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Assimilation of ozone data from the Michelson Interferometer for Passive Atmospheric Sounding

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SUMMARY

Global ozone profiles from the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) were added to an assimilation system that includes ozone data from the Solar Backscatter Ultraviolet/2 (SBUV/2) instrument. Substantial impacts were found and investigated. MIPAS ozone profiles have a vertical resolution close to 3 km, retrieved from infrared limb emission radiances, with a height-dependent error of 4–8%; they were used over 12 layers, spanning between 60–80 hPa and 0.15–0.25 hPa. As a research instrument, MIPAS provides variable coverage from day to day, with occasional data gaps of several days. The operational SBUV/2 data give regular temporal coverage in sunlit areas, yielding total columns and partial profiles, assimilated for Umkehr layers 3 (126–63 hPa) to 12 (<0.25 hPa), with errors comparable to MIPAS near the ozone maximum but increasing substantially at higher and lower levels. The higher accuracy of MIPAS data leads to substantial improvements in the assimilated ozone below the ozone maximum when compared to accurate *in situ* (ozonesonde) and space-based (occultation) data; vertical gradients in the lower stratosphere are improved. In the Arctic winter of 2002/03, the ability of MIPAS to sample the vortex interior leads to substantial beneficial impacts. In the tropics, assimilation of MIPAS profiles improves analyses in the lower stratosphere and provides substantially better agreement with occultation data in the middle stratosphere, near the ozone maximum. This offsets an underestimate in the SBUV-only analyses caused by transport errors in the forecast. The global improvements in the assimilation lead to local improvements when compared against individual measured ozone profiles, where vertical structures are determined by height dependence in horizontal advection from diverse regions. The spatio-temporal variability in the assimilation is more realistic when MIPAS data are included. Experiments to examine the impacts of temporal gaps in the MIPAS data reveal a 'memory' of 5–10 days in the transport-dominated lower stratosphere. In the middle stratosphere, the impact of missing MIPAS data is more complex; transport errors cause a large initial impact followed by ozone values typical of SBUV assimilation.

KEYWORDS: Global model Limb sounder Lower stratosphere

1. INTRODUCTION

Middle atmospheric ozone plays major roles in the terrestrial radiation balance and in shielding the surface from ultraviolet radiation. This motivates efforts to monitor ozone through the production and analysis of global time-dependent fields. With only a sparse ground-based observational network, it is left to space-borne sensors to provide near-global coverage. Such sensors provide good information on the distribution of total ozone and on some aspects of the vertical profile. The satellite data are well suited for producing global three-dimensional (3D) ozone distributions using various mapping techniques. Data assimilation is a method that provides both spatial mapping and a consistent temporal evolution of the ozone distribution.

Sequential data assimilation combines a short-term model forecast with observations using statistical analysis, according to error characteristics of the data and the forecast (e.g. Stajner *et al.* 2001). Geophysically realistic temporal evolution of ozone is provided by the underlying chemistry and transport model (CTM), which is used to generate the forecasts. This approach can be used to produce sequences of 3D ozone

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fields that rely heavily on observations from multiple instruments with various viewing geometries.

The nadir-viewing Solar Backscatter UltraViolet/2 (SBUV/2) instrument provides limited information on the stratospheric ozone profile (Miller *et al.* 1997), including a partial-column estimate for a deep layer below the ozone maximum. This limits the utility of such data for studies of the radiative forcing of climate, which is sensitive to the lower-stratospheric ozone profile (e.g. Hansen *et al.* 1997). Nevertheless, the demonstrated accuracy of these profiles in the middle and upper stratosphere (Bhartia *et al.* 1996) and their operational availability have motivated their use in assimilation systems. The profile information from SBUV/2 alongside total-column data facilitates attempts to produce 3D global fields with high temporal resolution (e.g. Stajner *et al.* 2001; Stajner *et al.* 2004).

Limb sounding of infrared or microwave emissions provides more detailed daytime and night-time profiles. Ozone data from the Microwave Limb Sounder (MLS) on the Upper Atmosphere Research Satellite were assimilated into middle atmospheric models (Levelt *et al.* 1998; Khattatov *et al.* 2000) and also combined in assimilation with Global Ozone Monitoring Experiment (GOME) data (Struthers *et al.* 2002). The latter study showed that including MLS profiles adds information to the GOME total-column data, by improving the separation between tropospheric and stratospheric ozone.

The Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) (Endemann *et al.* 2000; Nett *et al.* 2001), on board the European Space Agency's Environmental Satellite (Envisat) launched in March 2002, is an infrared limb sounder. Retrievals extend down to cloud top, with a vertical resolution of about 3 km. This study evaluates the impact of adding the MIPAS data to the assimilation system described by Stajner *et al.* (2004). MIPAS data are assimilated in combination with the SBUV/2 total ozone data, with and without the use of SBUV/2 profile information. The impacts are evaluated using independent ozonesonde and solar occultation data. This study demonstrates improvements to the lower stratospheric ozone profile in the assimilated product, as a prelude to some detailed scientific applications of this product.

Of the aforementioned studies, this work bears the closest relationship to that of Struthers *et al.* (2002), where MLS was the only source of ozone profile data. Stajner and Wargan (2004) assimilated profile data from two instruments. They showed that the addition of data from the Polar Ozone and Aerosol Measurement III (POAM III) instrument, which measures at high latitudes, significantly improves the quality of lower-stratospheric assimilated ozone over Antarctica in the winter compared to SBUV/2-only assimilation. The wider range of latitudes observed by MIPAS allows investigation of the global stratospheric impact on the assimilation in this study. The focus is on the interplay among MIPAS data, SBUV/2 data and the evolution provided by the CTM within the assimilation system. Specific questions to be asked are:

(i) How substantial are the improvements in the global analyses when MIPAS data are added to the assimilation?

(ii) How does information from the MIPAS and SBUV/2 datasets combine in the analyses, and what do we learn about the error characteristics assigned to the two data types and the model?

(iii) How does the assimilation system respond to temporal voids in the MIPAS data?

The experiments were performed for December 2002 and January 2003 in order to study the impact of MIPAS data in the northern polar night.

An overview of the ozone assimilation system used in this work is given in section 2, followed by a brief overview of the SBUV/2 data in section 3. A description and validation of the MIPAS data are then given in section 4. Section 5 gives a detailed analysis of the global and regional impacts of adding MIPAS data to the assimilation system, with additional examination of synoptic structures in section 6. The impacts of temporal gaps in the MIPAS data record are examined in section 7. Some effects of changing the selection of data on the quality of the lower-stratospheric assimilated ozone profiles are shown in section 8. Finally, a closing discussion and summary are given in section 9.

2. Assimilation system

In the ozone assimilation system (Stajner *et al.* 2001), 15-minute forecasts generated by a CTM with parametrized ozone chemistry are blended with observations. The Physical-space Statistical Analysis System with specified forecast error covariances is used (Cohn *et al.* 1998). Forecast error variances are modelled as being proportional to the ozone field. Vertical forecast-error correlations are non-zero for up to five model levels above and below any given model level. Horizontal forecast-error correlations are modelled using a second-order autocorrelation function on a cylindrical surface, which provides longer length-scales in the zonal than in the meridional direction, especially in the tropics. Further details about the error covariance models are given by Stajner *et al.* 2001. Here we use a horizontal length-scale of 500 km, as in previous assimilation of SBUV/2 total ozone columns and profiles (Stajner *et al.* 2004). For this study, the system was modified to ingest MIPAS profiles either with or without SBUV/2 profiles; in either case the SBUV/2 total-column data were used.

The CTM is based on the flux-form semi-Lagrangian transport scheme (Lin and Rood 1996), using a horizontal resolution of $2.5° \times 2°$ (longitude by latitude) with 29 levels, which follow the terrain near the surface and transition to pure pressure by 161 hPa for the top 20 levels. This configuration sets a clear focus on middle atmospheric ozone, since the resolution is inadequate for detailed tropospheric study. As in Stajner *et al.* (2004), a simple ozone chemistry scheme is included, adapted from Fleming *et al.* (2001). Time-averaged (in this case, 12-hour mean) winds from the Goddard Earth Observing System, version 4, (GEOS-4) meteorological assimilation are used to drive the CTM.

