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Contract Report to the European Space Agency

Monitoring and assimilation of MIPAS, SCIAMACHY and GOMOS retrievals at ECMWF

November 2004

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Annual report for ESA contract 17585/03/I-OL: Technical support for global validation of ENVISAT data products (ENVISAT II)

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Monitoring and Assimilation of MIPAS, SCIAMACHY and GOMOS retrievals at ECMWF

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European Centre for Medium-Range Weather Forecasts

Shinfield Park, Reading, Berkshire, UK

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Abstract

Contracted by ESA, ECMWF is involved in the validation and monitoring of atmospheric data from several instruments on board Envisat. Under contract 17585/03/I-OL (Technical support for global validation of Envisat data products (ENVISAT II)), which runs from 1 October 2003 to 31 December 2005, ECMWF monitors near-real-time level 2 data products from MIPAS, SCIAMACHY, and GOMOS. This paper is the annual report for ESA contract 17585/03/I-OL and describes results from the monitoring statistics and assimilation experiments for MIPAS, SCIAMACHY and GOMOS data for the period October 2003 to September 2004.

1 Introduction

ECMWF is contracted by ESA under project 17585/03/I-OL to give technical support for the global validation of Envisat data products. This includes the monitoring and validation of a subset of the Envisat level 2 retrievals, the so called Meteo products, which are available in near-real-time (NRT) in BUFR format. These Meteo data include temperature, ozone and water vapour profiles from MIPAS (MIP_NLE_2P) and from GOMOS (GOM_RR__2P), as well as total column ozone retrievals from SCIAMACHY nadir measurements (SCI_RV__2P). The project continues the work carried out under ESA contract 14458/00/NL/SF (Dethof 2003a).

The monitoring statistics shown in this paper cover the period 8 October 2003 to 30 September 2004. 8 October 2003 was chosen as a start date because on 7 October 2003 the ECMWF operational model was updated to model cycle CY26R3. In CY26R3 ozone profiles from MIPAS were actively assimilated and so were radiances from the Advanced InfraRed Sounder (AIRS) on Aqua. Both changes affected the monitoring statistics of the atmospheric Envisat data. Another model change (CY28R1) took place on 9 March 2004, but it did not affect the Envisat monitoring activities. A further change (CY28R2) was implemented on 29 June 2004. This included the change to the so called Early Delivery System. The Early Delivery System comprises two main 6-hour 4D-Var analysis and forecast cycles for 00 and 12 UTC with two additional 12-hour 4D-Var analysis and first-guess forecast cycles. The 6-hour 4D-Var analysis and forecast cycles of the early delivery system have a shorter cut-off time, allowing the forecast products to be made available to the member states 3-4 hours earlier. The additional 12-hour 4D-Var cycles are run with a delayed cut-off time of 14 hours. The monitoring statistics for Envisat data are based on the delayed cut-off analyses after 29 June 2004. This has the advantage that more Envisat data have been received by the time the analysis is started, so that more data go into the monitoring statistics.

Ozone retrievals from the SBUV/2 (Solar Backscatter Ultra Violet) instrument on NOAA-16 have been assimilated in the operational ECMWF system since April 2002. The SBUV/2 data come from NESDIS (see http://orbit-net.nesdis.noaa.gov/crad/sit/ozone/ for more information). They are given as 12 ozone layers and are combined at ECMWF into 6 ozone layers (0.1-1 hPa, 1-2 hPa, 2-4 hPa, 4-8 hPa, 8-16 hPa, 16 hPa-surface) to reduce observation error correlation. From 7 October 2003 until 26 March 2004 MIPAS ozone retrievals were also assimilated in the ECMWF system.

In the ECMWF analysis system no humidity observations are assimilated in the stratosphere. A simple parameterization of the upper-stratospheric moisture source due to methane oxidation is included in the model to avoid an unrealistically drying of the stratosphere in the ECMWF model (Simmons pers. communication). Stratospheric humidity values from the 45-year re-analysis project (ERA-40) are about 10-15% lower than UARS retrievals in the upper stratosphere and lower mesosphere at high latitudes where air moistened by methane oxidation has descended. Since then, the parameterization of methane oxidation has been modified to take into account a more recent climatology of methane, so that the dry bias of the current operational ECMWF model should be smaller than in ERA-40. In the lower stratosphere the ECMWF water vapour field shows a too rapid upward progression of the annual cycle of drying and moistening in the tropics.

This paper is structured in the following way. Section 2 summarizes the results of the monitoring of MIPAS temperature and water vapour retrievals, and of the assimilation of MIPAS ozone profiles. Section 3 gives results of the monitoring and assimilation of SCIAMACHY total column ozone retrievals, Section 4 shows results of the monitoring of GOMOS data, and Section 5 provides the conclusions.

2 Monitoring and assimilation of MIPAS NRT products (MIP_NLE_2P)

MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) is a limb-viewing high-resolution Fourier-transform spectrometer that measures atmospheric emissions in the mid infrared part of the spectrum (4.15 microns to 14.6 microns), allowing the retrieval of concentration profiles of more than 20 atmospheric trace gases, from 70 km down to 7 km, with a vertical resolution of 3-5 km (http://Envisat.esa.int). MIPAS provides global coverage, including coverage of the polar regions, independent of illumination conditions. The six main species (O_3, H_2O, HNO_3, CH_4, N_2O and NO_2) as well as temperature and pressure profiles are routinely retrieved by the ESA ground segment.

At ECMWF a subset of these retrieved products is monitored that is available in NRT (MIP_NLE_2P). These data include temperature, water vapour and ozone profiles. In research experiments the assimilation of MIPAS ozone profiles had been shown to have a positive impact on the ECMWF ozone analysis (Dethof 2003b). As a result of these experiments the assimilation of MIPAS ozone profiles was included in the operational ECMWF system (cycle 26R3) on 7 October 2003. Temperature and water vapour retrievals from MIPAS continued to be monitored passively.

The monitoring results for MIPAS data presented in this paper are for the period 8 October 2003 to 31 March 2004. Because of instrument problems there have been no MIPAS level 2 data since 27 March 2004.

2.1 Monitoring of MIPAS temperatures retrievals

Figure 1 shows area averaged MIPAS and ECMWF temperature profiles for the areas 90-65°N (top left), 0-20°S (middle left) and 65-90°S (bottom left) averaged over the period 8 October to 31 December 2003. The right panels show the corresponding MIPAS departures. Figure 2 shows MIPAS temperature profiles and departures averaged over the period 1 January to 31 March 2004. On the whole, MIPAS temperature profiles agree well with the ECMWF temperatures, and the differences between MIPAS and ECMWF temperatures are less than 1% (less than 2 K) for most levels in the stratosphere. Larger departures are seen in the mesosphere, and the largest departures are found at the model top. MIPAS temperatures are larger than ECMWF temperatures throughout the stratosphere. In the mesosphere the sign of the departures varies depending on the area and the time of year. Averaged over 90-65°N MIPAS temperatures are higher than the ECMWF values by up to 4% in the time average, averaged over 0-20°S and 65-90°S MIPAS temperatures are lower than ECMWF temperatures, by up to -6%. Departures can be larger for shorter periods, as illustrated by the large standard deviations of the departures near the model top.

Figures 3 to 5 show timeseries of area averaged temperatures and departures at 20 hPa (averaged over 6-hourly analysis cycles) for the areas 90-65°N, 0-20°S, and 65-90°S, respectively. These figures illustrate that MIPAS data delivery deteriorated from December 2003 onwards and was particularly poor early in 2004, when the instrument went into heater-refuse-mode more and more often. Almost no MIPAS data were available in January 2004 and the early part of February 2004. However, the data quality remained good in 2003, apart from

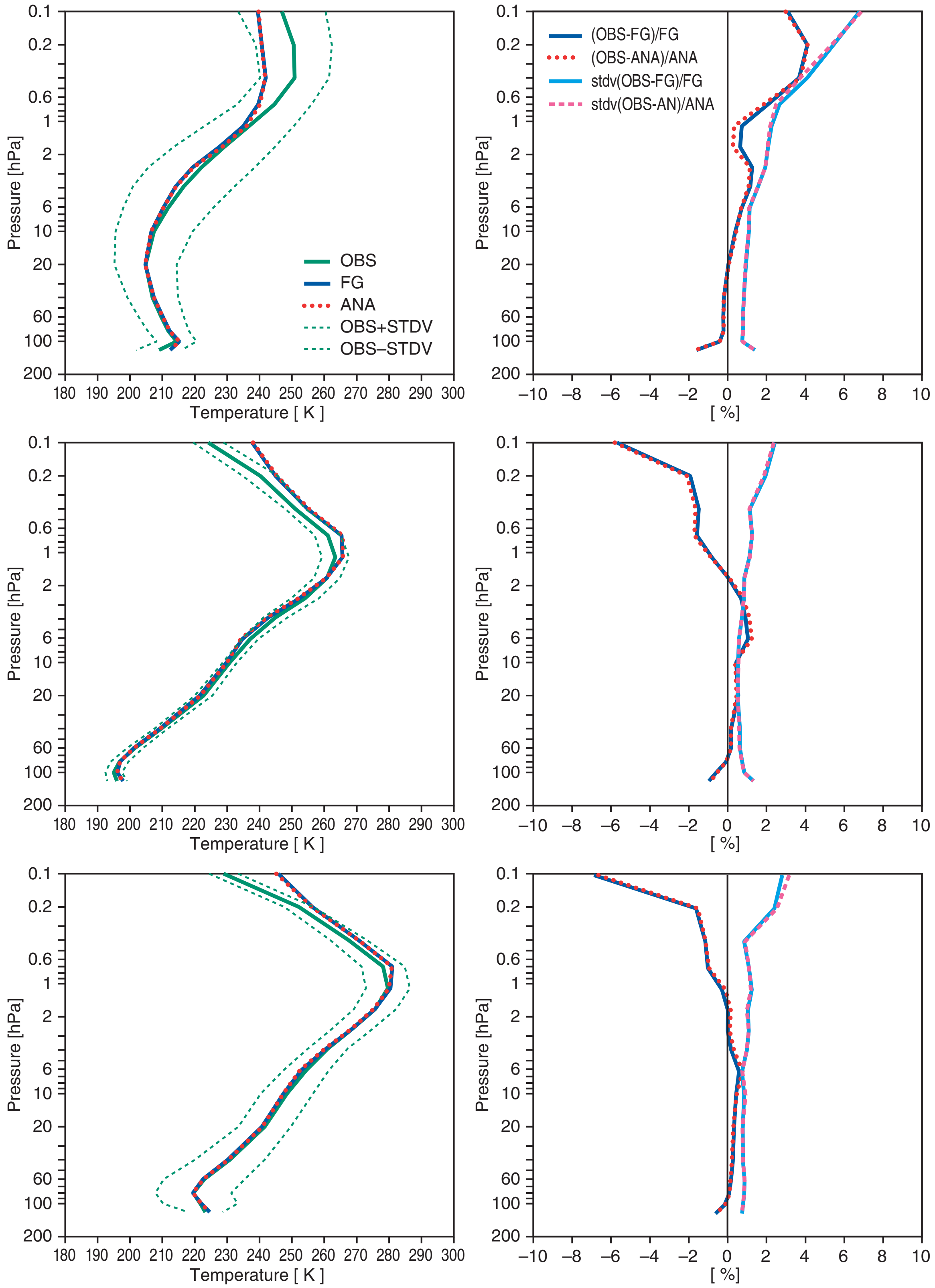


Figure 1: Profiles of time and area averaged MIPAS and ECMWF temperatures in K (left) and MIPAS departures in % (right) for the areas 90-65°N (top), 0-20°S (middle), and 65-90°S (bottom). Averaging period is 8 October to 31 December 2003.

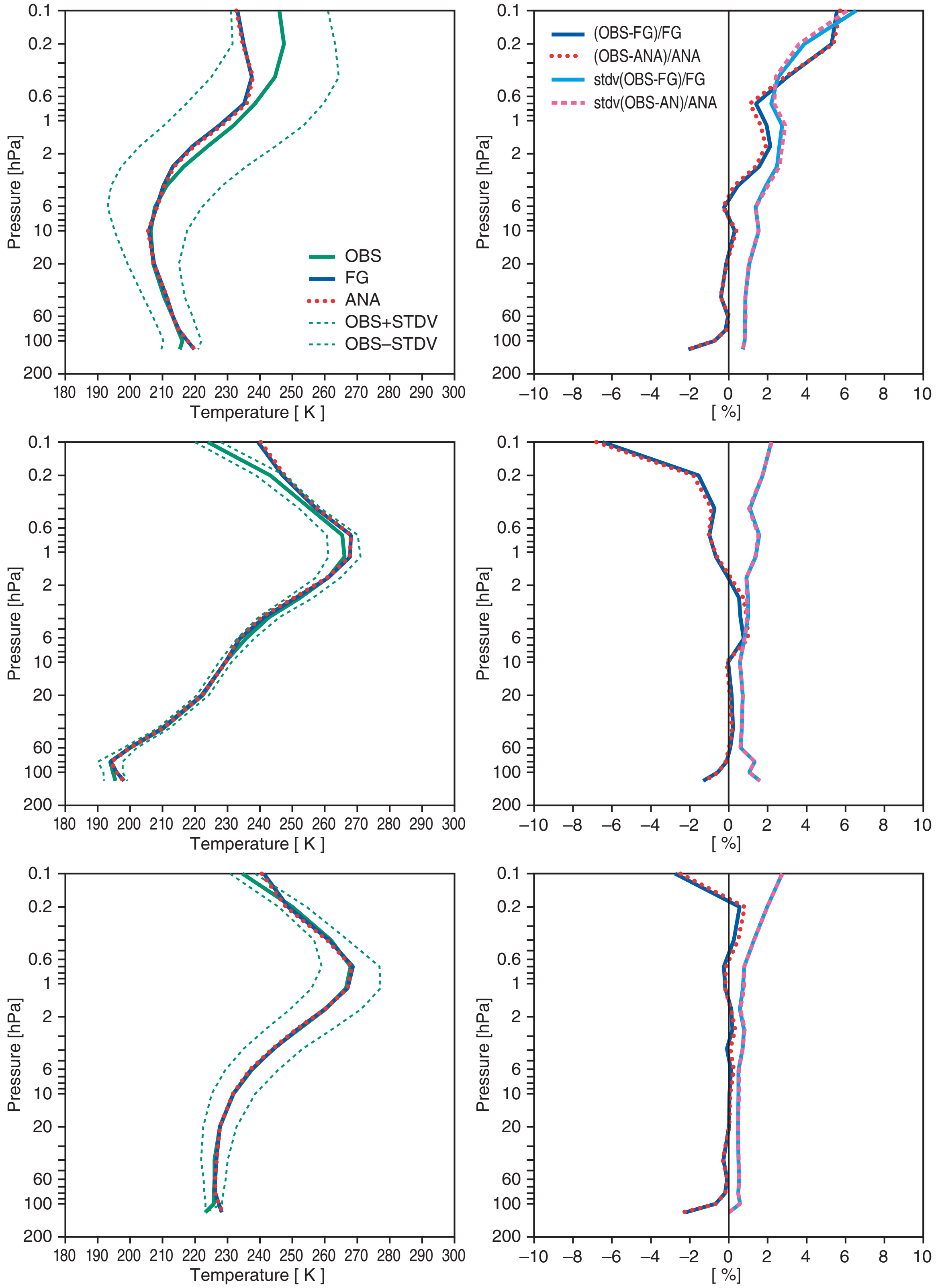


Figure 2: Like Figure 1 but for averaging period 1 January to 31 March 2004.

