2003. Middle: BASCOE MIPAS monitoring of HALOE. Bottom: BASCOE GOMOS monitoring of HALOE. The red circles indicate the daily mean latitude of HALOE sunrise occultations (right axis).*

6. NITROGEN DIOXIDE RESULTS

Figure 5 shows the NO_2 zonal mean at noon on Sep. 30, 2003 from BMIP and BGMS. The agreement between both panels is very good although we can see some differences (unlike for the ozone case in Figure 1). The main differences occur south of 60°S around 10 hPa, where BGMS is higher than BMIP.

Regarding the OmA differences, we found (not shown) that the best agreement is found between 1 to 10 hPa, around the NO_2 vmr maximum. In this region, biases are lower than $\pm 10\%$ for both analyses.

Figure 6 shows a time series of HALOE sunrise observations of NO_x from August to November 2003. The corresponding analyses BMIP and BGMS obtained by the monitoring of HALOE are also shown. From mid–August to December, the observed NO_x vmr are well reproduced by the analyses. Before this time period, high values observed by HALOE, due to the production of NO_x in the mesosphere and transported downward into the polar stratosphere (Funke et al., 2005) are not well reproduced by the analyses. This is because the OIQC filter rejects these data, and the NO_x intrusion from the mesosphere is not modelled by the BASCOE CTM. This suggests we need to improve our data filter, filter the data off–line and/or take into acount the mesospheric NO_x production in our model. BMIP shows values of unperturbed stratosphere (≈ 5 ppmv) during that period/region. Values estimated by BGMS are higher ($\approx$ 10 ppmv) but still very different from HALOE. These differences are due to the different set-up of both experiments. As mentioned earlier, the first five assimilation days of GOMOS are done with a background error of 50%, allowing BGMS to assimilate “perturbed” NO_2 data.

Figure 4 shows the bias and standard deviations between both analyses and HALOE and POAM. Statistics with respect to HALOE are done from Sep. to Nov. 2003 (three months) and for NO_x instead of NO_2. For statistics with respect to POAM, we focus on the October 2003, during a period of unperturbed stratospheric NO_x. Around the NO_2 maximum, between 1 and 10 hPa, the biases are within ±10% and the standard deviations are almost lower than 20% (being around 10% at the NO_2 maximum). This is in agreement with the instrument errors. In other altitude regions, especially below 10 hPa, biases and variability increase. The amount of NO_2 being much lower in these regions, the instrument signal to noise ratio decreases and the instrumental error increases. It is thus difficult to make any conclusions in these regions

7. CONCLUSIONS

This study has presented two assimilation experiments of O_3 and NO_2 by the BASCOE system: one used MIPAS v4.61, the other used GOMOS v6.0f. The analyses are evaluated by data monitoring of HALOE and POAM–III. With respect to these instruments, MIPAS and GOMOS analyses exhibit a bias of less than 10% in the high and middle stratosphere. On the other hand, around 0.5 hPa, MIPAS assimilated data and MIPAS analyses are significantly biased (+20%), showing an incompatibility between ozone observed by MIPAS and modelled ozone by the BASCOE CTM. Since no disagrement is found between BASCOE and the other ozone assimilated data (HALOE and GOMOS), this indicates a bias in MIPAS ozone data (v4.61).

Comparison of NO_2 analyses with independent data is good between 1 and 10 hPa, around the NO_2 maximum volume mixing ratio. Comparison with HALOE NO_x shows a bias below 15% while comparison with POAM–III during unperturbed stratospheric conditions shows a bias lower than 20% (for both set of analyses). Data filtering used by BASCOE to avoid outliers entering the system prevents the assimilation of Polar NO_2 data during stratospheric perturbation by Solar Proton Events or by mesospheric prodution of NO_x. This suggests a need to improve our data filtering method and/or to model these NO_x sources.

Overall, few differences are found between MIPAS and GOMOS data, suggesting a general good agreement between O_3 and NO_2 retrieval from both instruments.

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