3. SBUV data

A series of SBUV/2 sensors on the National Oceanographic and Atmospheric Administration (NOAA) satellites has provided ozone profiles and total columns in near-real time. The present study uses version 6 data from the NOAA-16 SBUV/2 instrument, with profile information provided in 5 km thick layers in the middle and upper stratosphere. The NOAA-16 platform is in a sun-synchronous orbit with equatorial crossing time 1430. The nadir-sounding SBUV/2 instrument has a 250 km $\times$ 250 km footprint.

The SBUV/2 total columns and partial columns for Umkehr layers 3 (126.66–63.33 hPa) to 12 (for pressure less than 0.25 hPa) are included in the assimilation, as in Stajner *et al.* (2004). This choice of levels is guided by the validation of the data, in studies such as Bhartia *et al.* (1996), with appropriately chosen error specifications (Stajner *et al.* 2001).

4. MIPAS DATA

MIPAS is an infrared Fourier spectrometer, measuring mid-infrared radiance (4.15–14.6 μm) at high spectral resolution of 0.035 cm^{-1} (Endemann *et al.* 2000). The space-borne instrument was developed from the balloon MIPAS-B (Fischer 1992) and the aircraft-borne MIPAS-FT instruments (Gulde *et al.* 1994), which demonstrated the feasibility of the spectral measurements and retrievals for a number of trace gases, including ozone. The Envisat platform completes about 14 orbits per day at a 98.55° inclination with a descending-node mean local solar time of 1000. In the nominal mode, consecutive scans of the Envisat MIPAS instrument are separated by the horizontal distance of 530 km along the orbit track. The limb-viewing geometry of MIPAS allows high-precision vertical scans with a vertical resolution of 3 km and a horizontal resolution of 30 km across the line of sight (Endemann *et al.* 2000).

Level 2 (version 4.53) along-track products are used in this work. The assimilation includes the retrieved tangent-level pressures and ozone volume mixing ratios. The retrieval algorithm, which relies on horizontal homogeneity, is described by Ridolfi *et al.* (2000).

(*a*) *Comparisons with other observations*

Migliorini *et al.* (2004) compared MIPAS ozone data with sondes in winter 2002/03. In the middle and lower stratosphere (above about 18 km altitude, i.e. for MIPAS levels 12 or less) they found that MIPAS profiles agree with ozonesondes within the theoretical MIPAS accuracy, with no significant biases.

This study uses two sources of independent ozone data for direct comparisons with MIPAS ozone profiles: the Halogen Occultation Experiment (HALOE) (Bruhl *et al.* 1996) and the POAM III instrument (Randall *et al.* 2003). Both instruments make solar occultation measurements, yielding accurate (well-calibrated) profiles with high vertical resolution at a limited number of latitudes. For the comparisons, separations of less than 4° longitude, 2° latitude, and 24 hours are used as a compromise between strict collocations and the need to obtain an adequate number of samples; this is also consistent with the horizontal averaging inherent to limb-viewing instruments. For December 2002, this gives 79 HALOE–MIPAS and 31 POAM–MIPAS profile pairs for comparison. Each HALOE, POAM and MIPAS profile was interpolated linearly in log pressure to a set of standard pressure levels (1, 2, 3, 5, 7, 10, 20, 30, 40, 50, 70, and 100 hPa).

Most collocated MIPAS and HALOE profiles are in northern middle latitudes. The mean ozone profiles agree within 1 mPa (Fig. 1(a)). The relative differences between MIPAS and HALOE mean ozone are under 4% for pressures between 2 and 7 hPa, and increase outside that pressure range to over 11% at 0.4 hPa and over 7% at 50 hPa. The relative r.m.s. differences range between 8% and 10% in the middle and upper stratosphere (1–40 hPa), increase to about 15% at 0.4 and 50 hPa, and further increase to over 20% in the lower stratosphere (70 and 100 hPa). The reported HALOE errors at 100 hPa often exceed 50%. We used only those HALOE data with errors lower than 20%.

The collocated pairs of MIPAS and POAM profiles are in northern high latitudes. The mean MIPAS and POAM profiles agree to better than 1.5 mPa (Fig. 1(b)) with the closest agreement of 1% in mid-stratosphere between 10 and 20 hPa. At pressures lower than 1 hPa, the MIPAS mean is more than 2% lower than that of POAM. The MIPAS mean exceeds the POAM mean by up to 9% at pressures higher than 20 hPa. The relative r.m.s. difference between the two instruments is between 7% (at 30 hPa) and 18%

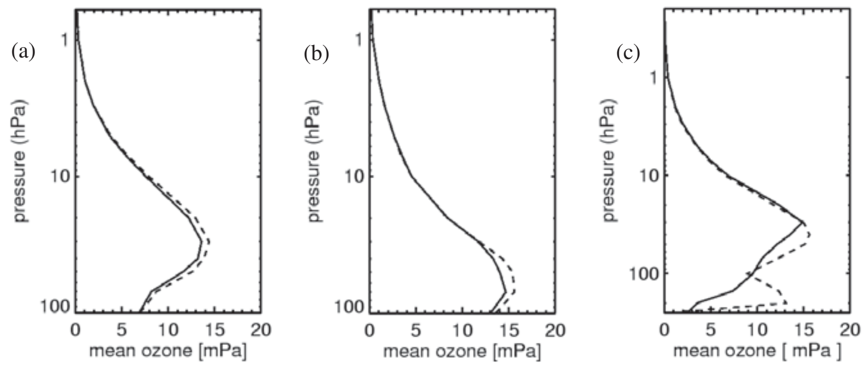

Figure 1. Comparison of the mean of coincident (see text for tolerance) MIPAS ozone profiles (dashed) in December 2002 against (a) HALOE data, 25°–48°N (79 profiles), (b) POAM data, 63.5°–64.5°N (31 profiles), and (c) SBUV assimilation, 30°–60°N (2075 profiles). Note that the vertical range on (c) is greater than on the other two panels.

(at 0.4 hPa). Note that random retrieval errors that are reported in POAM data have typical values around 5% throughout most of the stratosphere.

(*b*) *Comparisons with SBUV/2 analyses*

Global 3D ozone fields from the control experiment that used SBUV/2 data (SBUV assimilation) allow comparisons of all MIPAS profiles with tightly collocated assimilated ozone profiles. Comparisons using a large number of profiles can rapidly provide robust estimates of the differences, while simultaneously resolving the underlying geophysical variability. This type of monitoring is typically done before the assimilation of a new dataset, in order to examine the global structure of bias and typical differences from the existing analyses, which will require careful attention in the assimilation process.

Comparison of MIPAS profiles with nearest profiles from the SBUV assimilation is shown in Fig. 1(c). MIPAS profiles were interpolated linearly in log pressure to the analysis pressure levels. In the latitude band 30°–60°N, where there is good coverage by both instruments, this comparison includes 2075 profile pairs in December 2002. At 150 and 200 hPa, the cloud contamination of MIPAS data is evident as a large bias. This motivated the exclusion of MIPAS data for pressures higher than approximately 70 hPa in this study. (Note that a later version (4.61) of the retrieval algorithm uses a new cloud filtering scheme.) In the upper stratosphere and mesosphere (pressure lower than 2 hPa), there is excellent agreement between the MIPAS data and the analysis. Between 100 hPa and about 40 hPa, the MIPAS data are higher than the SBUV/2 analyses. This is a region with strong vertical ozone gradients which are not resolved by the thick SBUV/2 layers. In this region there is low confidence in the fidelity of the SBUV/2 data (Bhartia *et al.* 1996) and, given a better agreement of MIPAS with HALOE data in this altitude range, this discrepancy is indicative of the poor quality of ozone from assimilation of SBUV/2 data. In the middle stratosphere, MIPAS data are biased low relative to the SBUV/2 analyses in the northern middle latitudes.