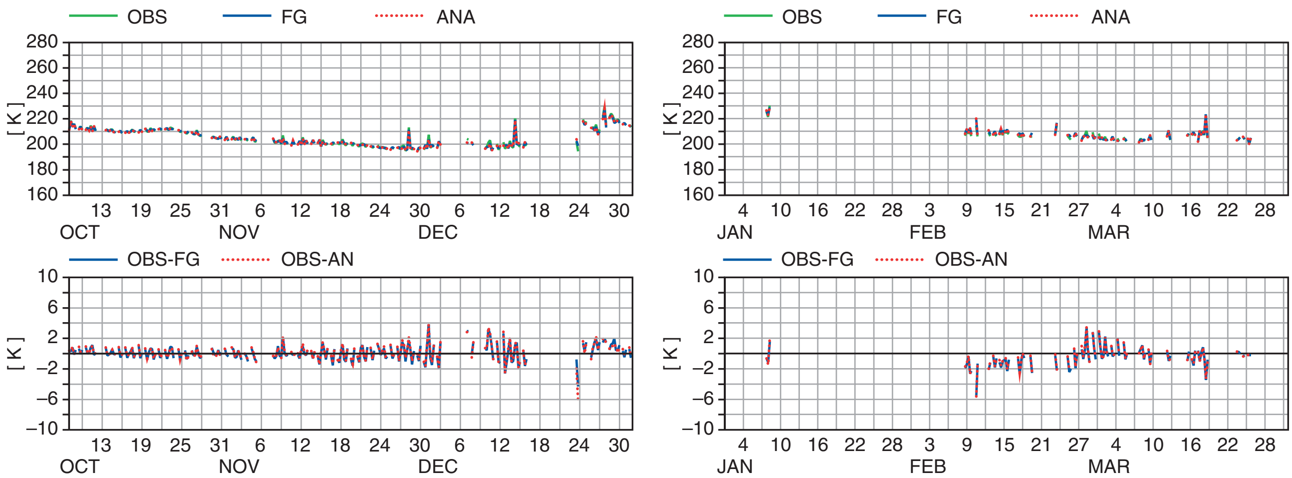


Figure 3: Timeseries of temperature data at 20 hPa averaged over 90-65°N covering the periods 8 October to 31 December 2003 (left) and 1 January to 31 March 2004 (right). The top panels show MIPAS temperatures, first-guess and analysis values, the bottom panels first-guess and analysis departures. All temperature values are in K.

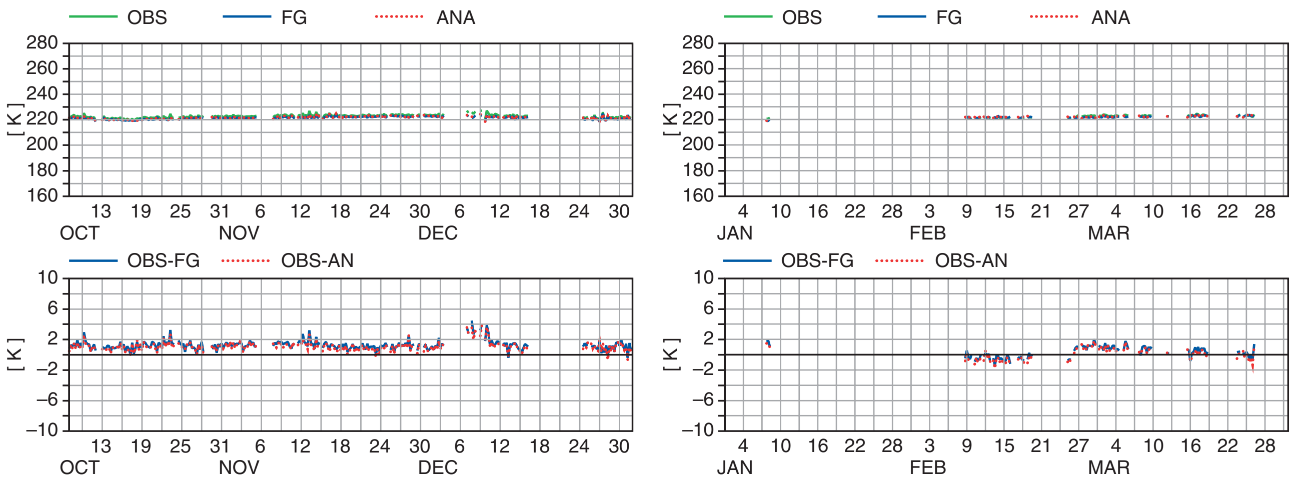


Figure 4: Like Figure 3 but averaged over 0-20°S.

some short problem periods. The plot of departures shows that the agreement between MIPAS and ECMWF temperatures between October and December is good, with departures of less than 2K in the area mean.

In 90-65°N (Figure 3) temperatures decrease from 220 K in October to values around 200 K in December 2003 in the polar night. At the end of December 2003 a stratospheric warming occurs (see also http://strat-www.met.fu-berlin.de/cgi-bin/alert) and temperatures increase from 200 K to 230 K within a few days. The data received during February and March 2004 show a discontinuity around 27 February.

In the tropics temperatures at 20 hPa are relatively constant around 220-230 K between October 2003 and March 2004 (Figure 4). However these timeseries also show discontinuities around 27 February 2004 and also around 6-9 December 2003 after periods of instrument switch-offs. As mentioned in Dethof (2003)a these problems occurred frequently during 2003, when pre-switch-off gain calibrations were applied to the post-switch-off data. After new gain calibrations were performed, MIPAS values always went back to pre-switch-off levels. Apart from these offsets, MIPAS temperatures are relatively stable and agree with ECMWF temperatures to within 2K.

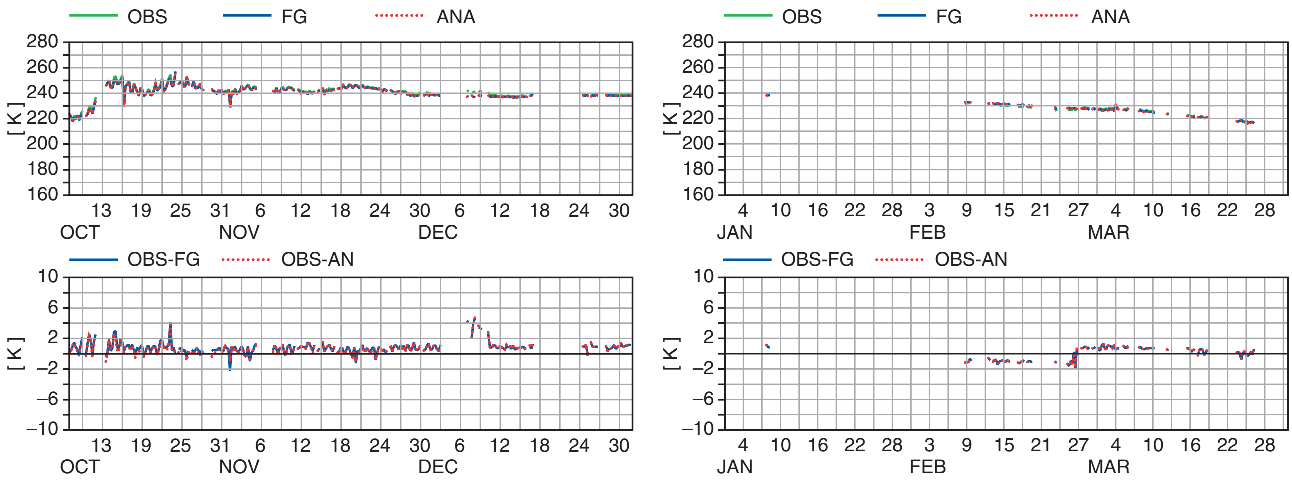


Figure 5: Like Figure 3 but averaged over 65-90° S.

In 65-90° S temperatures increase from 220 K to 250 K in October at the end of the austral spring and return to values around 240 K in December 2003. From February to March 2004 they decrease from 230 K to below 220 K. The timeseries for 65-90° S (Figure 5) also shows discontinuities in December 2003 and February 2004.

2.2 Monitoring of MIPAS water vapour retrievals

In the ECMWF assimilation system water vapour layers or partial columns (unit kgm^{-2}) are monitored, not water vapour profile points. These partial layers are calculated for MIPAS data during the conversion from PDS to BUFR format.

Time and area averaged MIPAS water vapour departures in % for the areas 90-65° N, 0-20° S, and 65-90° S are shown in Figure 6 averaged over the periods 8 October to 31 December 2003 (left) and 1 January to 31 March 2004 (right). MIPAS water vapour values are larger than ECMWF values in almost all layers and areas. The sign of this bias is in agreement with a dry bias the ECMWF model shows compared to UARS data in the stratosphere (Simmons pers. communication). However, the differences seen between MIPAS and ECMWF data are greater than 20% over much of the stratosphere, which is larger than the ECMWF dry bias. This bias was 10-15 % for ERA-40 data, but should be smaller in the current operational model after a change in the parameterization of methane oxidation. This suggests that MIPAS retrievals have a moist bias and overestimate stratospheric water vapour.

The largest water vapour departures are seen in the lower stratosphere and upper troposphere in the tropics, where the time and area averaged MIPAS water vapour data are up to 80% higher than the ECMWF values. These unrealistically large MIPAS values are likely to be a sign of cloud contamination, a problem limb sounders are often affected by, particularly in the tropics. Even though a cloud clearing algorithm was implemented on 23 July 2003 in the retrieval, it is not flagging the cloudy data properly in the MIPAS NRT data, and unrealistically large water vapour and ozone values continue to be seen in the MIPAS data in the tropics.

Figure 7 shows timeseries of globally averaged MIPAS water vapour values and departures for a layer between 20-40 hPa. The timeseries clearly show the moist bias of the MIPAS water vapour data relative to the ECMWF values, which is between 100-150 mg/m^2 in the global mean. The timeseries show that the discontinuities seen in the temperature retrievals around 6-9 December 2003 and 27 February 2004 propagate into the water vapour retrievals and lead to discontinuities in the MIPAS water vapour timeseries. MIPAS water vapour values are

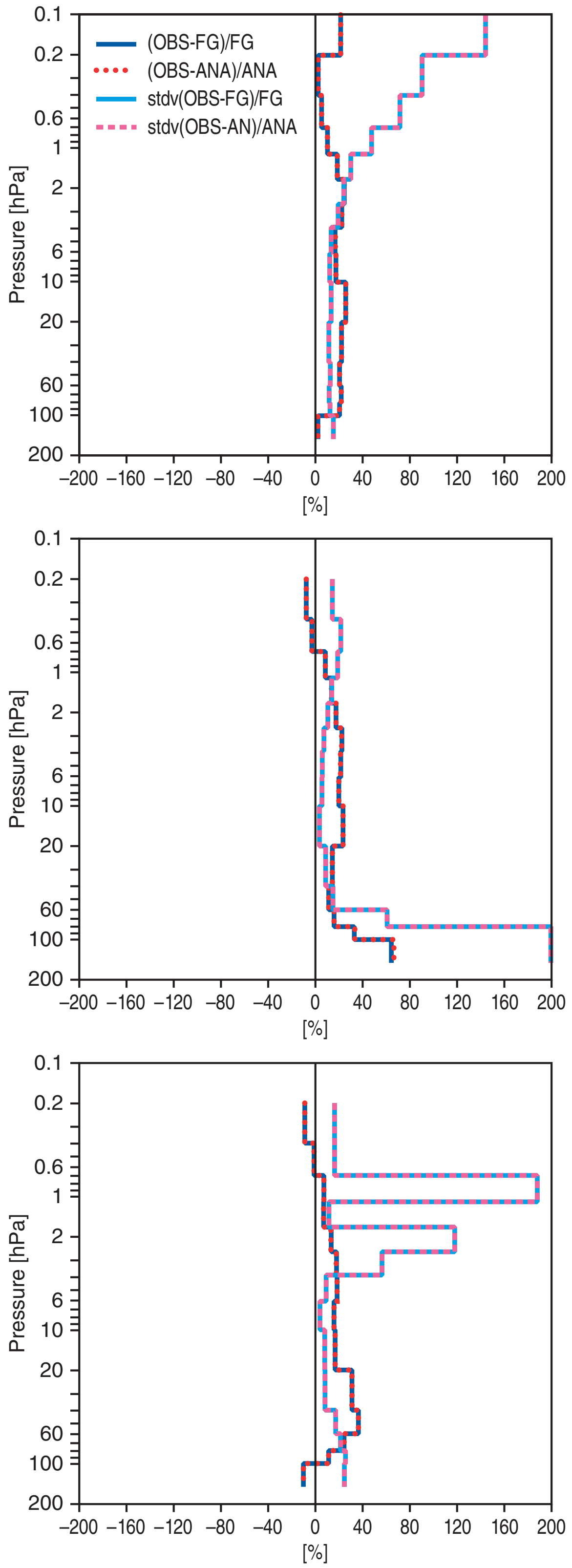


Figure 6: Profiles of time and area averaged MIPAS water vapour departures in % for the areas 90-65°N (top), 0-20°S (middle), and 65-90°S (bottom). Averaging periods are 8 October to 31 December 2003 (left) and 1 January to 31 March 2004 (right).

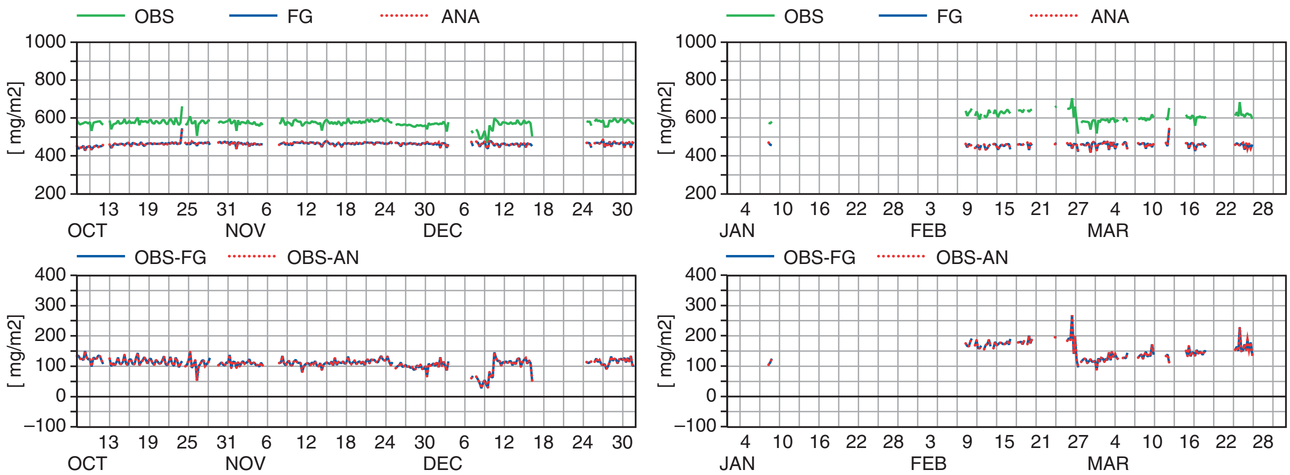


Figure 7: Timeseries of globally averaged water vapour data in a layer between 20-40 hPa covering the periods 8 October to 31 December 2003 (left) and 1 January to 31 March 2004 (right). The top panels show MIPAS water vapour layers, first-guess and analysis values, the bottom panels first-guess and analysis departures. All water vapour values are in mg/m^2.

generally lower and departures are smaller when the temperature departures are larger.

2.3 Assimilation of MIPAS ozone retrievals

In the ECMWF assimilation system ozone layers or partial columns (unit kgm^{-2} or Dobson Units (DU)) are monitored, not ozone profile points. These partial layers are calculated for MIPAS data during the conversion from PDS to BUFR format.

The assimilation of MIPAS ozone retrievals had been tested in research experiments and had been found to have a positive impact on the ECMWF ozone analysis (Dethof 2003b). As a result of those experiments the assimilation of MIPAS ozone profiles was included in the operational ECMWF system (CY26R3) on 7 October 2003. This means that an independent validation of MIPAS ozone values against ECMWF data is not possible anymore. Hence, other independent data are used to validate the ECMWF ozone field.

2.3.1 Monitoring results

Figure 8 shows profiles of time and area averaged MIPAS ozone departures in % for the averaging periods 8 October to 31 December 2003 and 1 January to 31 March 2004. The profile plots show that the analysis is drawing to the MIPAS data (analysis departures smaller than first-guess departures; standard deviation of analysis departures smaller than standard deviation of first-guess departures).

Figure 9 shows timeseries of global mean MIPAS ozone values and departures in DU for a layer between 20-40 hPa for the periods 8 October to 31 December 2003 and 1 January to 31 March 2004. The timeseries illustrate again that the analysis is drawing to the data.