(*c*) *Data coverage and error specifications*

Complementary coverage of SBUV/2 and MIPAS partially motivated the choice of December 2002 and January 2003 as the time period for the study. Infrared MIPAS measurements are made on sunlit and dark sides of the earth, while SBUV/2 provides daytime-only data. Additionally, MIPAS data are available in the polar night, and

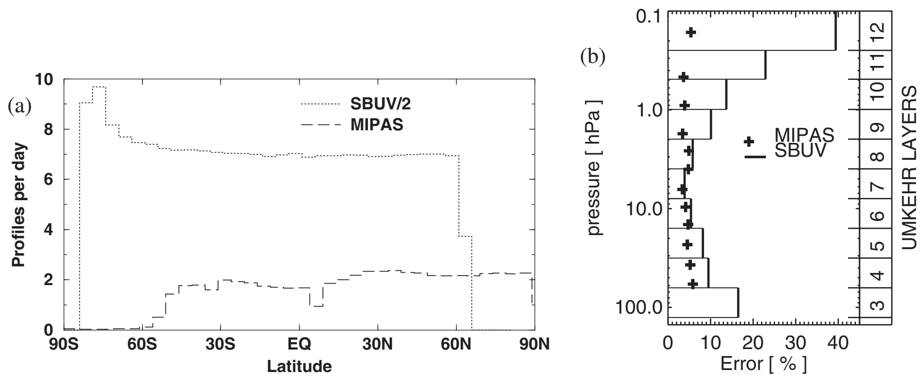

Figure 2. (a) Average daily number of MIPAS (dashed) and SBUV/2 (dotted) profiles per 1° latitude. (b) Typical profiles of error standard deviations that are used in assimilation of MIPAS (crosses) and SBUV/2 (solid line) data, with Umkehr layers 3–12 marked on the right axis.

SBUV/2 data are available in the southern (summer) hemisphere, where MIPAS data density is low (Fig. 2(a)). Although MIPAS provides global coverage, the retrievals available for this study include profiles between 60°S and 90°N. Note that MIPAS observations were missing on 14 December and 15, 18, and 19 January. The SBUV/2 data were available for all days except 1 January.

The MIPAS data were included in the assimilation using an observation operator that interpolates model values horizontally and vertically to MIPAS locations. Note that model values represent grid box means, rather than point values, at a resolution that is comparable to that of MIPAS. The MIPAS error standard deviations are specified for each profile from the random error covariance matrices provided with the retrievals. For example, MIPAS errors for 46°N on 20 December 2002 vary slightly with pressure between about 3% and 6% (Fig. 2(b)). The off-diagonal (covariance) components were not used, meaning that vertical correlations of errors are neglected. Note that limb-sounding retrieval errors for neighbouring levels tend to be anticorrelated, with correlation coefficients ranging from −0.2 to −0.8. It is also assumed that errors for different profiles are uncorrelated. The SBUV/2 error standard deviations are modelled as the lowest in the upper stratosphere and increase towards the top and the bottom of the profile (Stajner *et al.* 2001). Regardless of the data combination being used, the observation and forecast error covariance models were not changed.

5. Impacts of assimilating MIPAS data

In this section, the results of assimilating MIPAS data alongside SBUV/2 data are discussed, focusing on different regions of the atmosphere. The control SBUV assimilation ran from 30 November 2002 to 31 January 2003. The main perturbation experiment (SBUV + MIPAS assimilation) includes the same SBUV/2 data and MIPAS mixing ratios for levels 1 (with tangent pressures varying from 0.15–0.25 hPa) to 12 (60–80 hPa). This choice of levels was motivated largely by monitoring the MIPAS data against the SBUV/2 assimilation (section 4(b)). Because research instruments like MIPAS are subject to interruptions in the data supply, SBUV/2 profiles were included alongside MIPAS.

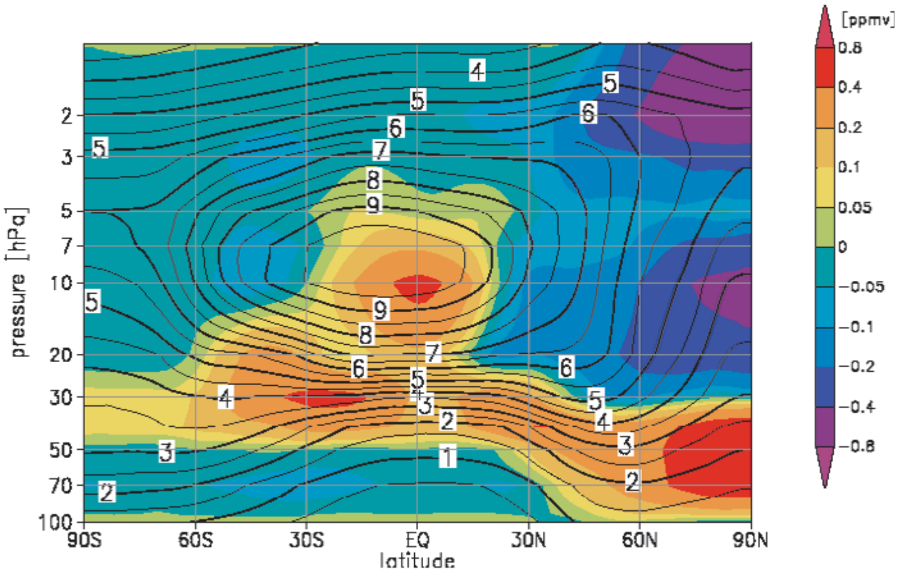

Figure 3. Monthly zonal-mean ozone for December 2002 in the SBUV assimilation (black contours with interval 0.5 ppmv). Colour shading shows the difference between SBUV + MIPAS and SBUV assimilations, with positive values indicating greater mixing ratio in SBUV + MIPAS. The shading interval increases with larger differences.

(*a*) *Impacts on the ozone distribution*

The impact of adding MIPAS data into the ozone assimilation is illustrated by zonal means in December 2002 (Fig. 3). Differences between SBUV + MIPAS and SBUV analyses are shown, along with the SBUV ozone analyses. Large impacts are seen at all levels in the polar night, below the ozone maximum at all latitudes, and near the ozone maximum in the tropics.

When interpreting Fig. 3, it is important to note that there are documented deficiencies in the SBUV assimilation (e.g. Stajner *et al.* 2001), that arise from both data limitations and problems with the transport model. The limited information on vertical structure available from SBUV-like instruments, especially the strong impact of the a priori used in the retrievals (e.g. Bhartia *et al.* 1996), means that the analyses below the ozone peak are subject to only weak data constraints (Fig. 2(b)). In this region, ozone is long-lived, meaning that chronic biases in the transport will have a substantial impact on the assimilated product. Transport errors with various assimilated wind fields are documented by Schoeberl *et al.* (2003), Tan *et al.* (2004) and van Noije *et al.* (2004). In particular, Schoeberl *et al.* (2003) show that rapid vertical dispersive mixing results from noise in kinematic vertical velocities. Excessive horizontal mixing across the subtropics in the low stratosphere was isolated by Tan *et al.* (2004). Douglass *et al.* (2003) show corresponding transport deficiencies in a CTM driven by GEOS-4 analyses, with too little ozone simulated at the tropical maximum and excessive transport across the subtropical barrier. Given that MIPAS data offer stronger constraints on the assimilated ozone, the impacts summarized in Fig. 3 are not unexpected; in the next three subsections these are discussed for different latitude bands.

(*b*) *The polar night: 60°–90°N*

At high latitudes (60°–90°N) in winter, SBUV/2 provides very limited coverage (Fig. 2(a)) and the available measurements are made under unfavourable high solar

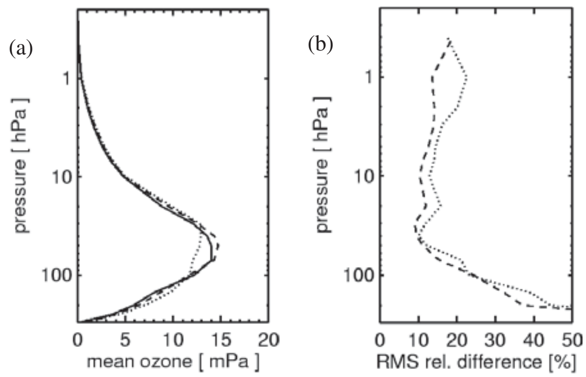

Figure 4. Comparison of the analyzed ozone mean profile against POAM data for December 2002 (300 profiles) and January 2003 (400 profiles), in the latitude band 63°–65°N: (a) mean ozone partial pressure from POAM (solid), SBUV assimilation (dotted), and SBUV + MIPAS assimilation (dashed), and (b) r.m.s. difference profiles for POAM minus SBUV assimilation (dotted) and POAM minus SBUV + MIPAS assimilation (dashed).

zenith angle conditions. Given that the polar vortex boundary typically lies close to 60°N and that transport across the vortex edge is limited, the inner vortex air is largely unconstrained by SBUV/2 data.