2.3.2 Validation against independent observations

The ECMWF ozone field is compared with independent observations to assess its quality and hence indirectly the quality of the MIPAS ozone profiles that are used in the analysis. The ECMWF ozone field is compared

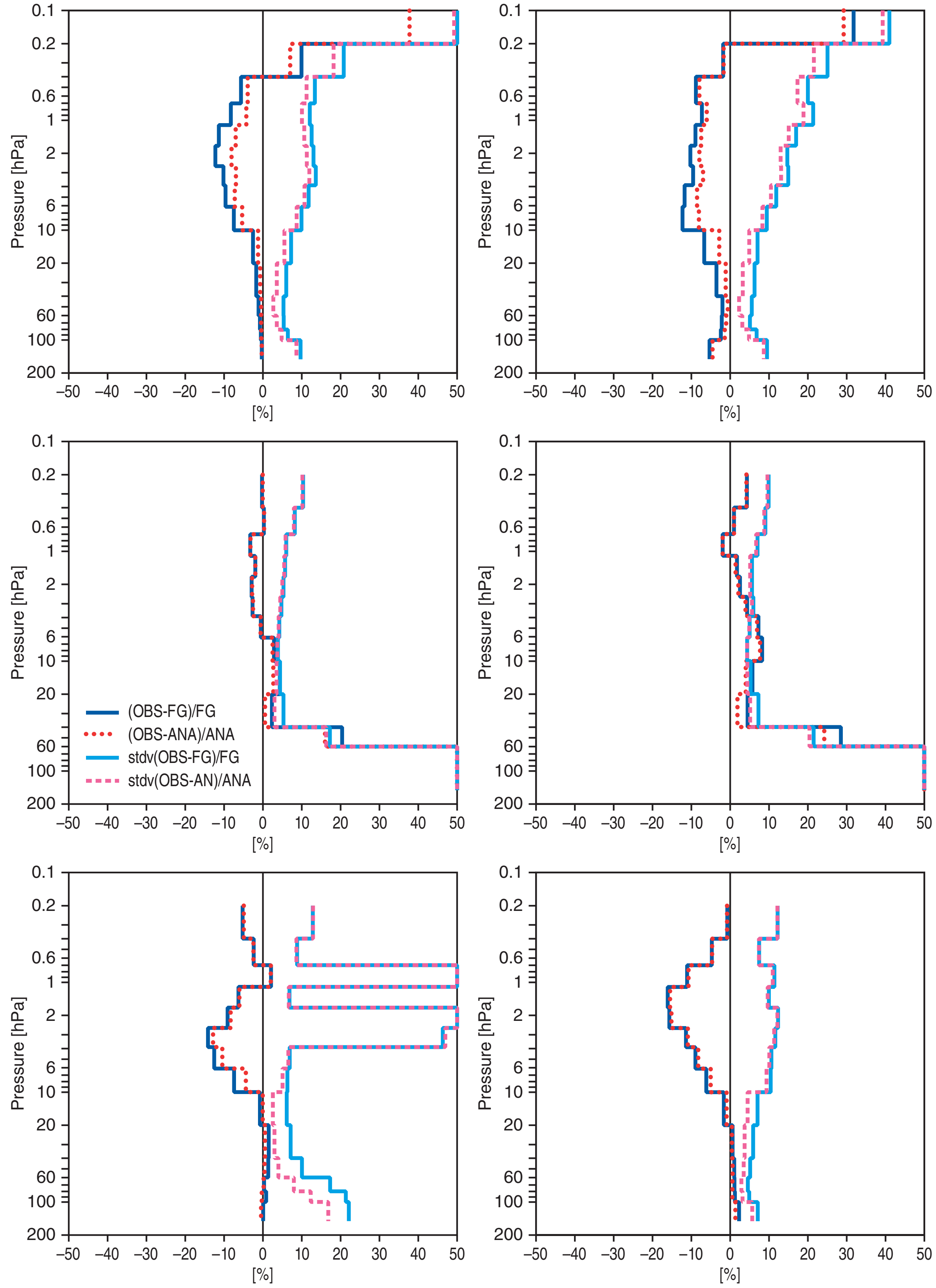


Figure 8: Profiles of time and area averaged MIPAS ozone departures in % for the areas 90-65° N (top), 0-20° S (middle), and 65-90° S (bottom). Averaging periods are 8 October to 31 December 2003 (left) and 1 January to 31 March 2004 (right).

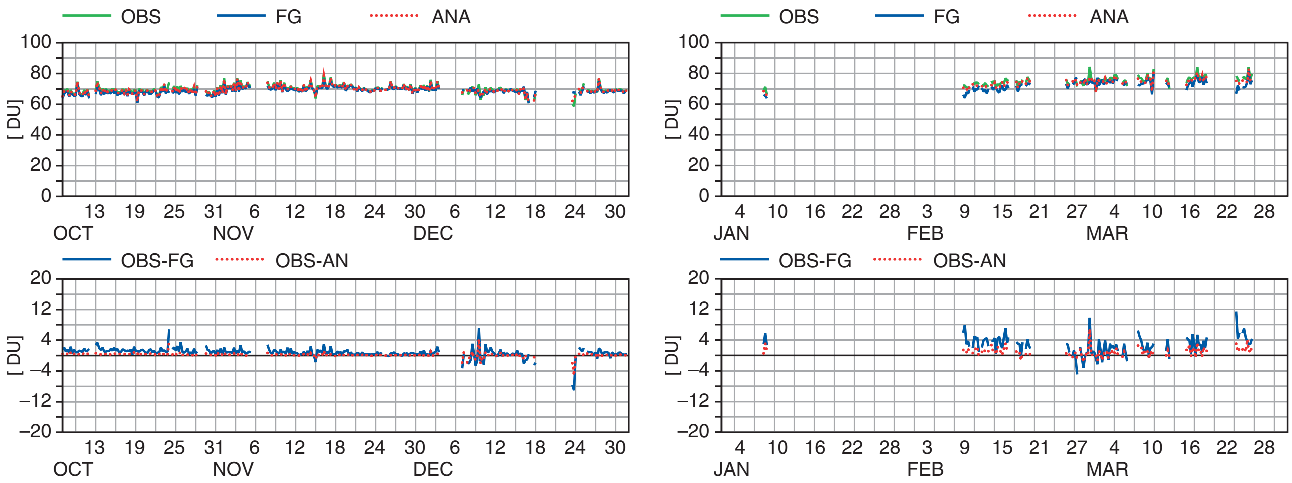


Figure 9: Timeseries of globally averaged ozone data in a layer between 20-40 hPa covering the periods 8 October to 31 December 2003 (left) and 1 January to 31 March 2004 (right). The top panels show MIPAS ozone layers, first-guess and analysis values, the bottom panels first-guess and analysis departures. All ozone values are in DU.

with TOMS total column ozone data and with ozone sonde profiles.

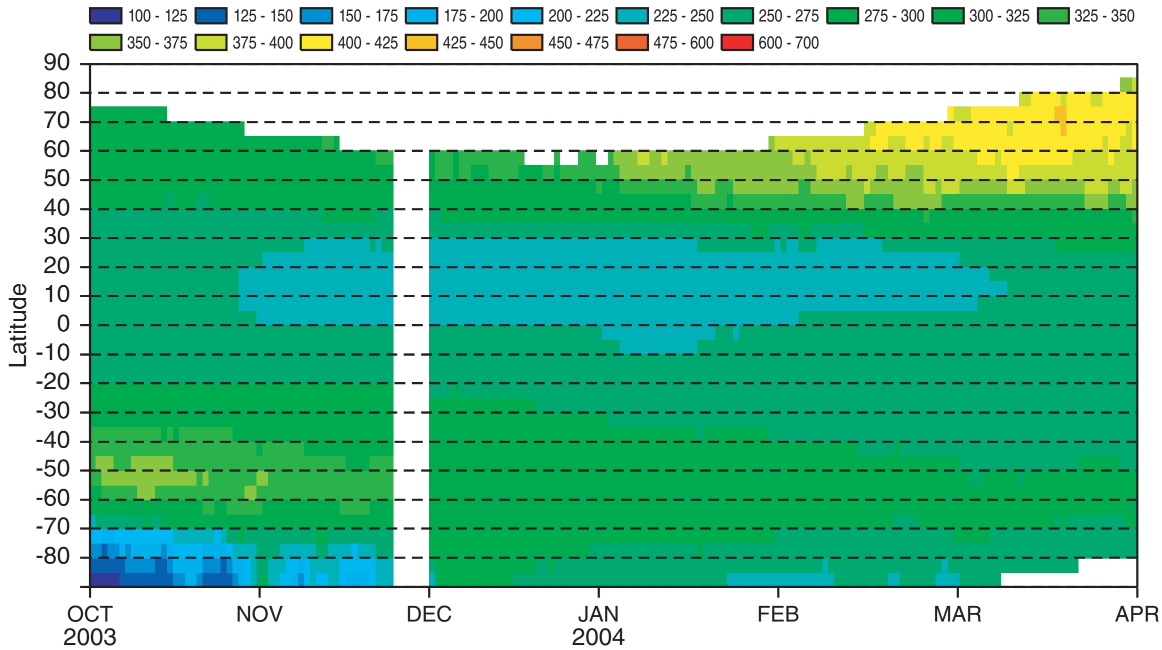
Figure 10 shows a timeseries of zonal mean total column ozone from TOMS (http://toms.gsfc.nasa.gov/index.html) and from the ECMWF analysis from 8 October 2003 to 31 March 2004. The ECMWF ozone analysis captures well the seasonal cycle of the ozone field (e.g. ozone hole during October, change to lower ozone values in the circum-antarctic belt from October to March, increased Ozone column at high latitudes in northern winter/spring). However, ECMWF ozone values are larger than TOMS values in the tropics and in the northern hemisphere (NH).

This bias is also apparent in Figure 11 that shows total column ozone from TOMS and from the ECMWF analysis on 15 November 2003. In the zonal mean the ECMWF total column ozone values are 5-10% larger than TOMS data, with the largest differences in the NH.

Next, comparisons with ozone sonde profiles are carried out for four NH, four tropical and one Antarctic station. The NH sondes were obtained from the Norwegian Air Research Institute (NILU), the tropical sondes from the Southern Hemisphere Additional Ozonesondes (SHADOZ) project website (http://croc.gsfc.nasa.gov/shadoz/) (Thompson, et al. 2003a,Thompson, et al. 2003b), and the sondes at the Antarctic Neumayer stations were obtained from the World Ozone and UV Radiation Data Centre (http://www.msc.ec.gc.ca/woudc/). Seasonal mean ozone profiles for October to December 2003 (OND), and for January to March 2004 (JFM) are calculated. Only sondes reaching above 40 hPa are used in the validation studies, and the ERA-40 ozone profiles are the analysis profiles from the grid point closest to the sonde location at the closest analysis time.

The NH seasonal mean profiles (Figure 12) generally show good agreement between the analysis and the sonde profiles. The analysis slightly overestimates the magnitude of the ozone maximum compared to the sondes, but on the whole the mean profiles and the standard deviations agree well. Differences between the sondes and the analysis are larger in JFM than in OND. The reason for this is that the ECMWF model has a positive ozone bias in the NH extratropics during winter and spring (Dethof and Hólm 2004). Because there are fewer MIPAS data available in JFM than in OND, MIPAS data have less impact on the analysis.

The tropical profiles (Figure 13) also show a good agreement between the analysis and the sondes. There is no systematic overestimation of the ozone maximum at the stations shown in Figure 13, despite the positive total column ozone bias seen in comparison with TOMS (Figure 11). At Samoa and Nairobi the analysis



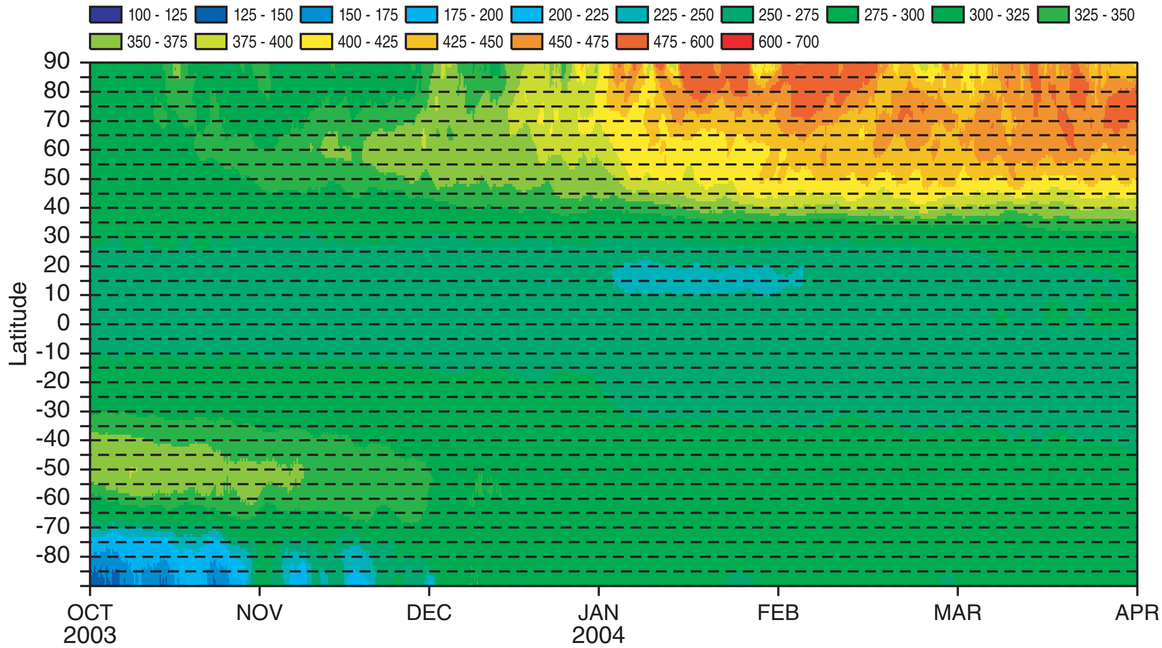


Figure 10: Timeseries of zonal mean total column ozone in DU from TOMS (top) and ECMWF analysis (bottom) from 8 October 2003 to 31 March 2004.

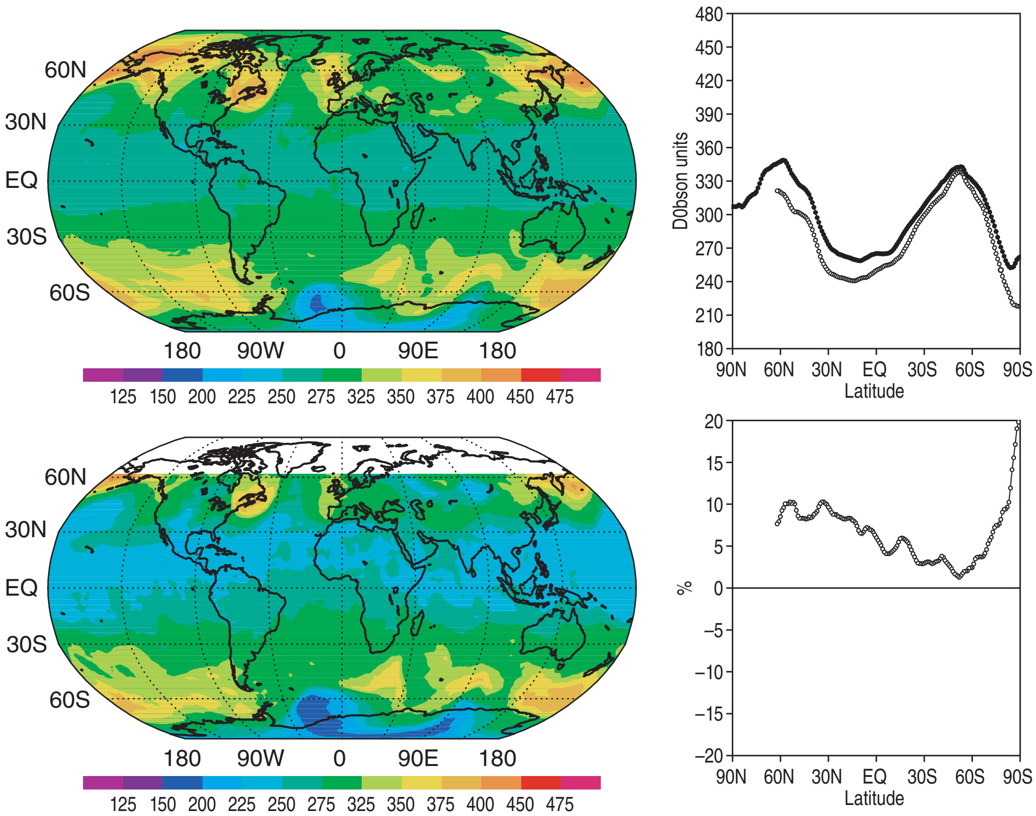


Figure 11: Left: Total column ozone in DU on 15 November 2003 from the operational ECMWF analysis (top) and from gridded daily TOMS data (bottom). Right: The top panel shows the zonal mean ozone values from the analysis (solid line) and from TOMS data (open circles), the bottom panel shows the relative difference in % between the analysis and TOMS.

overestimates the ozone maximum, at Paramaribo and Irene it underestimates it. Ozone values near the surface are overestimated in the analysis at all stations.

At the Antarctic Neumayer station the agreement between the analysis and the ozone sondes is good, both for the mean profile and for the standard deviation. The analysis captures the large variability between October, when ozone is almost completely depleted between 60-100 hPa, and December 2003. Ozone near the surface is again overestimated in the analysis.

While the comparisons with the ozone sondes show a good agreement between the analysis ozone profiles and the independent data, the agreement between TOMS and the total column ozone analysis is less good (Figure 11). These differences in the total column ozone fields are surprising because they were not seen in earlier assimilation experiments of MIPAS ozone profiles (Dethof 2003b), and they were also not seen in the CY26R3 experimental suite (e-suite) that preceeded the operational implementation of CY26R3, and that was run from 1 June to 6 October 2003. The e-suite total column ozone analyses generally show good agreement with TOMS (zonal mean differences less than 5%), but from the second half of October 2003 onwards the differences with TOMS increase in the operational suite. This is due to a change to lower total column ozone values in the tropics seen in TOMS data from the second half of October onwards, that is not reproduced by the analysis. The reason for the differences between TOMS and the analysis is not clear. It might be due to a seasonal change that is not captures in the analysis or the MIPAS data. Unfortunately, we do not have any good quality SCIAMACHY data available for this period, that would allow an independent validation of TOMS data and the analysis' ozone column.

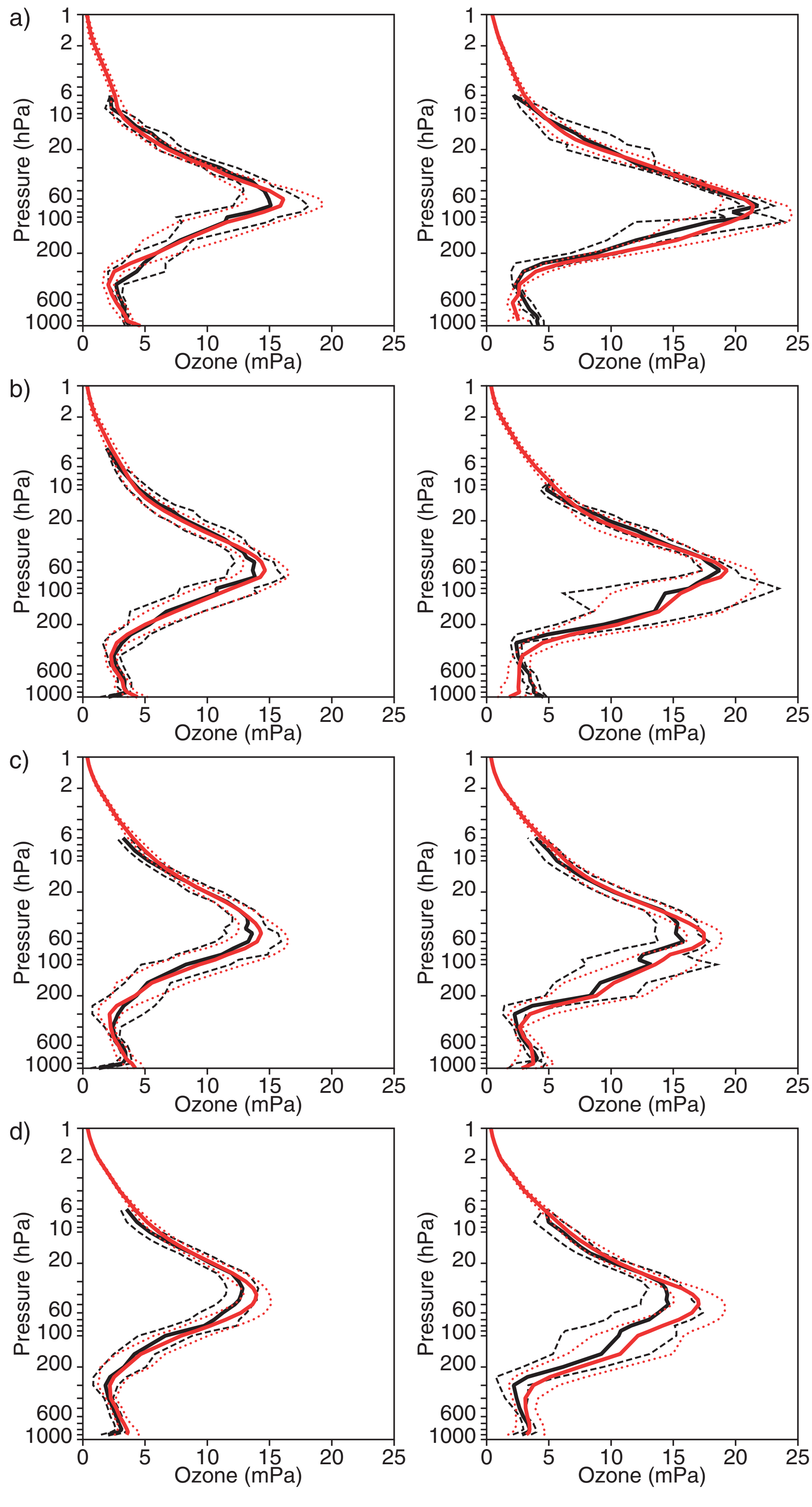


Figure 12: Mean ozone profiles for the period 8 October to 31 December 2003 (left) and 1 January to 31 March 2004 (right) at (a) Ny-Aalesund (79°N, 12°E), (b) Sodankyla (67.2°N, 26.4 °E), (c) Legionowo (52°N, 21°E) and (d) Hohenpeissenberg (47.8°N, 11.0°E). Shown are sondes (black solid) ± standard deviation (black dashed) and analysis profiles (red solid) ± standard deviation (red dotted).

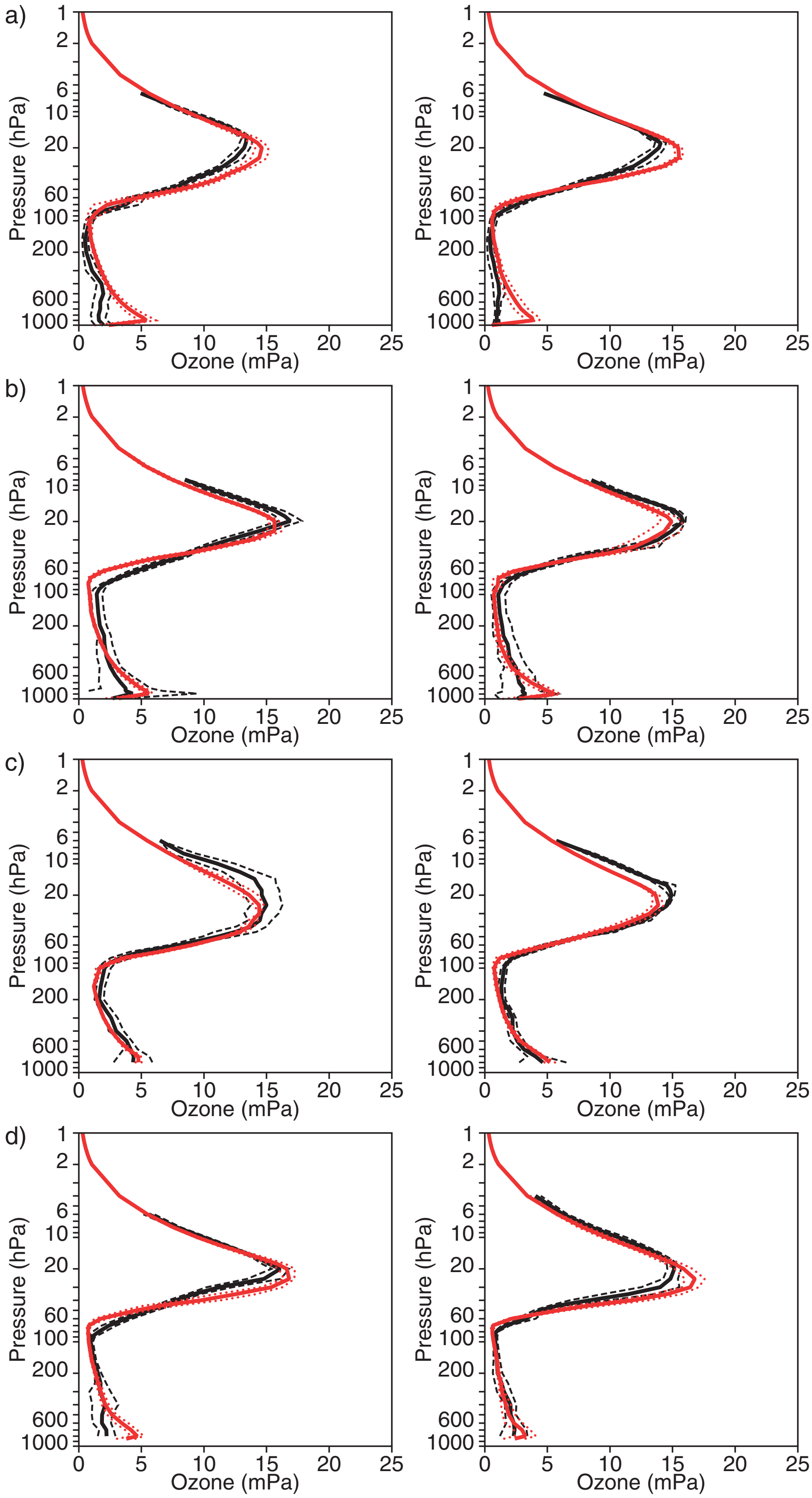


Figure 13: Like Figure 12 but for the tropical stations (a) Samoa (14.2°S, 170.6°W), (b) Paramaribo (5.8°N, 55.2°W), (c) Irene (25.9°S, 28.2°E) and (d) Nairobi (1.3°S, 36.8°E).

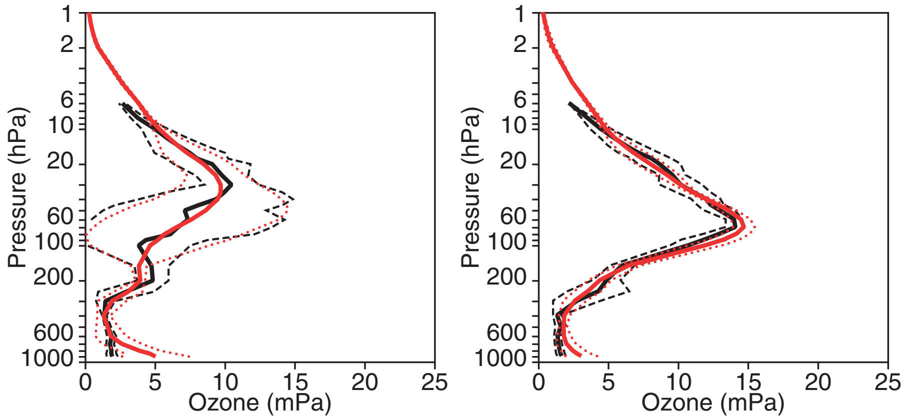


Figure 14: Like Figure 12 but for the Antarctic Neumayer station (70.7°S, 8.3°W).

To assess if the assimilation of MIPAS ozone profiles improves or degrades the fit of the total column ozone analysis field with TOMS data, two assimilation experiments (CY26R3, resolution T159) are run. Both experiments are started from the operational analysis on 1 November 2003, 0z, and are run until 15 November 2003, 18z. The control experiment (Exp-A) uses the operational set up (MIPAS ozone actively assimilated), while in Exp-B MIPAS data are not assimilated.

Figure 15 shows the difference of the total column ozone field in DU of Exp-B and Exp-A on 15 November 2003. Without the assimilation of MIPAS ozone data, total column ozone values in Exp-B are 10-20 DU lower than in Exp-A between 60°N and 60°S. Only at high northern latitudes and at the remains of the ozone hole in the SH are values lower if MIPAS data are assimilated. Without the assimilation of MIPAS data the agreement with TOMS in the zonal mean is improved between 55°N and 60°S (Figure 16), with the largest improvement in the tropics.

Comparisons with tropical ozone sondes from the SHADOZ project (Figure 17) show that analysis ozone values around the ozone maximum are increased if MIPAS ozone retrievals are assimilated. The differences between Exp-A and Exp-B at the maximum are large enough to explain the total column differences seen between the experiments in Figure 15. However, the profiles from Exp-A (MIPAS assimilated) agree better with the sondes than the profiles from Exp-B, suggesting that the assimilation of MIPAS ozone data improves the ozone analysis around the ozone maximum in the tropics. The tropical profiles also show differences between the analysis and the sondes in the troposphere (Figures 14 and 17). In most cases the analysis overestimates ozone near the surface compared to the sondes. If MIPAS data are assimilated this difference is slightly reduced, but the overestimation remains. Hence, a possible explanation for the worse fit of the analysis to TOMS data if MIPAS ozone profiles are assimilated is the following. Without the assimilation of MIPAS data there are two problems with the ECMWF ozone profiles in the tropics that have an opposite impact on the ozone column (underestimation of the ozone maximum, overestimation of tropospheric ozone). The assimilation of MIPAS ozone profiles improves the stratospheric ozone by increasing the ozone values around the ozone maximum. However, because it does not cure the problem of too high ozone values in the lower troposphere, the total column values of the analysis increase, degrading the agreement with TOMS.

2.4 Summary MIPAS

MIPAS temperature values are larger than ECMWF temperatures in the stratosphere, but departures are smaller than 1%. Larger departures can be seen at the model top.

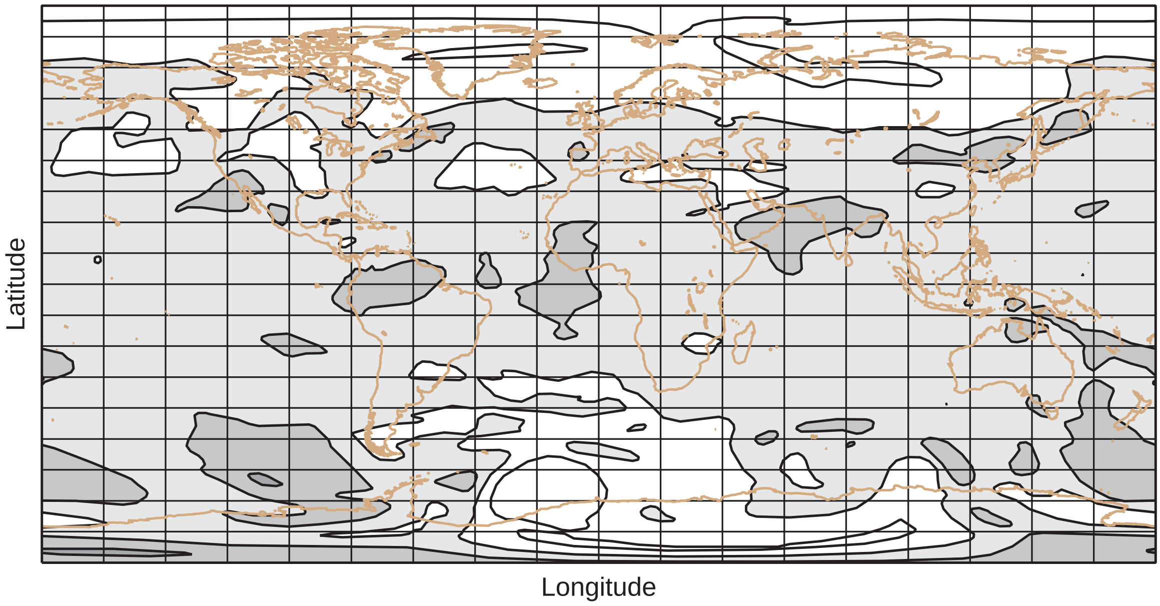


Figure 15: Difference of total column ozone in DU of Exp-B and Exp-A on 15 November 2003, 12z. Contour interval is 10 DU and negative values are shaded.