Ozone profiles from SBUV and SBUV + MIPAS assimilations have been compared to data from POAM III, which observes in the latitude band 63°–65°N (Fig. 4). In passing, we note that the mapping inherent in the assimilation allows comparisons with all POAM profiles (more than 300 in December), in contrast to only 31 collocated profiles used in the characterization of MIPAS data in Fig. 1(b). The comparison reveals a large improvement in the analyses when MIPAS data are included. The MIPAS data increase the mean ozone by up to about 2 mPa between 70 and 50 hPa, correcting the profile shape around the maximum partial pressure and causing a small overestimation. The reduction of ozone values between 100 and 200 hPa also contributes to improved representation of vertical ozone gradients in the lower stratosphere. Assimilation of MIPAS data reduces the r.m.s. differences between analysis and POAM III data and improves ozone profiles throughout the polar stratosphere (Fig. 4(b)).

Although sparse, ozonesonde observations are a valuable source of validation data, owing to their high vertical resolution and accuracy. Comparison of the two analyses with the mean profile calculated from ozonesonde measurements in the northern high latitudes in December and January (Fig. 5(a)) verifies that inclusion of MIPAS significantly improves the ozone analyses. Note in particular the reduction in the mean error from 4.9 to 0.24 mPa at 70 hPa, and the correction to the profile shape.

(*c*) *Northern midlatitudes: 30°–60°N*

Results from the monitoring of MIPAS data in the middle latitudes were discussed in section 4(b). Figure 3 reveals large impacts of the MIPAS assimilation in this latitude band, especially in the lower to middle stratosphere.

Profiles from ozonesondes and HALOE data were used to evaluate these middle latitudinal impacts. The mean sonde profile is shown in Fig. 5(b). The impacts of MIPAS are not as pronounced here as in the high latitudes but they reduce the mean analysis error from about 1.4 to 0.14 mPa at the 40 hPa pressure level. Comparison of the assimilations with HALOE profiles, for December and January in the latitude band 36°–47°N, are shown in Fig. 6. Differences in the profiles indicate that assimilation of

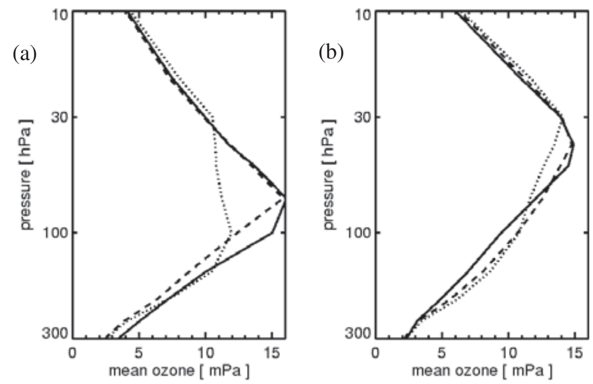

Figure 5. Comparison of mean assimilated ozone profiles (SBUV dotted and SBUV + MIPAS dashed) against mean sonde data (solid) between 300 and 10 hPa in December 2002 and January 2003: (a) 67 profiles 60°–90°N (44 from Canada and 23 from Norway), and (b) 122 profiles 30°–60°N (69 from Europe, 31 from North America, 20 from Japan, and 2 from the Middle East).

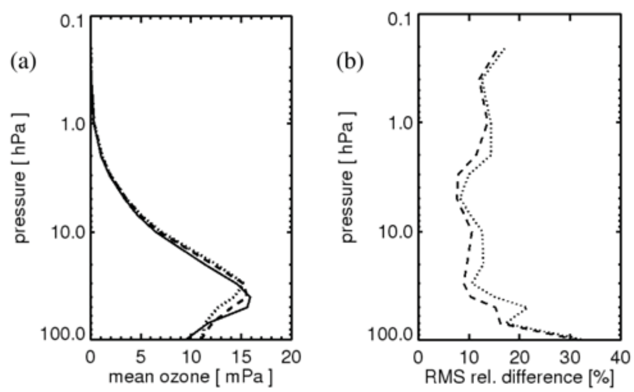

Figure 6. As Fig. 4, but comparison of SBUV (dotted) and SBUV + MIPAS (dashed) assimilations with collocated HALOE profile data (solid) for December 2002 (200 profiles) and January 2003 (139 profiles), in the latitude band 36°–47°N: (a) mean ozone partial pressure, and (b) r.m.s. difference.

MIPAS data indeed leads to improvement. In the middle and upper stratosphere, the improvements are modest, but at 50 hPa the MIPAS data reduce the bias in ozone partial pressure from 2.9 to 1.6 mPa. There is a corresponding decrease from 22% to 15% in the r.m.s. difference. Addition of MIPAS data to SBUV assimilation improves the comparisons with independent data for pressures lower than 100 hPa, but it has very little impact on regional statistics at 100 hPa.

(*d*) *The tropics: 30°S–30°N*

In the middle stratosphere, there is a small impact of the MIPAS data on the mean ozone distribution in midlatitudes. A large ozone increase (peaking near 0.8 ppmv) is seen in the tropics (Fig. 3) which persists through January 2003.

High-resolution observations from the Stratospheric Aerosol and Gas Experiment (SAGE) II have been extensively validated (e.g. Wang *et al.* 2002). The SAGE II reported error standard deviations typically do not exceed 3% between 50 and 8 hPa. As seen in Fig. 7, inclusion of MIPAS data in the assimilation increases ozone by

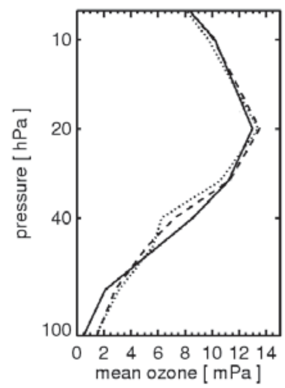

Figure 7. The mean SAGE II (solid) and mean assimilation profiles from SBUV (dotted) and SBUV + MIPAS (dashed) assimilations between 8 and 100 hPa from 113 profiles between 22 and 28 January 2003 as SAGE observations cross the 20°S–20°N latitude band.

around 10 hPa, reducing the mean difference between SAGE data and analyses from about 0.5 to 0.1 mPa. The r.m.s. difference (not shown) decreases from about 7% to 4%. The MIPAS-induced increase of ozone in the layer between 40 and 30 hPa also improves the agreement with SAGE data.

The impact of using MIPAS data could arise for two reasons. First, the availability of night-time as well as daytime data will allow less time for model error to increase between successive observations. Second, simply increasing the number of observations will better constrain the system. To investigate which effect is dominant, two additional assimilations were performed, including only either the ascending- or descending-node MIPAS data. We recall that descending-node observations made by MIPAS (equatorial crossing time 1000) precede those of SBUV/2 by over 4 hours. The impacts are examined using time series of observed-minus-forecast (O–F) residuals, which provide a very sensitive measure of performance for data assimilation systems (e.g. Stajner *et al.* 2004).

Time series of daily mean of SBUV/2 O–Fs in the Umkehr layer 5 (16–32 hPa) are shown (Fig. 8(a)) for four experiments that include all, daytime, night-time, or no MIPAS data. The time mean of SBUV/2 O–Fs is about 3.75 Dobson units (DU) in the SBUV-only experiment. Assimilation of night-time or daytime MIPAS data reduces the time mean to near 2.2 or 2 DU, respectively. The slightly larger reduction with daytime data is likely due to the larger number of daytime profiles. Larger improvements from daytime data are seen following the days on which the difference between the number of daytime and night-time data is larger (see arrows between Figs. 8(b) and (a)). Assimilation of all MIPAS data further reduces the time mean of SBUV/2 O–Fs to 1.1 DU. The size of this reduction from combining daytime and night-time data is largely due to their complementary coverage. Night-time and daytime observations were available in two different longitude intervals (70°–170°E and 250°–350°E; see Fig. 8(c)).

The bias in the ozone forecasts in the tropical middle stratosphere decreases as more MIPAS data are assimilated. Complementary coverage of night-time and daytime MIPAS data leads to larger improvements when all MIPAS data are used than when only ascending- or descending-node data are used. The forecast error variances are now being re-tuned, since increasing them will provide a larger impact of observations in the tropical middle stratosphere, and should improve the ozone representation.

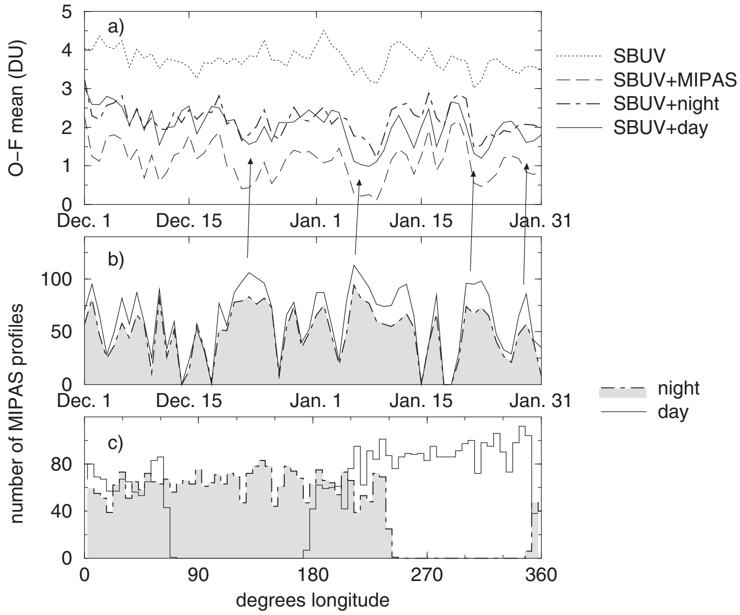

Figure 8. Time series for December 2002 and January 2003 over 30°S–30°N: (a) mean of SBUV/2 O–F residuals in Umkehr layer 5 (16–32 hPa) for SBUV assimilation (dotted), SBUV + MIPAS assimilation (dashed), SBUV + daytime MIPAS assimilation (solid) and SBUV + night-time MIPAS assimilation (dot-dashed), and (b) the number of MIPAS profiles for each day. (c) shows the cumulative number of profiles in 5° longitude bins. This coverage is specific to version 4.53 MIPAS data over the period of our study.

6. Synoptic features in the assimilated ozone field

In this section, some features in the synoptic distribution of ozone in January 2003 are discussed, with an emphasis on their representation in the flow and their sensitivity to the ozone data that are assimilated.

(*a*) *Geographical distributions*

Figure 9 shows the analyses at 70 hPa for 1–15 January 2003, a relatively undisturbed period preceding a major stratospheric warming. The temperature and geopotential height reveal a pronounced polar vortex, with the core located over the Barents Sea. Low temperatures (about 197 K) are centred over the North Sea, with warmer air (230 K over the Sea of Okhotsk) extending from eastern Russia to the western tip of Alaska. As is typical for the northern hemisphere (e.g. Harvey *et al.* 2002), the highest assimilated ozone values are evident in this same region, with values exceeding 3 ppmv in the SBUV + MIPAS assimilation (Fig. 9(c)).

The largest differences between the SBUV + MIPAS and SBUV-only assimilations (Fig. 9(d)) exceed 1 ppmv and are aligned with the polar vortex. This is because the inner vortex is not sampled by SBUV in early January, so these values are model determined in the SBUV-only assimilation. Ozone profiles at 75°N, 60°E (Fig. 10(a)) reveal the substantial impact of including ozone data in the polar vortex; the near-identical profiles in the SBUV + MIPAS assimilation and an additional MIPAS assimilation experiment (that used only MIPAS profiles and SBUV/2 total columns) highlights this.

Profiles at 60°N, 180°E (Fig. 10(b)), near the ozone maximum in Fig. 9(c), show that the change in the profile shape due to the assimilation of MIPAS data is less pronounced. The air masses here have been constrained by SBUV/2 data, both because they

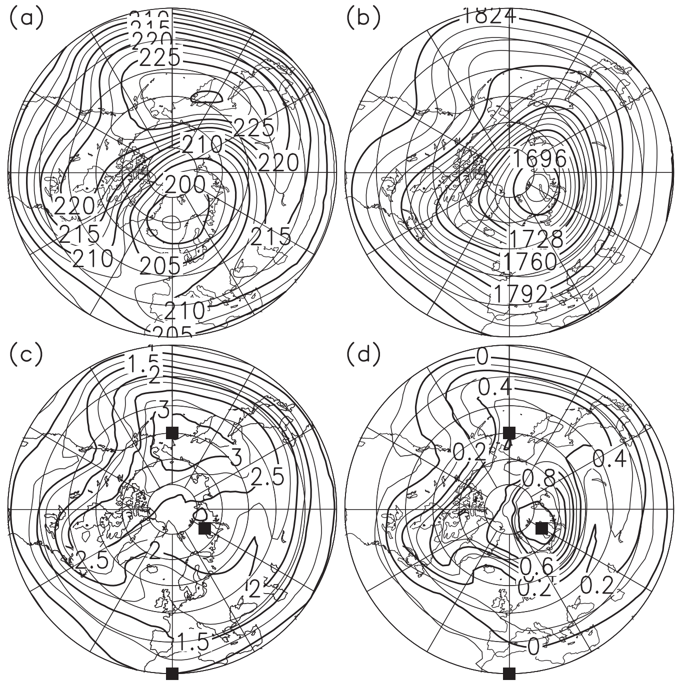

Figure 9. Polar stereographic plots, showing monthly mean fields at 70 hPa in January 2003, north of 30°N: (a) temperature, with contour interval 2.5 K, (b) geopotential height, with interval 8 gpdm, (c) ozone from the SBUV + MIPAS assimilation, with interval 0.25 ppmv, and (d) ozone difference (SBUV + MIPAS minus the SBUV assimilation), with interval 0.1 ppmv. The points marked on (c) and (d) are 75°N 60°E, 60°N 180°E and 30°N 0°E.

lie further south than the inner-core profile and because the air flows through this region from lower latitudes. However, the MIPAS + SBUV and MIPAS-only assimilations are virtually identical at pressures greater than 40 hPa, indicating the substantial impacts of MIPAS data in the combined analysis.

Subtropical profiles (30°N, 0°E) show a different impact (Fig. 10(c)); while at higher latitudes the MIPAS + SBUV curves lie close to the MIPAS curves, in this region the combined assimilation falls midway between the two single-dataset assimilations. As with the other two locations, the profile shape is markedly different when MIPAS data are assimilated.

(*b*) *Day-to-day variations and layering*

The day-to-day variability of the ozone at 52°N, 20°E is now discussed. This is the closest grid point to Legionowo (52.4°N, 20.97°E), where eight ozonesondes were launched in January 2003. Differences in the ozone assimilations at Legionowo will be discussed in the context of the synoptic evolution and ozone transport, including comparison with the available ozonesonde data.

Legionowo lies on the outer edge of the polar vortex (near the 1792 gpdm contour on Fig. 9(b)), so it is subject to substantial dynamical disturbances. Figure 11 shows time–height sections, for January 2003, of 'scaled' potential vorticity, temperature and ozone (from SBUV + MIPAS assimilation). These time–height sections reveal a typically rich structure for a midlatitude location, with evidence of passing tropical (e.g. 9 January) and polar air masses. There is a coherent pattern of warming, high

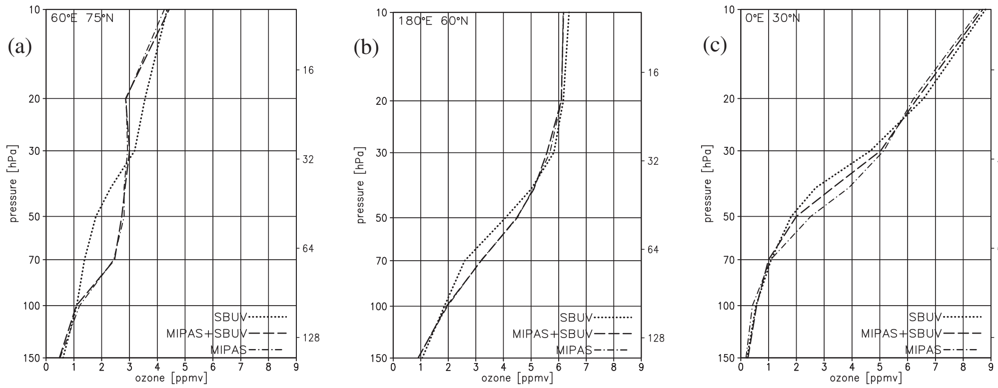

Figure 10. Monthly-mean ozone profiles for January 2003 from the three assimilation experiments SBUV (dotted), MIPAS (dash-dotted) and SBUV + MIPAS (dashed), for points marked by the black squares in Fig. 9(c) and (d): (a) 75°N, 60°E close to the vortex core, (b) 60°N, 180°E near the ozone maximum, and (c) 30°N, 0°E in the subtropics. The pressures on the right-hand axis mark the boundaries of the Umkehr layers for which SBUV partial columns are reported.

ozone and strong vertical gradients in potential vorticity in the 20–70 hPa layer in the second half of the month. The last ten days of the month are dominated by high ozone values at pressures lower than 50 hPa, along with low potential vorticity and warming. In the lower stratosphere (near 150 hPa), the highest potential vorticity of the month is seen on 31 January together with the highest ozone values.