Even though MIPAS temperatures have never been assimilated in the ECMWF data assimilation system, they proved to be a useful independent data set in the past and helped to identify problems with the ECMWF temperatures caused by the assimilation of radiances from the AIRS instrument (Dethof 2003a).

MIPAS water vapour values are larger than ECMWF values almost everywhere. The departures are greater than 20% over much of the stratosphere. While the ECMWF model is known to have a dry bias, this bias should not be larger than 10-15%, and is hence not large enough to explain all of the departures. MIPAS water vapour values in the stratosphere are too high.

The assimilation of MIPAS ozone profiles leads to a good agreement of the analysed ozone profiles with independent ozone sondes (see also Dethof (2003)b). However, the fit of the total column ozone analysis to independent TOMS data is degraded, because the assimilation of MIPAS data increases ozone around the ozone maximum which leads to an increased ozone column and worse agreement with TOMS. This disagreement is puzzling, because it had not been observed in previous assimilation experiments that had shown an improved fit to TOMS if MIPAS ozone profiles were assimilated. When MIPAS operations resume, the impact of the assimilation of MIPAS ozone profiles on the total column ozone analysis will have to be carefully studied before the operational assimilation of MIPAS ozone data will be continued. SCIAMACHY total column ozone data might then serve as a useful independent data set.

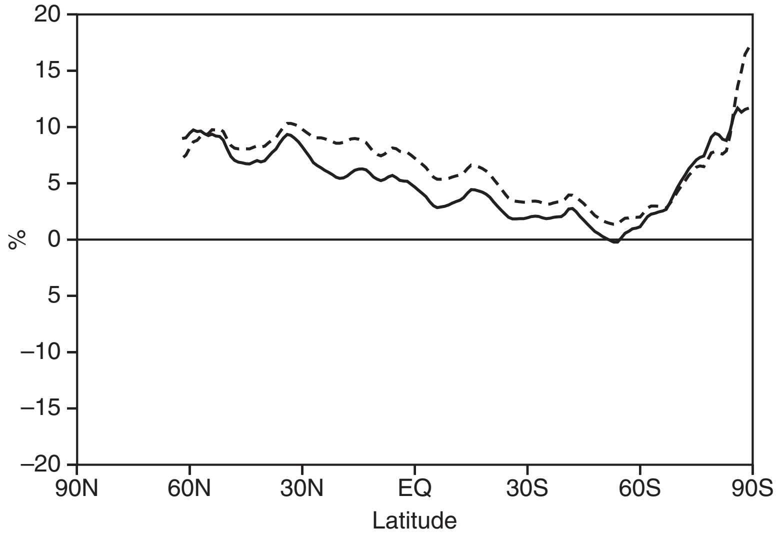


Figure 16: Relative difference in % of zonal mean total column ozone from Exp-A and TOMS (dashed) and Exp-B and TOMS (solid) on 15 November 2003.

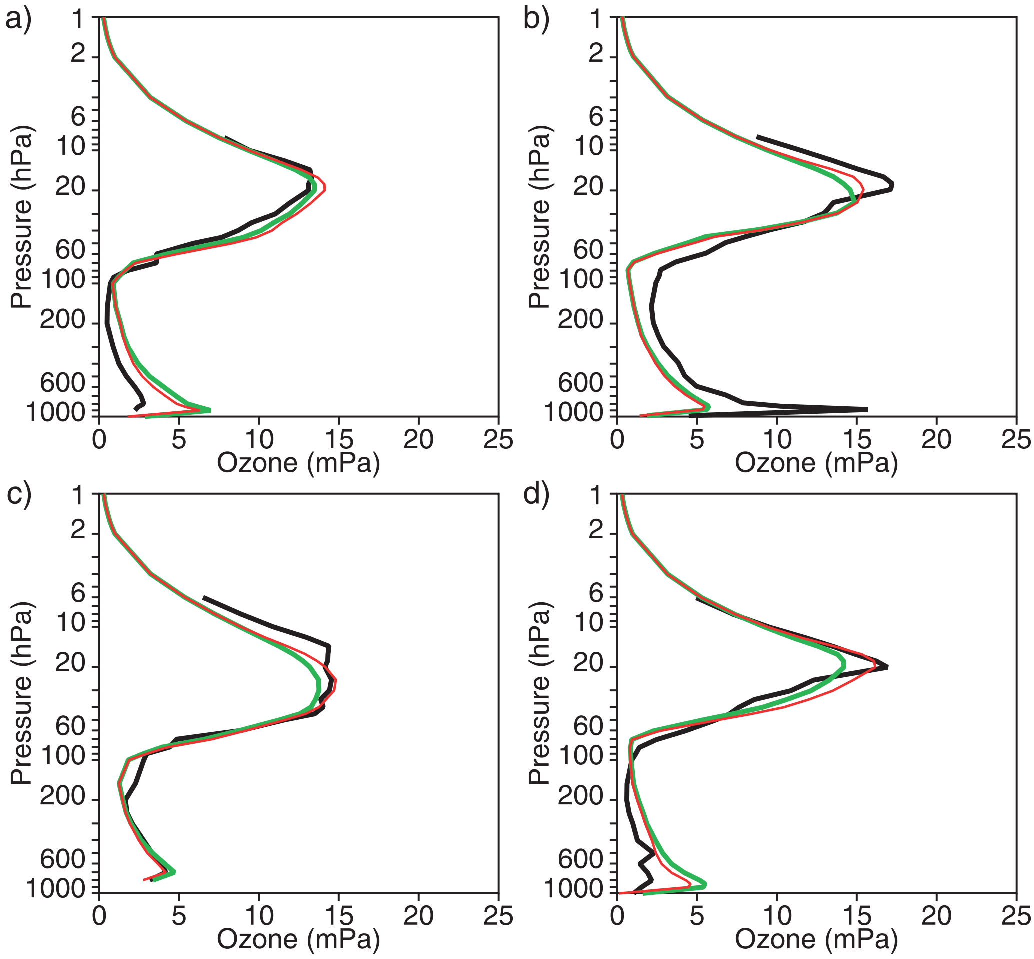


Figure 17: Ozone profiles for the tropical stations (a) Samoa (14.2° S, 170.6° W) on 7 November 2003, (b) Paramaribo (5.8° N, 55.2° W) on 12 November 2003, (c) Irene (25.9° S, 28.2° E) on 12 November 2003 and (d) Malindi (3.0° S, 40.2° E) on 13 November 2003. Shown are sondes (black), profiles from Exp-A (red) and profiles from Exp-B (green).

3 Monitoring and assimilation of SCIAMACHY NRT total column ozone retrievals

SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY) (Burrows et al. 1998) measures radiation in the wavelength region 240-2380 nm at moderate spectral resolution (0.2 nm - 1.5 nm). SCIAMACHY provides global measurements of various trace gases including ozone in the troposphere and stratosphere, as well as information about aerosols and clouds. SCIAMACHY measures in three viewing modes: nadir, limb and occultation. NRT total column ozone retrievals from the nadir measurements are produced operationally by ESA and also by KNMI. Both ESA and KNMI NRT SCIAMACHY ozone retrievals have been monitored passively at ECMWF in the operational suite, the NRT data produced by ESA (SCI_RV__2P) since February 2003, and the KNMI NRT data since March 2004.

3.1 Monitoring of NRT SCIAMACHY ozone columns produced by ESA (SCI_RV__2P)

Figure 18 shows timeseries of globally averaged SCIAMACHY total column ozone data (ESA's SCI_RV__2P product), as well as globally averaged departures (averaged over 6-hourly analysis cycles) between 8 October 2003 and 30 September 2004. The SCIAMACHY data have a negative bias with respect to the ECMWF analysis. This bias is around -30 DU in the global mean from October 2003 to April 2004, and decreases to values of less than -20 DU after an algorithm change on 27 April 2004. At least part of the remaining bias is due to problems in the ECMWF model that is known to overestimate ozone in the extratropics at certain times of year (Dethof and Hólm 2004).

From mid-March 2004 to the end of April 2004 SCIAMACHY ozone data were not stable, and Figure 18 shows several sudden changes in the data during this period. A change to unrealistically large SCIAMACHY ozone columns (greater than 400 DU in the global mean) occurred on 13 March 2004. This was the result of the use of a wrong initialization file in the retrieval. This error was corrected, and on 24 March 2004 SCIAMACHY values returned to what they had been before 13 March. However, another change, this time to lower SCIAMACHY values, occurred around 26 March 2004 after a PMD/SF ADC calibration was performed, resulting in global mean analysis departures of -60 DU from the end of March 2004 onwards. After an algorithm update was implemented on 27 April 2004 the situation improved and SCIAMACHY ozone values increased. Since then, they have been closer to ECMWF values, with global mean analysis departures of around -20 DU. Another problem period with increased departures is seen between 18 and 28 June 2004, when the instrument was decontaminated (heated to reduce the ice build-up that affects various channels). Apart from this decontamination period SCIAMACHY data have been relatively stable since 27 April 2004.

The changes that affected the SCIAMACHY NRT data can also be seen when looking at timeseries of zonal mean total column ozone values (Figure 19) and of zonal mean total column analysis departures (Figure 20). For example, unrealistically large ozone values (greater than 500 DU) can be seen in the tropics during March 2004, as can the change to lower ozone values and increased analysis departures after 27 March 2004, the change to larger ozone values and smaller departures on 27 April 2004, and changes during the decontamination period from 18 to 28 June 2004. The plots of the zonal mean analysis departures (Figure 20) also show large departures at high latitudes in both hemispheres. These departures are likely to occur at high solar zenith angles (SZA) and could point to a problem with the retrieval at high SZA. Unfortunately, the NRT SCI_RV__2P data do not include any geolocation information like SZA, which are included in the off-line level 2 data. Consequently, data or retrieval problems related to these parameters can not be identified by monitoring the NRT data.

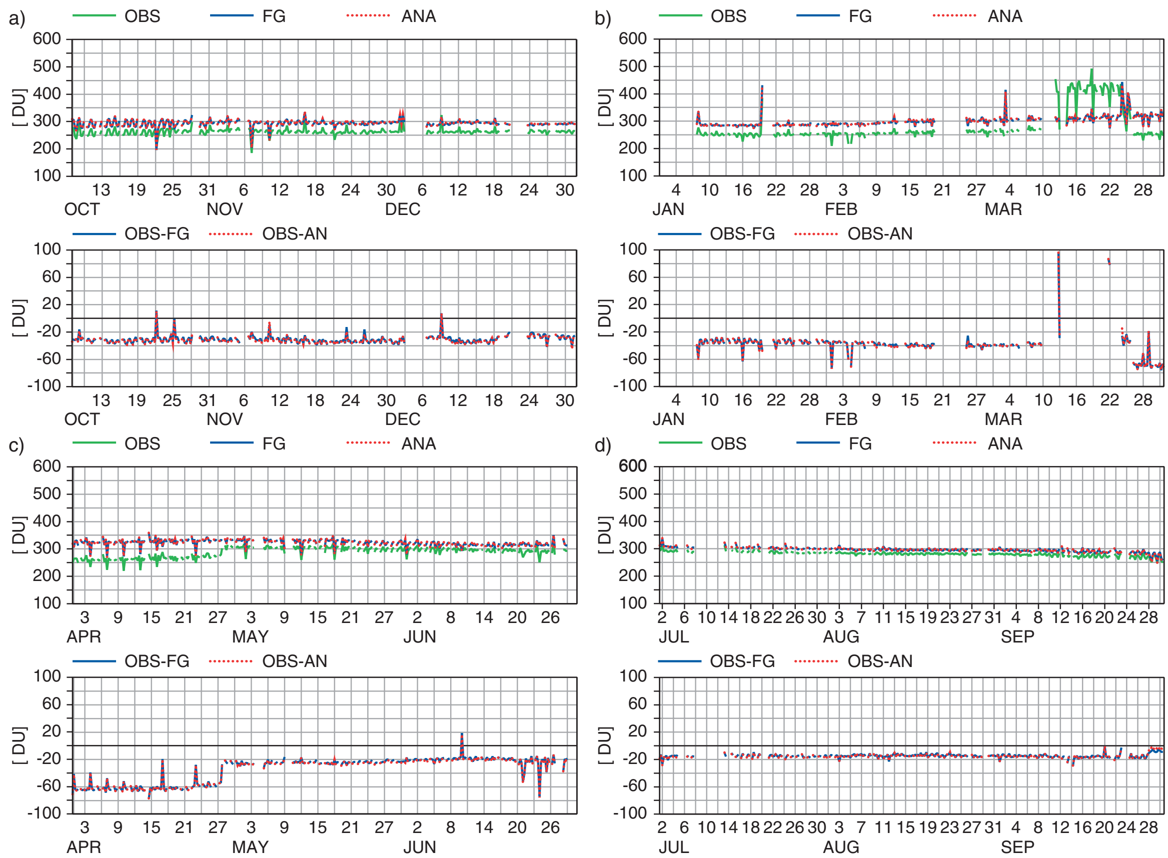


Figure 18: Timeseries of globally averaged data covering the periods (a) 8 October to 31 December 2004, (b) 1 January to 31 March 2003, (c) 1 April to 30 June 2004 and (d) 1 July to 30 September 2004. The top panels show SCIAMACHY NRT total ozone observations, first-guess and analysis values, the bottom panels first-guess and analysis departures. All ozone values are in DU.

3.2 Monitoring and assimilation of NRT TOSOMI SCIAMACHY ozone column retrievals produced by KNMI

3.2.1 *Monitoring of TOSOMI total column ozone data*

In addition to the ESA NRT SCIAMACHY ozone columns, NRT total column ozone retrievals from SCIAMACHY produced by KNMI have also been monitored passively at ECMWF since March 2004. The KNMI retrieval uses the TOSOMI algorithm, a modified version of the DOAS method that had been developed to retrieve total column ozone fields from OMI (Ozone Monitoring Instrument) (Veefkind and de Haan 2001). The TOSOMI SCIAMACHY data compare well with ground based observations (Brinksma 2004). The monitoring statistics accumulated at ECMWF show the TOSOMI data to be more stable than the ESA NRT product and to agree better with the ECMWF analysis. This is illustrated in the timeseries of observations and departures of ESA and KNMI SCIAMACHY data from 1 March to 30 June 2004 (Figure 21). While the ESA data show several changes during March and April 2004, the KNMI data are stable during this period. Also, the low bias seen in the ESA data prior to the algorithm update on 27 April 2004 is not seen in the KNMI data. Since the algorithm update on 27 April 2004 the two datasets agree well in the global mean. The standard deviations of both datasets and of their analysis departures also agree well.