Figure 12 shows ozone profiles from two soundings made at Legionowo in January 2003. On 8 January, the ozone profile was relatively smooth above a partial-pressure maximum of 19 mPa near 50 hPa, with substantial layering lower down, including a local peak near 200 hPa and a deep minimum between the two peaks (Fig. 12(a)). Comparison with the assimilated profiles at the closest grid-box (52°N, 20°E) shows that the SBUV assimilation fails to capture the 50 hPa peak and the lower minimum and the MIPAS assimilation agree well with the observed profile shape at all levels. The SBUV + MIPAS result lies between these two at pressures lower than 70 hPa, but close to the SBUV result at lower levels. The MIPAS data are not assimilated below the 60–80 hPa level, so the improvement is caused by the combined impact of the model and multiple data sources in the assimilation. The discussion will be separate for higher and lower levels.

Between 70 hPa and 30 hPa, the MIPAS data clearly improve the assimilation, since the SBUV/2 data are biased low (Figs. 4–6) and do not resolve vertical structure with only one partial column (Umkehr layer 4) between 32 and 64 hPa.

At 100 hPa the SBUV + MIPAS and SBUV assimilations are similar, while the MIPAS assimilation differs from them but agrees with the sonde. The biases in SBUV + MIPAS and SBUV assimilations in the tropics and northern midlatitudes are also evident in the earlier comparisons (Figs. 5–7).

Backward Lagrangian trajectories indicate that the air between 50 and 150 hPa in the 8 January profile came from the eastern Pacific within seven days (Fig. 13). The air mass ending at 70, 100, and 150 hPa at Legionowo originated in the subtropics where ozone values are typically low. The air ending at 50 and 200 hPa originated in the higher-ozone region north of 40°N. Interestingly, the trajectory ending at 200 hPa travelled through latitudes north of 70° within the four preceding days. The trajectory ending at 100 hPa is representative of the air mass; trajectories ending at neighbouring

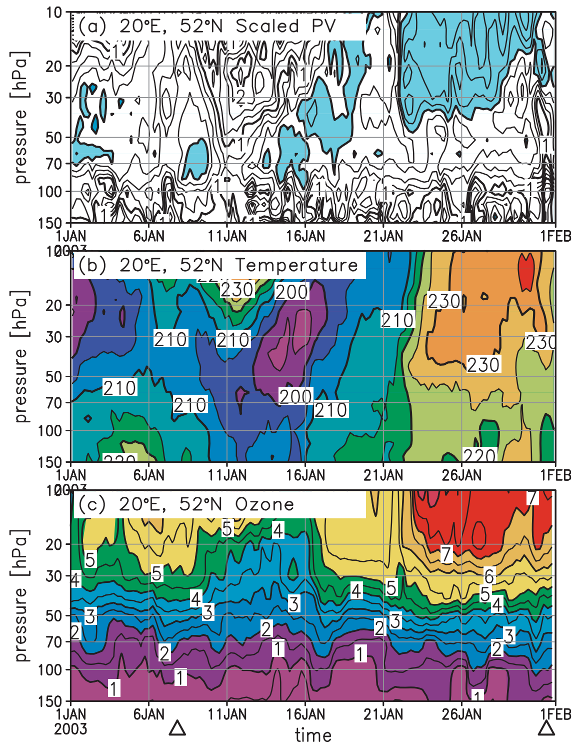

Figure 11. Time–height sections, between 150 and 10 hPa, at model grid point 52°N, 20°E in January 2003: (a) a scaled, non-dimensional form of the potential vorticity, with the scaling performed by normalizing the values according to the zonal mean at 30°N, and with negative values (blue shading) indicating transport of tropical air into these middle latitudes, (b) the analysed temperature (K), and (c) the analysed ozone (ppmv) from the SBUV + MIPAS assimilation. 8 and 31 January are marked by triangles on the lowest axis.

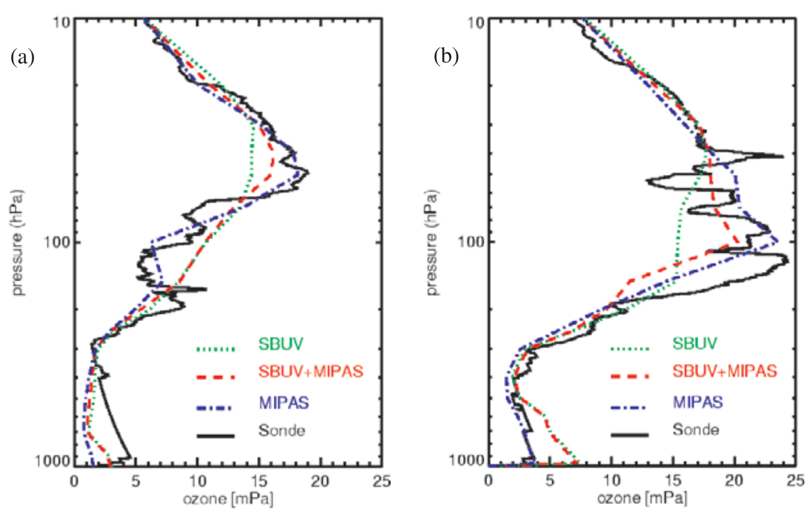

Figure 12. Profiles of the ozone sounding (solid line) at Legionowo (52.4°N, 20.97°E) on (a) 8 January and (b) 31 January 2003. The three other curves show the ozone profiles at the nearest grid point (52°N, 20°E) from the SBUV (dotted), SBUV + MIPAS (dashed) and MIPAS (dash-dotted) assimilations.

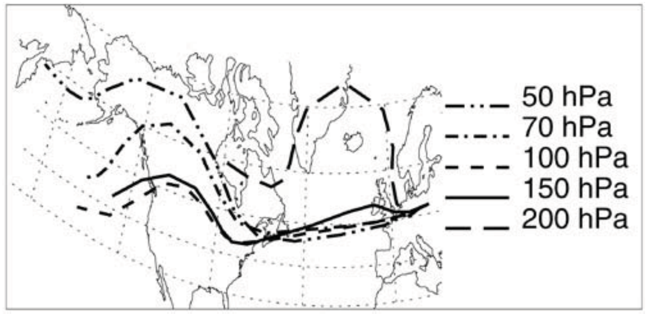

Figure 13. Back trajectories for 7 days, starting from different pressure levels in the profile at 52°N, 20°E on 8 January 2003.

grid points originated at similarly low latitudes in the eastern Pacific. The analyses that include SBUV/2 data (SBUV and SBUV + MIPAS) were shown to overestimate lower-stratospheric ozone in the tropics (Fig. 7), but the analysis that uses only MIPAS profile data has less ozone near 100 hPa in the tropics (Fig. 10(c)). Thus, omitting SBUV/2 profile data improves the representation of the profile at Legionowo on 8 January, likely due to a more accurate representation of ozone near 100 hPa in the tropics. (This is discussed further in section 8.)

On 31 January, the Legionowo profile contains many fine layers (Fig. 12). These layers are too shallow to be captured by either assimilation. In this case, the SBUV assimilation shows a similar low bias to that on 8 January, but the MIPAS assimilation brackets the higher peaks of the profile. At pressures below 100 hPa, the SBUV + MIPAS assimilation most closely matches the sonde profile averaged to the vertical resolution of the model. The synoptic structure at 70 hPa (Fig. 14), shows a region of high ozone over Europe, with a tongue of low ozone (and low potential vorticity) air extending from the tropics over Russia. Enhanced horizontal gradients, with less ozone in the tongue and a stronger ozone maximum over Europe in the SBUV + MIPAS assimilation, are consistent with the mean values for the appropriate 'source regions' shown in Figs. 9 and 10.