While the datasets agree well in the global mean after 27 April 2004, there are still some regional differences between the retrievals. Figure 22 shows scatter plots of SCIAMACHY ozone columns for June 2004 plotted

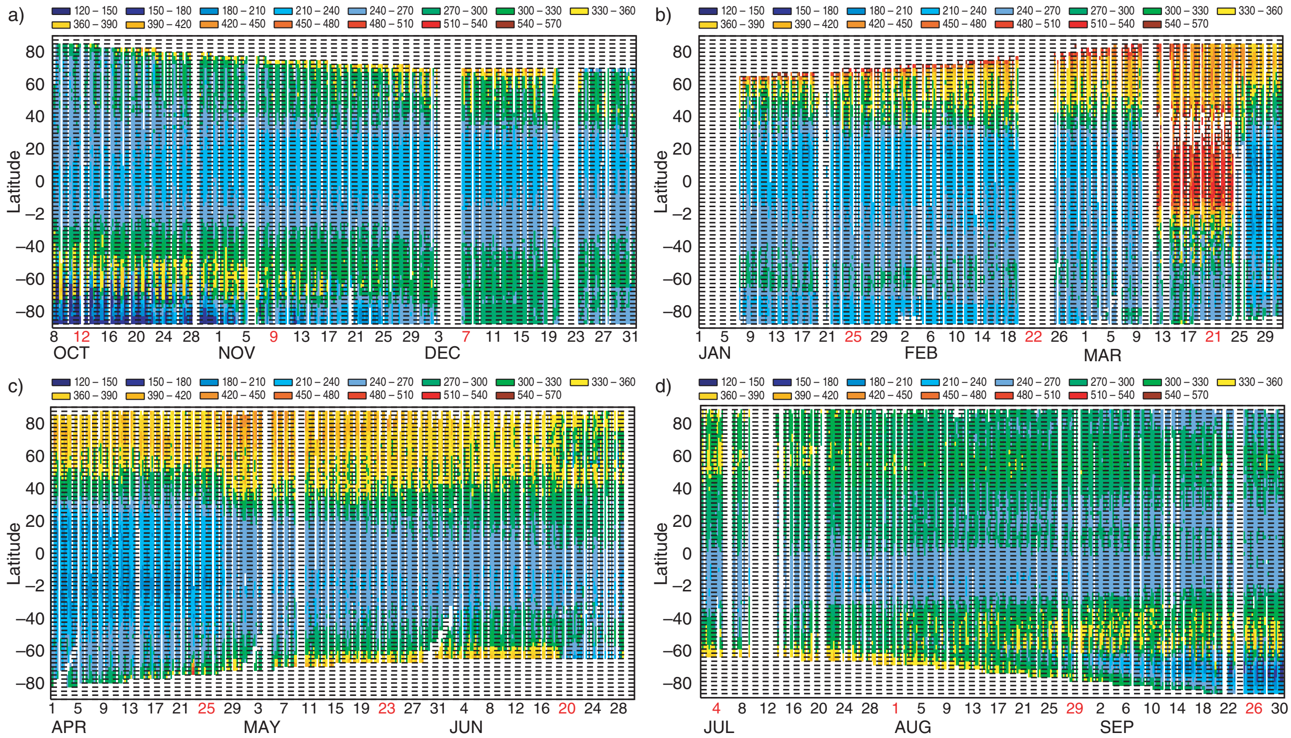


Figure 19: Timeseries of zonal mean NRT SCIAMACHY total column ozone values in DU for the periods (a) 8 October to 31 December 2003, (b) 1 January to 31 March 2004, (c) 1 April to 30 June 2004, and (d) 1 July to 30 September 2004.

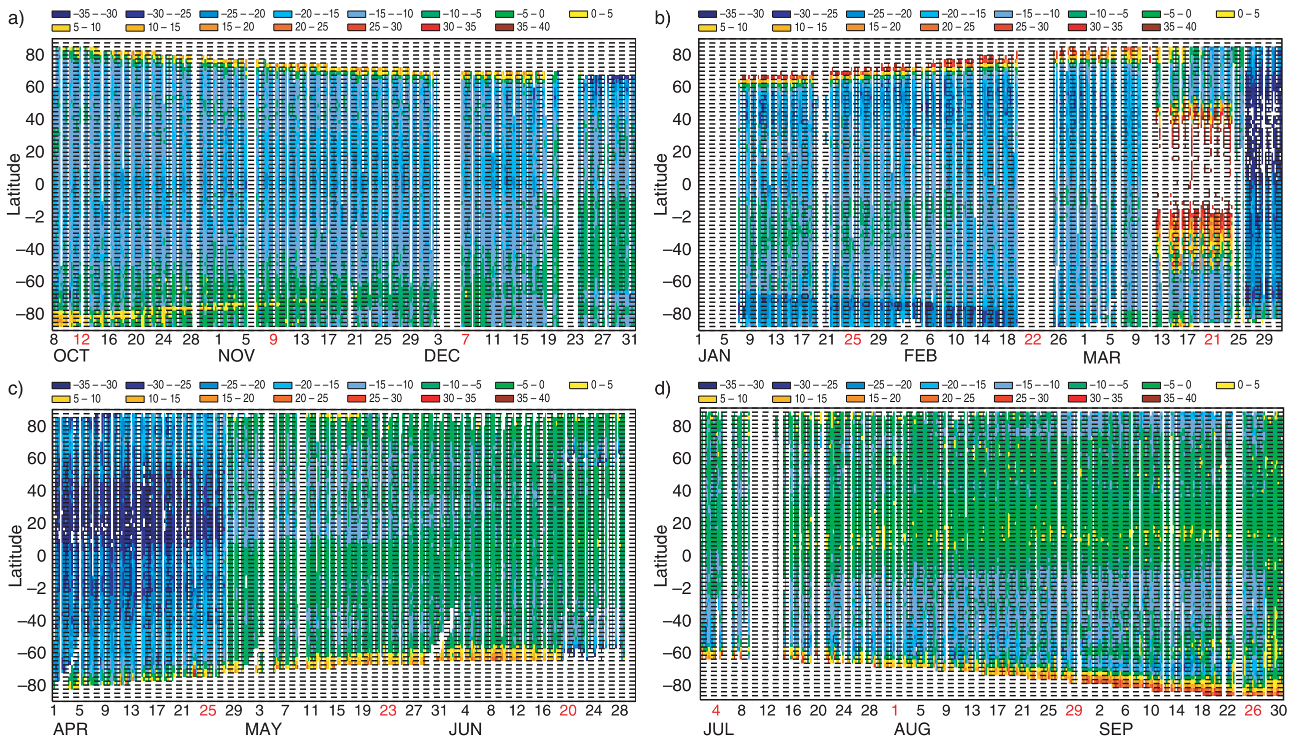


Figure 20: Like Figure 19 but showing NRT SCIAMACHY total ozone analysis departures in %.

against latitude for ESA and KNMI retrievals. The figure illustrates that while the data agree well in the tropics there are differences in the extratropics in both hemispheres. The ESA retrievals have values as low as 120 DU between 50-60°N and also around 60-70°S, which are not seen in the KNMI retrievals. The ESA data also show larger ozone values (up to 460 DU) south of 60°S, which are again not seen in the KNMI data. Looking at the geographical distribution of analysis departures for both data sets (Figure 23) shows that these large ozone values correspond to large analysis departures for the ESA data around 60°S (already seen in Figure 20). Again this points to problems with the retrieval at high SZA. The geographical plots also show areas around 60° in both hemispheres where the ESA data have unrealistically low values, leading to large negative analysis departures.

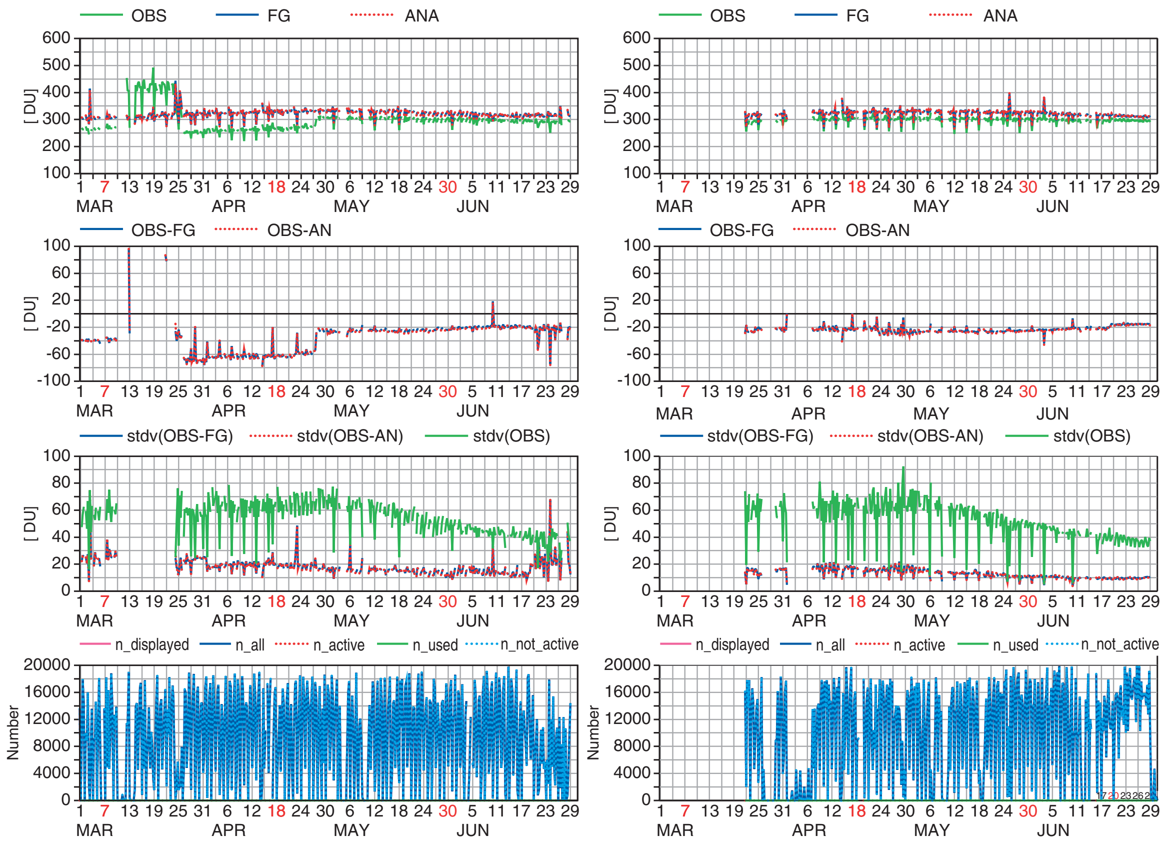


Figure 21: Timeseries of global mean ESA (left) and KNMI (right) NRT SCIAMACHY data for the period 1 March to 30 June 2004. The top panels show SCIAMACHY observations, first-guess and analysis values, the second panels first-guess and analysis departures, the third panels the standard deviation of the observations and departures, and the fourth panel the number of observations per 6-hour cycle. All ozone values are in DU.

3.2.2 Impact of the assimilation of TOSOMI total column ozone data

A number of T159, 6-hour 4D-Var assimilation experiments (model cycle 28r2) are run to assess the impact of the assimilation of KNMI SCIAMACHY ozone columns on the ECMWF system. Two experiments are started on 24 April 2004 and run until 23 May 2004. The control experiment (Exp-1) uses the operational setup, which includes the assimilation of SBUV/2 ozone layers from NOAA-16. In the other experiment (Exp-2), NRT TOSOMI SCIAMACHY ozone columns are assimilated in addition to the SBUV/2 data. Two further experiments (Exp-3 and Exp-4) are started on 15 February 2004 and run until 29 February 2004. Exp-3 is the control experiment and in Exp-4 SCIAMACHY data are active. These two experiments include the assimilation

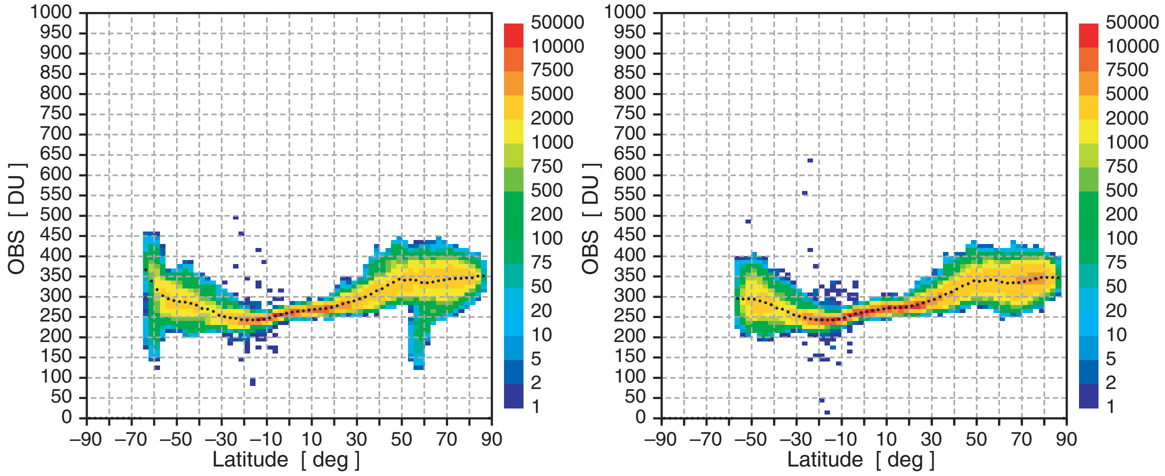


Figure 22: Scatter plots for June 2004 of ESA (left) and KNMI (right) NRT SCIAMACHY total column ozone in DU plotted against latitude. The colours give the number of observations per bin, and the black dots the mean per bin.

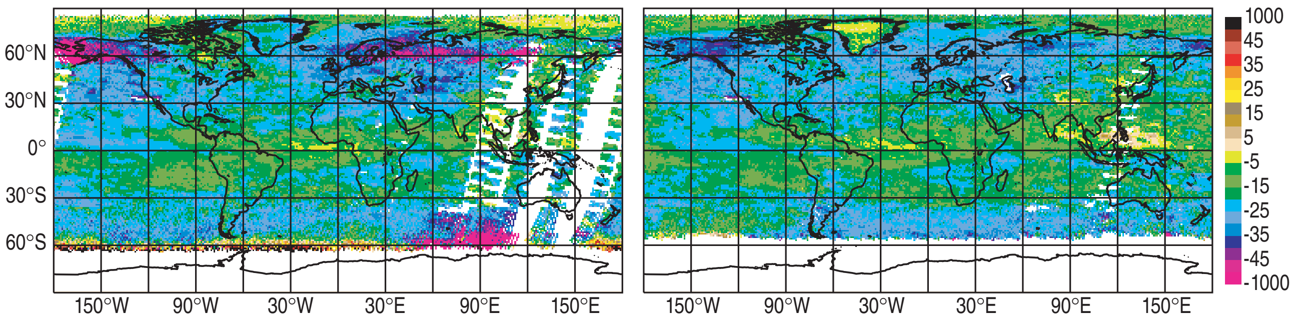


Figure 23: Geographical distribution of monthly mean analysis departures in DU for June 2004 for ESA (left) and KNMI (right) NRT SCIAMACHY data.

of ozone profiles from MIPAS and of ozone layers from SBUV/2 on NOAA-16. The SCIAMACHY data have a horizontal resolution of 30 km x 60 km, but are pre-thinned to a horizontal resolution of 1°x1° in all experiments.

Results of the April/May experiments The timeseries in Figure 24 shows that in control experiment Exp-1 the SCIAMACHY data are about 20 DU lower than the analysis in the global mean. When SCIAMACHY data are assimilated the analysis is drawing to the data, and the analysis departures are reduced to global mean values of less than -5 DU. The standard deviation of the analysis departures is also reduced.

The differences between the ozone analyses of the two experiments at the end of the experiments (23 May 2004) are shown in Figure 25. Total column ozone in Exp-2 is lower that total column ozone in the control experiment Exp-1 almost everywhere with maximum differences greater than -40 DU (Figure 25, top panel). In the vertical, the largest differences (in mPa) are seen between 20-100 hPa where ozone values in Exp-2 are reduced by up to 3 mPa (Figure 25, bottom panel).