In summary, including MIPAS data leads to substantial improvements in both the profile shape and in the layering of the assimilated lower stratospheric ozone. Using SBUV/2 data alone produces biases and a lack of detail in the vertical structure. The structure obtained through layering involves vertical differences in horizontal advection, meaning that it is not only the local vertical resolution of the MIPAS data that is important; regional biases resulting from poor SBUV/2 information content and accuracy have an impact when air parcels are carried over large distances. Even though not all aspects of the vertical structure are obtained in the assimilated product, including the MIPAS data does lead to layering that is often similar to that detected by the *in situ* measurements.

7. Persistence of MIPAS information

This part of the study is motivated by likely uncertainties in data availability from research instruments. Limb-sounding profiles from research satellites often have temporal gaps, ranging from several orbits to several days. The impacts of such data voids on the resultant analyses need to be investigated. This contrasts with the continuous monitoring provided by SBUV/2 data (in the absence of unexpected failures).

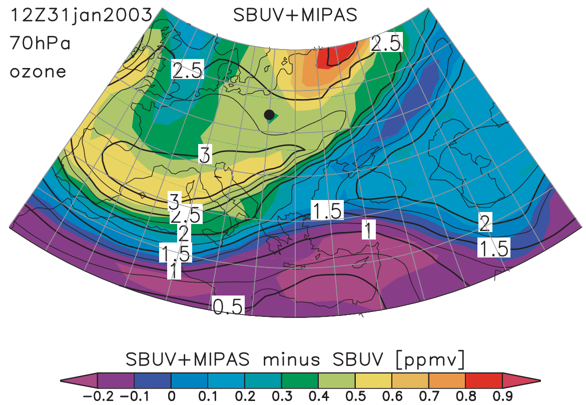

Figure 14. Synoptic structures in the ozone distribution at 70 hPa on 31 January 2003 for the area 30°–60°N and 10°W–60°E. The black contours (interval 0.25 ppmv) show the analysed ozone from SBUV + MIPAS, and the colour shading shows the difference SBUV + MIPAS minus SBUV. Legionowo is marked with a solid circle.

Understanding the impacts on the analyses of data gaps in MIPAS (or other such instruments) is of substantial interest. This section examines the response to withholding MIPAS data. Specifically, we investigate how long and to what degree the information that was introduced by assimilation of MIPAS data persists in the products after MIPAS data are no longer available.

A 20-member ensemble of assimilation experiments is examined. These were initialized from the SBUV + MIPAS experiment on each day between 10 and 31 December, except for 15 December following a day of missing MIPAS data. Each ensemble member assimilated SBUV/2 data and was run for 22 days. In order to measure the drift of ensemble members away from the SBUV + MIPAS run, we evaluated the average r.m.s. of MIPAS O–F residuals as a function of number of days after the initialization of each ensemble member and compared with average values from SBUV + MIPAS and SBUV runs.

In the northern midlatitudes (30°–60°N) in the lower stratosphere, near 70 hPa, the ensemble r.m.s. increases slowly towards the values from SBUV-only assimilation over about two weeks (Fig. 15(a)). The largest differences in ozone fields from runs that used or withheld MIPAS data generally originate at high latitudes, where MIPAS information can be retained because of the lack of SBUV/2 data. Moreover, larger SBUV/2 standard deviations (Fig. 2) and lower forecast error variances in the lower than in the middle stratosphere allow longer persistence of MIPAS information in the lower stratosphere.

Near 10 hPa, the average ensemble r.m.s. of O–F residuals exceeds that from the SBUV-only run in just two days (Fig. 15(b)). After about 10 days it declines to near the values from the SBUV-only run, while still showing day-to-day variability. At 10 hPa, the largest differences in ozone fields between runs that used or withheld MIPAS data generally come from the tropics. Assimilation of MIPAS data increases the tropical ozone maximum, and reduces ozone in middle latitudes (Fig. 3). The effect of the excessive transport of tropical air into middle latitudes is reflected strongly in the fields that were constrained with MIPAS data because of stronger initial horizontal gradients. Subsequent reduction in horizontal gradients from transport and constraints from SBUV/2 data leads to a balance similar to that in SBUV-only assimilation.

These experiments suggest that the length of temporal voids in MIPAS data that will not significantly degrade the performance of the assimilation system is about a week

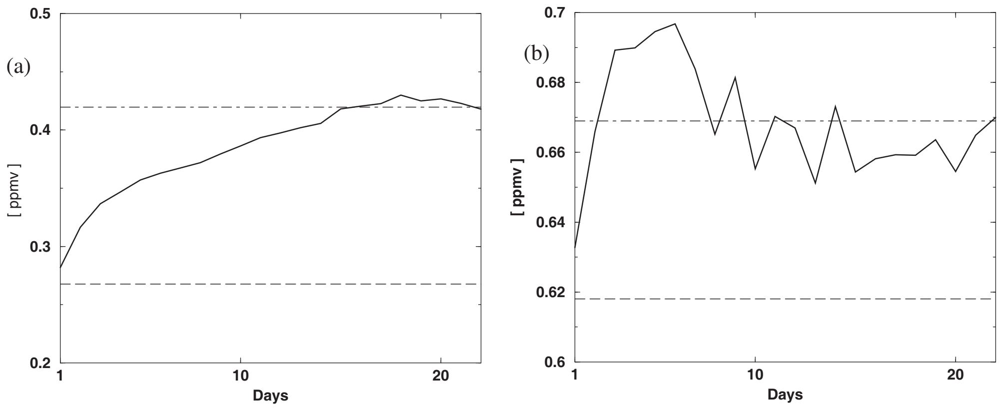

Figure 15. Daily r.m.s. of MIPAS O–F residuals in northern midlatitudes (30°–60°N) for (a) level 12 (60–80 hPa) and (b) level 8 (8–12 hPa). An ensemble of analyses that used only SBUV/2 data for 20 days were initialized from SBUV + MIPAS analyses on 10 to 29 December 2002. The time axis shows number of days after the initialization of each ensemble member. The average r.m.s. values are shown for all ensemble members (solid), MIPAS + SBUV analyses (dashed), and SBUV analyses (dash-dotted).

in the lower stratosphere and about a day in the middle stratosphere. In conclusion, given temporal voids in data from MIPAS, a constraint from another data source seems necessary in the middle, but not in the lower stratosphere, where even occasional insertion of accurate observations provides lasting information preserved by the model.

8. SBUV/2 DATA SELECTION

It has been demonstrated that assimilating MIPAS data in 12 layers at and above 80–60 hPa improves the representation of the lower stratospheric ozone. However, the MIPAS data did not reduce the high bias in assimilated ozone at 100 hPa in the northern midlatitudes and in the tropics (Figs. 3, 6(a) and 7). In contrast, the MIPAS-only assimilation had lower, more realistic, ozone values at 100 hPa in the subtropics (Fig. 10(c)) and at Legionowo on 8 January (Fig. 12(a)). This, along with the known limitations of vertical resolution in the SBUV data below the ozone peak, motivated a new SBUV–UL3 + MIPAS assimilation that excludes SBUV data for Umkehr layer 3 (63–126 hPa). Note that such data exclusion is a limiting case of increasing the specified observation error to infinity.

The quality of lower stratospheric ozone in northern middle latitudes is compared in four runs (SBUV, SBUV + MIPAS, SBUV–UL3 + MIPAS, MIPAS) that use decreasing amounts of SBUV data. At 70 hPa, the addition of MIPAS data improves the agreement with SAGE compared to the SBUV-only assimilation, especially for higher ozone values (Fig. 16(a)). To quantify the impacts of MIPAS and SBUV/2 data further, differences between the analyses and SAGE data are binned by the SAGE ozone values: ≤1.5 ppmv, 1.5–2.5 ppmv, and ≥2.5 ppmv. Adding MIPAS data improves the r.m.s. differences between analysis and SAGE data in the highest bin from 16% to 8% (Fig. 16(c)). A smaller improvement (∼3%) is seen in the middle bin. Withholding SBUV/2 data changes the agreement between analyses and SAGE data at 70 hPa only slightly.

Even though assimilation of MIPAS alongside SBUV/2 data causes only slight changes in the ozone at 100 hPa, withholding the UL3 data has a substantial impact. Agreement with SAGE data is significantly improved, especially for lower ozone values (Fig. 16(b)). The withholding of UL3 data improves the r.m.s. differences between

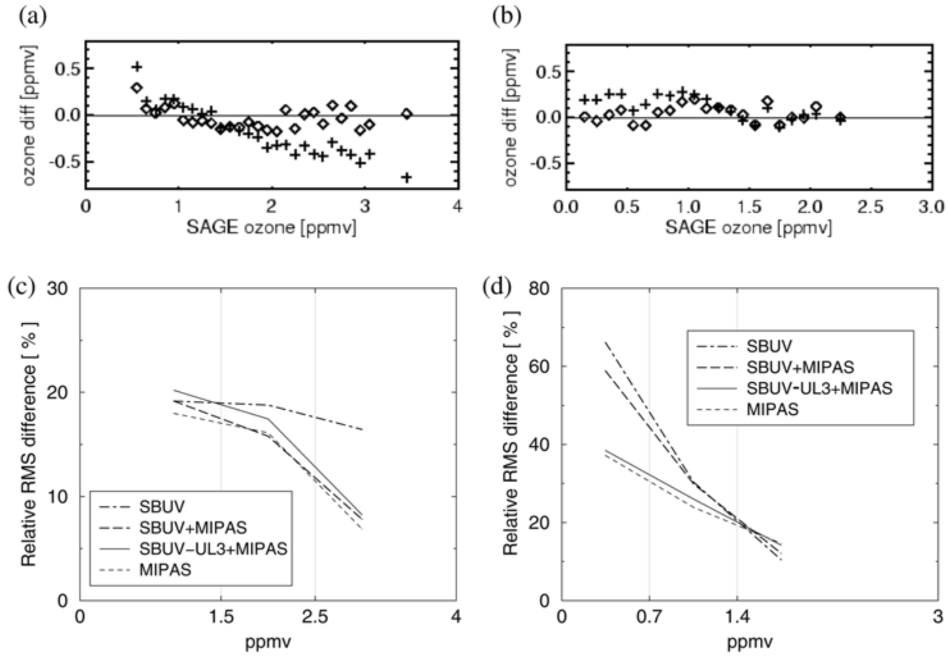

Figure 16. Comparison of assimilated ozone with SAGE data in northern midlatitudes: mean analysis-minus-SAGE differences in bins of 0.1 ppmv at (a) 70 hPa for SBUV (+) and SBUV + MIPAS (◇) analyses, and (b) 100 hPa for SBUV + MIPAS (+) and SBUV–UL3 + MIPAS (◇) analyses, and relative r.m.s. differences between SAGE and the four assimilation experiments for low, medium, and high ozone bins (see text for details) at (c) 70 hPa and (d) 100 hPa.

analysis and SAGE from 59% to 38% in the lowest ozone bin (<0.7 ppmv) and from 30% to 26% in the medium ozone bin (0.7–1.4 ppmv) (Fig. 16(d)). Withholding the entire SBUV/2 profile has a similar impact. The 8 January Legionowo case-study (Fig. 12(a)) revealed that the best agreement between the assimilated and measured ozone at 100 hPa was in the MIPAS run, with no SBUV/2 data. An almost identical improvement was found in the SBUV–UL3 + MIPAS run (not shown). This clearly reveals that the UL3 data are the cause of the overestimated ozone concentrations near 100 hPa.

These results motivated an experiment in which UL3 data were withheld from an SBUV-only assimilation. Similar improvements were found in this study, which used the GEOS-4 meteorological analyses. In contrast, when winds from the earlier GEOS-2 analyses were used, the transport errors were so large that the assimilation of UL3 data was beneficial (Stajner *et al.* 2001). Note that the UL3 data depend heavily on a priori information (Bhartia *et al.* 1996), and we found that even the use of first-guess values from SBUV/2 retrievals is beneficial in the ozone assimilation driven by GEOS-2 winds. This result reflects the improved transport in GEOS-4 compared to GEOS-2, an issue that will be addressed further elsewhere. In the present context, this result indicates the importance of interplay between the model and the observations in the assimilation.

In conclusion, the addition of MIPAS data together with withholding of SBUV/2 data between 63 and 126 hPa provides the best results in the lower stratosphere and maintains robust performance in the middle stratosphere when MIPAS data are absent.

9. DISCUSSION AND CONCLUSIONS

This study demonstrates the benefits of including stratospheric ozone profiles from the limb-sounding MIPAS instrument alongside the SBUV/2 data in an ozone assimilation system. Spatio-temporal coverage and vertical resolution of MIPAS and SBUV/2 differ. SBUV/2 provides data only over the illuminated portion of the planet, while MIPAS measures infrared emission on both sides of the globe and in the polar night. SBUV/2 retrievals provide total-ozone columns and coarse-vertical-resolution partial columns, which are strongly influenced by the a priori information below the ozone maximum (especially for pressures larger than about 63 hPa). The MIPAS data have a vertical resolution of about 3 km over the range that they were used in this study, up to pressure of 60–80 hPa.

Analysis of the MIPAS level-2 ozone data showed that they are of high quality, agreeing well with independent observations. Migliorini *et al.* (2004) found good agreement between MIPAS data and ozonesondes. Here, comparison of the MIPAS data with retrievals from high-quality occultation sounders, HALOE and POAM, was within about 10%, with better than 4% agreement in the upper and middle stratosphere. This is in broad agreement with the error variances provided with the MIPAS retrievals. In the assimilation, MIPAS error variances are smaller in the lower stratosphere than those used for SBUV/2 data (Stajner *et al.* 2001), thus more weight is given to MIPAS than to SBUV/2 data. The two datasets have comparable accuracy in the middle stratosphere. Inclusion of systematic error components would increase MIPAS errors (Dudhia *et al.* 2002), but also the errors of SBUV/2 and forecasts in the stratosphere.

Including MIPAS ozone substantially improves the analyses in the polar night and below the ozone maximum at all latitudes. This was established by comparisons of assimilated ozone fields with occultation datasets and ozonesondes. Additional improvements were found near the tropical ozone maximum, where the increased number of observations in the SBUV + MIPAS assimilation helps suppress the impact of transport errors in the model. Withholding of SBUV/2 data between 63 and 126 hPa yielded further improvements. This configuration provides the best results in the lower stratosphere and maintains robust performance in the middle stratosphere when MIPAS data are absent.

The case-studies presented in section 6 highlight the importance of both the integrity of the long-range transport with the GEOS-4 winds and the benefits of assimilating data that adequately constrain the geographical variations of vertical structure in the ozone distribution. Long-range transport from diverse latitudes produces layering in ozonesonde profiles over middle latitudes; without the MIPAS data, the assimilation was not able to reproduce these structures. Even though the layering is not perfect with the MIPAS data in the assimilation, there are demonstrable improvements at the limit of MIPAS resolution.

Future studies will examine impacts of ozone assimilation on meteorological analyses and forecasts, including the forecast of ozone itself. Research instruments like MIPAS do not guarantee non-stop operations, leading to gaps in the time series, making them potentially unsuited to such applications. Our data-withholding experiments in section 7 reveal that, in the lower stratosphere where ozone is chemically long lived, the GEOS-4 transport is adequate to maintain the distributions over data gaps of several days. At higher levels, where transport and chemistry are faster and where the winds are less well constrained, the absence of MIPAS data quickly leads to substantial biases in the assimilation. These results are again consistent with the decision that the UL3 SBUV/2 data may be omitted from the analyses, but that the near-uninterrupted SBUV/2 data should be included alongside the MIPAS data in the assimilation.

Successful assimilation of MIPAS data contributes to their validation under varying geophysical conditions. Superior vertical resolution and global coverage provided by the instrument improve assimilated ozone, especially in those regions that are poorly observed by SBUV/2 (the lower stratosphere, the polar night region) or whose dynamics were not captured accurately by the CTM (the tropical pipe). This study quantifies many of the benefits of including MIPAS alongside SBUV/2 (Umkehr layers 4 and higher) in the assimilation, and examines the mechanisms that led to the positive impacts. Significant improvements in the ozone profiles are attributed to compensation of errors in both the transport and the SBUV/2 data. Future work on assimilation of limb-sounder data will include revised forecast- and observation-error covariance models, and attempt to include ozone data at lower altitudes. We plan to examine in more detail the radiative impacts of ozone, the consequences for meteorological assimilation, the separation of stratospheric and tropospheric ozone columns, and the cross-tropopause ozone fluxes. The examination of long-term climate forcings by ozone in the lower stratosphere remains beyond reach with currently available data. Given the unsuitability of present operational sensors to adequately observe the lower stratosphere, global assimilation of ozone in the lower stratosphere requires limb-sounding instruments. MIPAS and instruments on NASA's Earth Observing System Aura provide high-quality data for a limited period, but there are presently no plans for long-term monitoring of this region.

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