In order to assess if the changes seen in the ozone analysis when TOSOMI SCIAMACHY data are assimilated are an improvement, the resulting ozone analysis fields are compared with independent observations. Comparison with daily gridded total column ozone data from TOMS (obtained from http://toms.gsfc.nasa.gov/index.html) on 23 May 2004 are shown in Figure 26. Total column ozone from the SCIAMACHY assimilation experiment

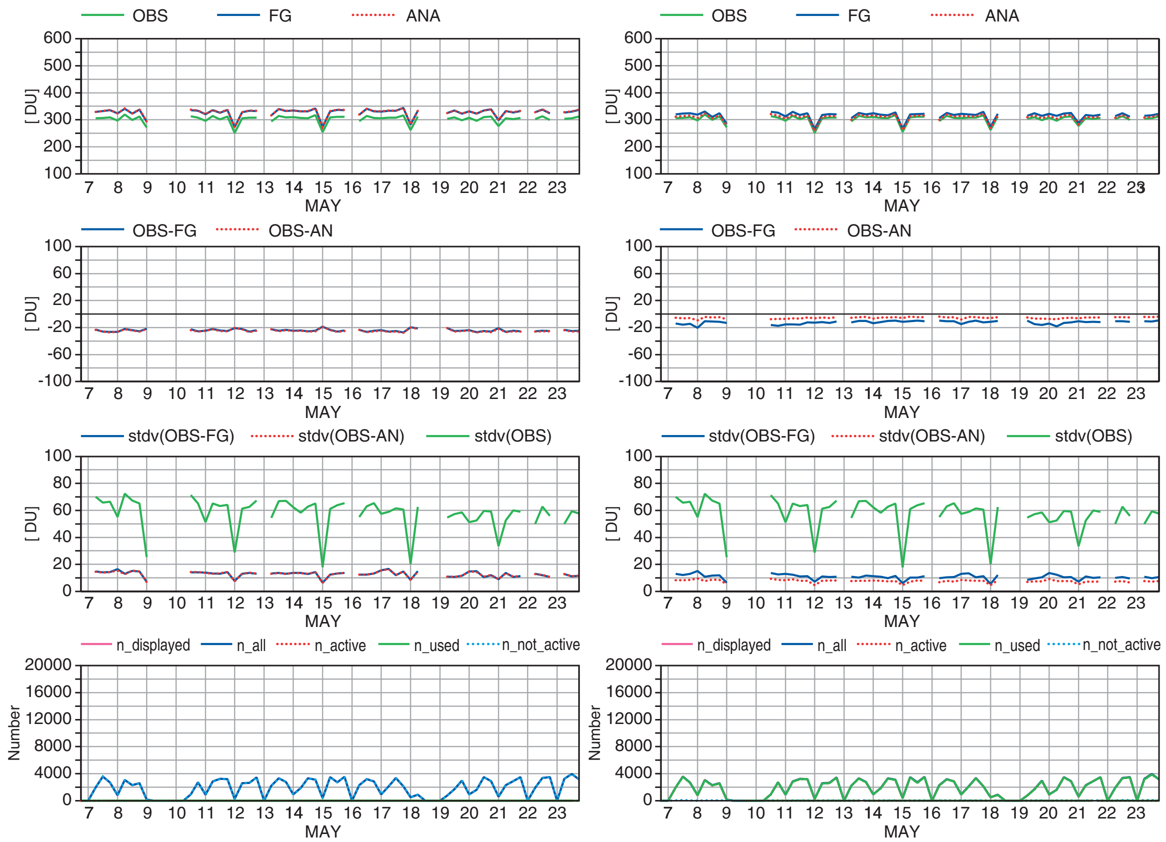


Figure 24: Timeseries of global mean SCIAMACHY and analysis values (top), analysis departures (2nd panel), standard deviations of observations and departures (3rd panel) and number of observation per 6-hour cycle (bottom panel) from the control experiment Exp-1 (left) and the SCIAMACHY assimilation experiment (Exp-2) for the period from 6 May 2004, 18z, to 23 May 2004, 18z.

Exp-2 agrees considerably better with the TOMS data, and the zonal mean differences between Exp-2 and TOMS are less than 5% everywhere.

Next, we look at analysis departures of SBUV/2 data from NOAA-16. These data are assimilated in both experiments. Figure 27 shows histograms of the SBUV/2 analysis departures for the lowest SBUV/2 layer (16 hPa - surface) from both experiments. The SBUV/2 analysis departures are reduced if SCIAMACHY data are assimilated. The global and time mean analysis departure is -10.5 DU in the control experiment Exp-1 and 3.2 DU in the SCIAMACHY experiment Exp-2.

Finally, ozone profiles from the two experiments are compared with ozone sondes (obtained from the Norwegian Institute for Air Research, NILU) for four European stations (Figure 28). Without the assimilation of SCIAMACHY data in Exp-1, the ozone maximum is overestimated at all four stations. In Exp-2 with the assimilation of SCIAMACHY ozone data, ozone values around the ozone maximum are reduced and the agreement with the sondes is improved.

Figure 29 shows forecast verification scores for 100 hPa vector wind root-mean square errors from the two experiments for 30 cases. The impact of assimilating SCIAMACHY data on the forecast scores is mainly neutral, with a slight degradation in the tropics that is significant at the 5% level.

Results of the February experiments The February experiments confirm that assimilating SCIAMACHY ozone columns leads to an improvement in the ozone field. This can be seen in Figures 30 to 32 showing

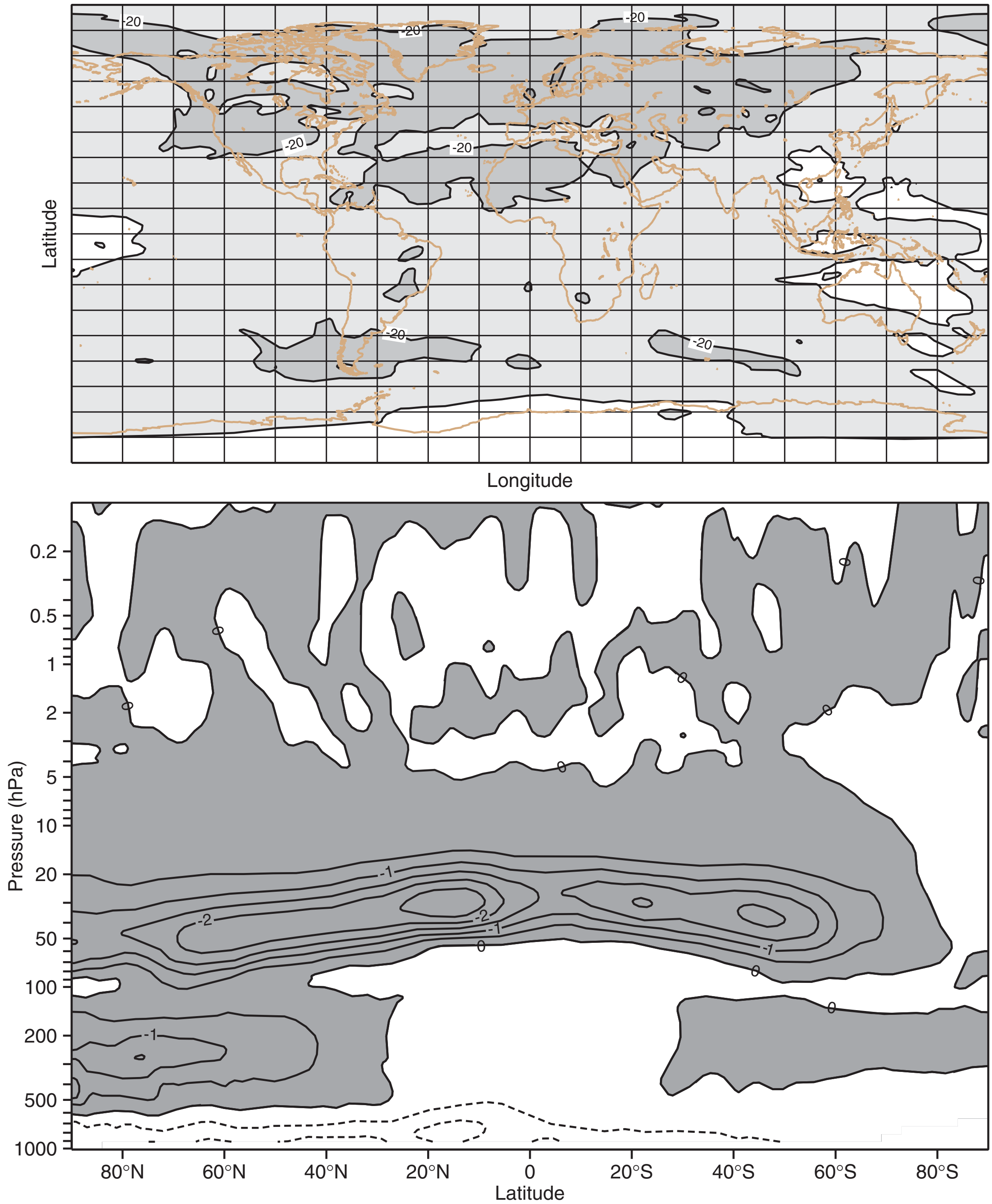


Figure 25: Top: Difference of total column ozone in DU of Exp-2 and Exp-1 on 23 May 2004, 12z. Contour interval is 20 DU and negative values are shaded. Bottom: Vertical cross section of zonal mean ozone differences in mPa of Exp-2 and Exp-1 on 23 May 2004, 12z. Contour interval is 1 mPa, negative values are shaded.

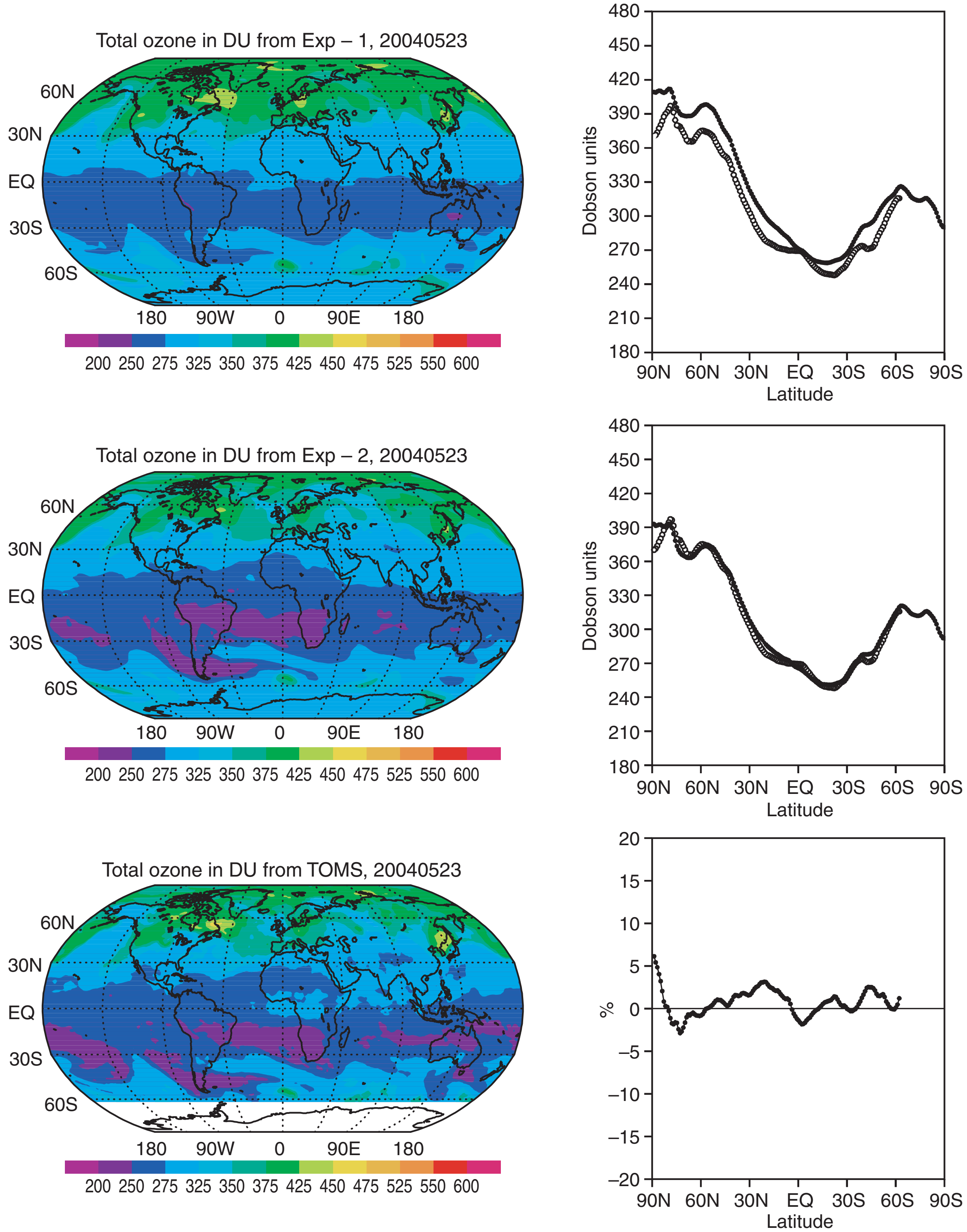


Figure 26: Left: Total column ozone in DU on 23 May 2004 from the control experiment Exp-1 (top), from the SCIAMACHY assimilation experiment Exp-2 (middle), and from gridded daily TOMS data (bottom). Right: The two top panels show the zonal mean ozone values from the experiments (solid line) and from TOMS data (open circles), the bottom panel shows the relative difference in % between Exp-2 and TOMS.

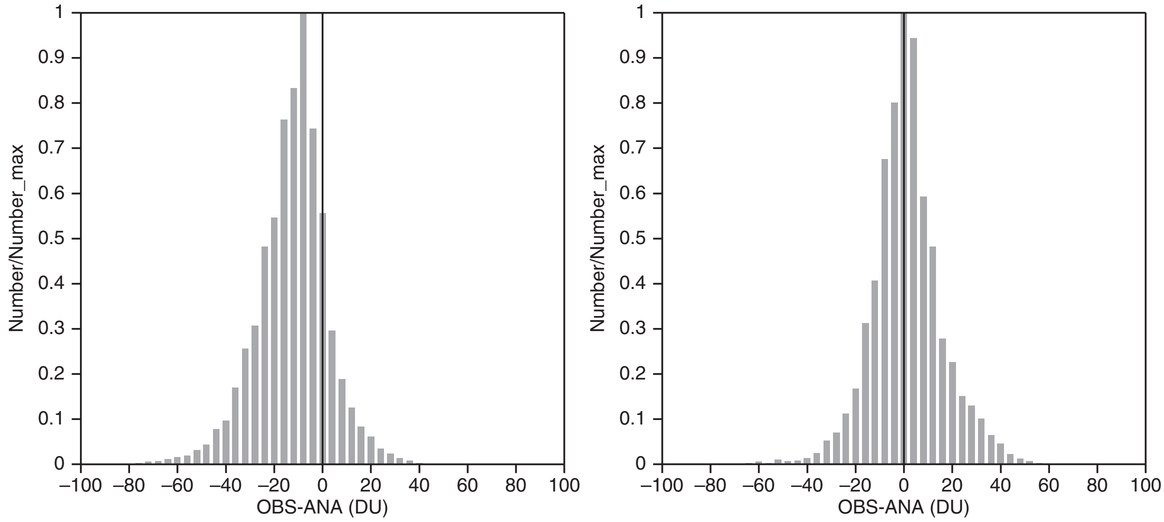


Figure 27: Frequency distribution of analysis departures of L6 (16 hPa-surface) from SBUV/2 from NOAA-16 from Exp-2 (left) and the control experiment Exp-1 (right) for the period 1 May 2004, 0z, to 23 May 2004, 18z.

comparisons with TOMS data, ozone sondes and SBUV/2 data from NOAA-16.

3.2.3 Summary SCIAMACHY

The assimilation of SCIAMACHY total column ozone data produced by KNMI's TOSOMI algorithm leads to a pronounced improvement of the analyzed ECMWF total column ozone field. Comparisons with ozone sondes show that the vertical distribution of the analysed ozone field is also improved in February and April/May 2004. The impact on the forecast scores of meteorological fields is mainly neutral, with a slight degradation at 100 hPa in the tropics. As a result of the research experiments it was decided to actively assimilate TOSOMI SCIAMACHY data in the operational ECMWF system. The assimilation of TOSOMI data underwent pre-operational testing (model cycle 28R3) from June to September 2004, and has been included in the operational ECMWF system since 28 September 2004. The impact of this can be seen in the monitoring timeseries for the ESA NRT SCI_RV__2P data (Figure 18). After 28 September 2004 the analysis departures of the SCI_RV__2P data are reduced to values around -5 DU, because the analysis is now drawing to the KNMI SCIAMACHY data. This also implies that from 28 September 2004 onwards the comparison of SCI_RV__2P with the ECMWF ozone analysis does not give an independent validation any more, but rather compares ESA and KNMI SCIAMACHY retrievals.

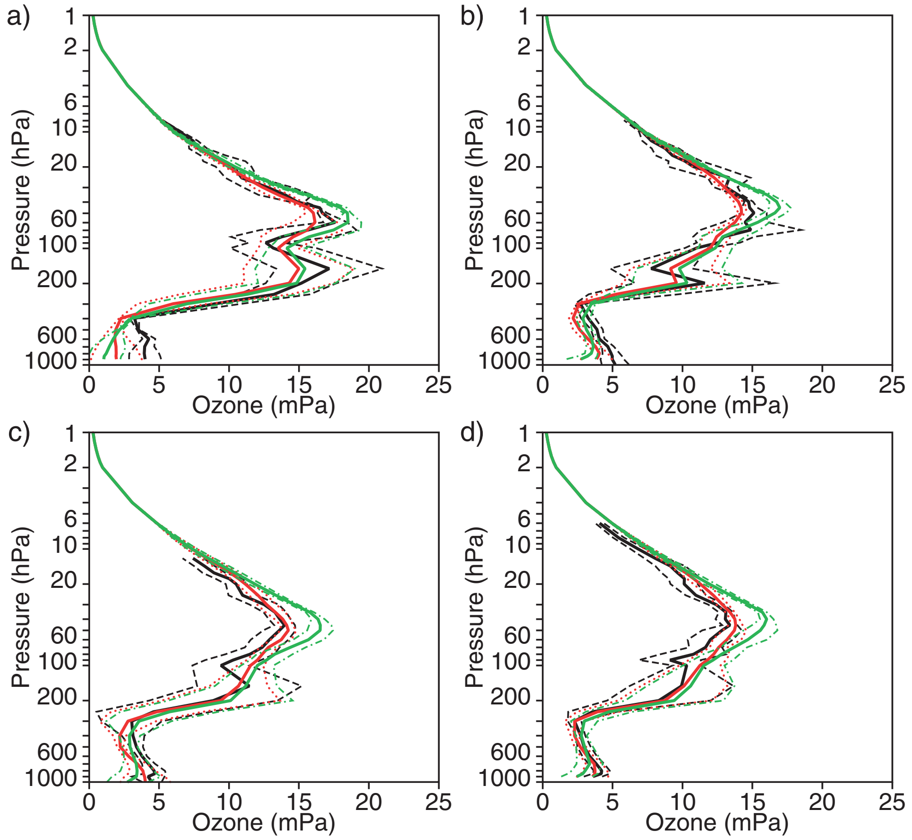


Figure 28: Mean ozone profiles in mPa for the period 24 April to 23 May 2004 at 4 European stations: (a) Sodankyla (67.2°N, 26.4°E), (b) Legionowo (52.2°N, 20.6°E), (c) Uccle (50.5°N, 4.2 °E) and (d) Hohenpeissenberg (47.8°N, 11.0 °E). Shown are sondes (black), profiles from the SCIAMACHY assimilation experiment Exp-2 (red), and profiles from the control experiment Exp-1 (green). The solid lines mark the mean profile, the dotted lines +/- one standard deviation.

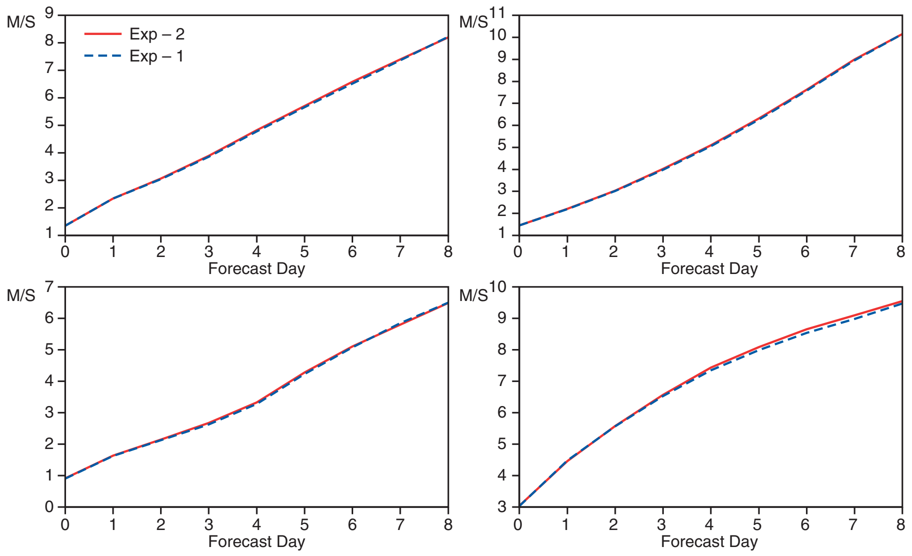


Figure 29: Forecast verification scores for 100 hPa vector wind root mean square errors from Exp-2 (red line) and Exp-1 (dotted blue line) over 30 cases for the NH (top left), the SH (top right), Europe (bottom left) and the tropics (bottom right).

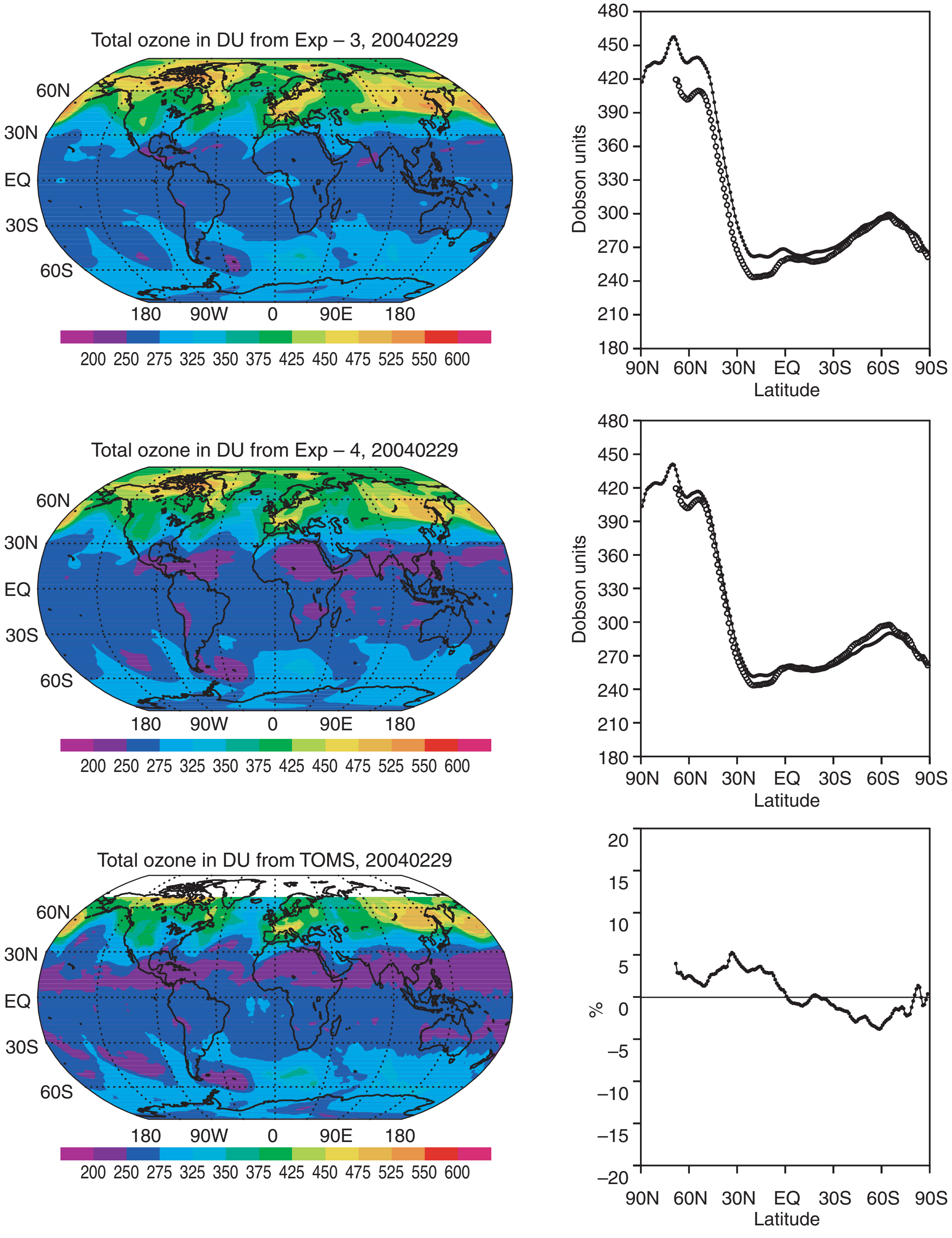


Figure 30: Left: Total column ozone in DU on 29 February 2004 from the control experiment Exp-3 (top), from the SCIAMACHY assimilation experiment Exp-4 (middle), and from gridded daily TOMS data (bottom). Right: The two top panels show the zonal mean ozone values from the experiments (solid line) and from TOMS data (open circles), the bottom panel shows the relative difference in % between Exp-4 and TOMS.

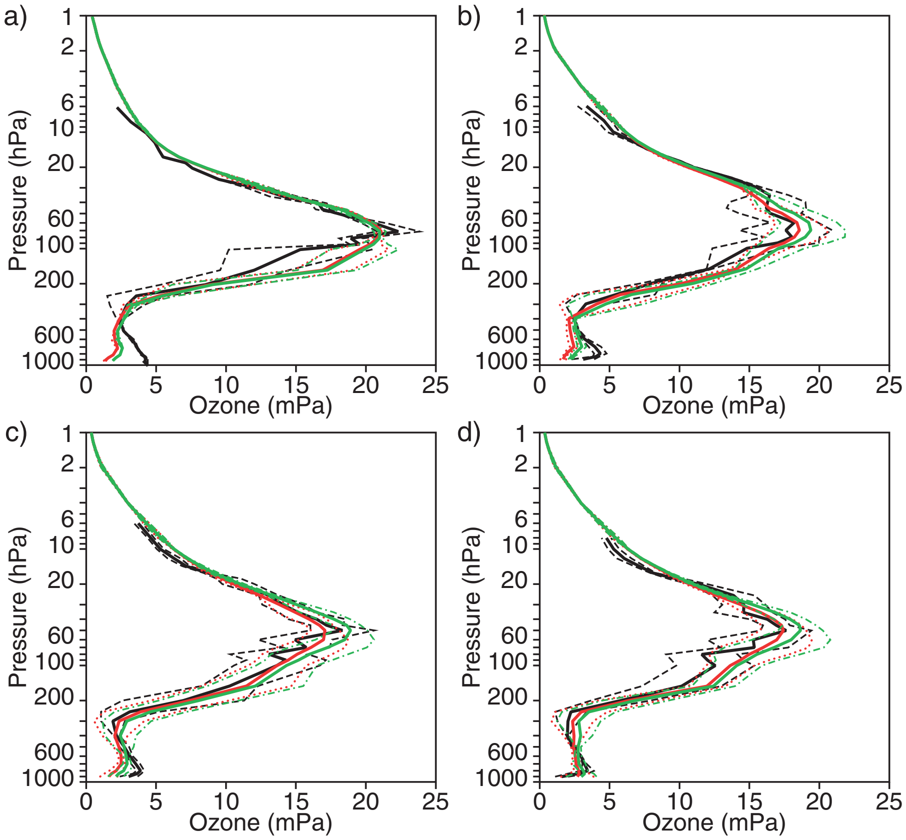


Figure 31: Mean ozone profiles in mPa for the period 15 to 29 February 2004 at 4 European stations: (a) Ny-Aalesund (78.9°N, 12.0°E), (b) Legionowo (52.2°N, 20.6°E), (c) Prague (50.0°N, 14.3 °E) and (d) Hohenpeissenberg (47.8°N, 11.0 °E). Shown are sondes (black), profiles from the SCIAMACHY assimilation experiment Exp-4 (red), and profiles from the control experiment Exp-3 (green). The solid lines mark the mean profile, the dotted lines +/- one standard deviation.

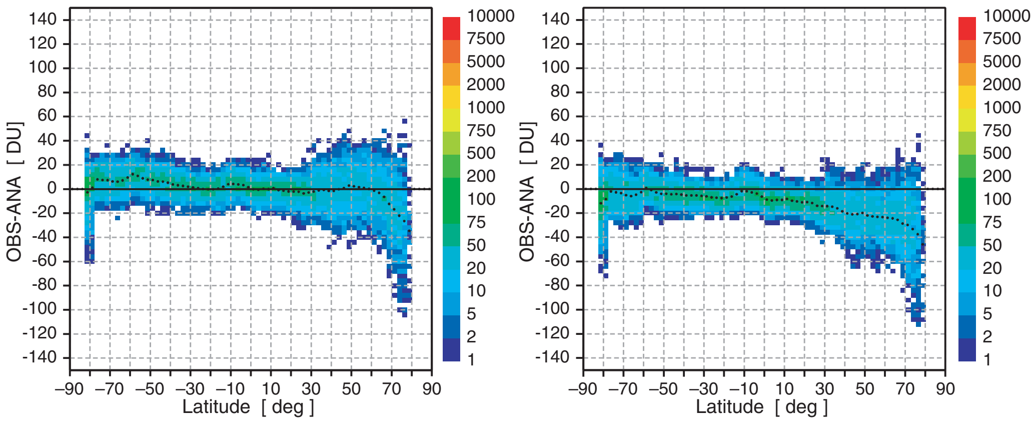


Figure 32: Scatter plot of analysis departures of L6 (16 hPa-surface) from SBUV/2 from NOAA-16 from Exp-4 (left) and the control experiment Exp-3 (right) for the period 15 to 29 February 2004. The colours show the number of observations per bin, the black dots are the mean per latitude bin.

4 Monitoring of GOMOS data

GOMOS (Global Ozone Monitoring by Occultation of Stars) makes use of the occultation measurement principle by tracking stars as they set behind the atmosphere. GOMOS has an UV-visible and a near-infrared spectrometer, covering the wavelength region 250-950 nm. It allows the retrieval of atmospheric trace gas profiles in the altitude range 100-20 km, with an altitude resolution better than 1.7 km. GOMOS gives day- and night time measurements with about 600 profiles per day. The primary GOMOS target species are O_3, NO_2, NO_3, OClO, H_2O and temperature.

At ECMWF a subset of these retrieved products is monitored that is available in NRT (GOM_RR__2P). This includes temperature, water vapour and ozone profiles. Unfortunately, there is currently no information about water vapour in the GOM_RR__2P BUFR files. All the water vapour values are set to missing values. Hence, only monitoring results for temperature and ozone data from GOMOS are described here. There is no information about star magnitude and limb conditions in the GOM_RR__2P BUFR files. Consequently, the monitoring statistics can not be compiled for subsets of the GOMOS data, but are averages over all available data.

The monitoring results for GOMOS data presented in this paper are for the period 1 April to 30 September 2004.

4.1 Monitoring of GOMOS temperature data

Figures 33 and 34 show area averaged GOMOS and ECMWF temperature profiles for the areas 90-60°N (top left), 30°N-30°S (middle left) and 60-90°S (bottom left) averaged over the period 1 April to 30 June 2004 and 1 July to 30 September 2004, respectively. The right panels show the corresponding GOMOS departures. GOMOS NRT temperatures show a good agreement with the ECMWF temperatures in the seasonal mean. Departures are generally less than 1% in the stratosphere and most of the mesosphere. Larger departures can be found at the model top. The timeseries of globally averaged data at 20 hPa (Figure35) also shows the good agreement of the NRT GOMOS data with the ECMWF temperature analysis.

4.2 Monitoring of GOMOS ozone data

Figures 36 and 37 show area averaged GOMOS ozone profiles and departures for the averaging periods 1 April to 30 June 2004 and 1 July to 30 September 2004, respectively. GOMOS and ECMWF ozone values agree less well than the temperatures. At the model top GOMOS ozone values are considerably lower than ECMWF values (departures greater than 50%) in all areas and both seasons. Apart from the differences near the model top, the largest differences between GOMOS and the ECMWF ozone data are found in 90-60°N (up to or greater than 50%), and below 80 hPa in 90-60°N and 30°N-30°S. The GOMOS profiles and the profiles of the departures show very large standard deviations (greater than 50% almost everywhere) indicating a lot of noise in the data. This noise can also be seen in the scatter plots of GOMOS ozone values and analysis departures for the layer 20-40 hPa in June 2004 (Figure 38). The scatter plot of the GOMOS ozone values also shows that there are unrealistically low ozone values (around 0 DU) as well as unrealistically large ozone values (up to 300 DU) in the layer 20-40 hPa.

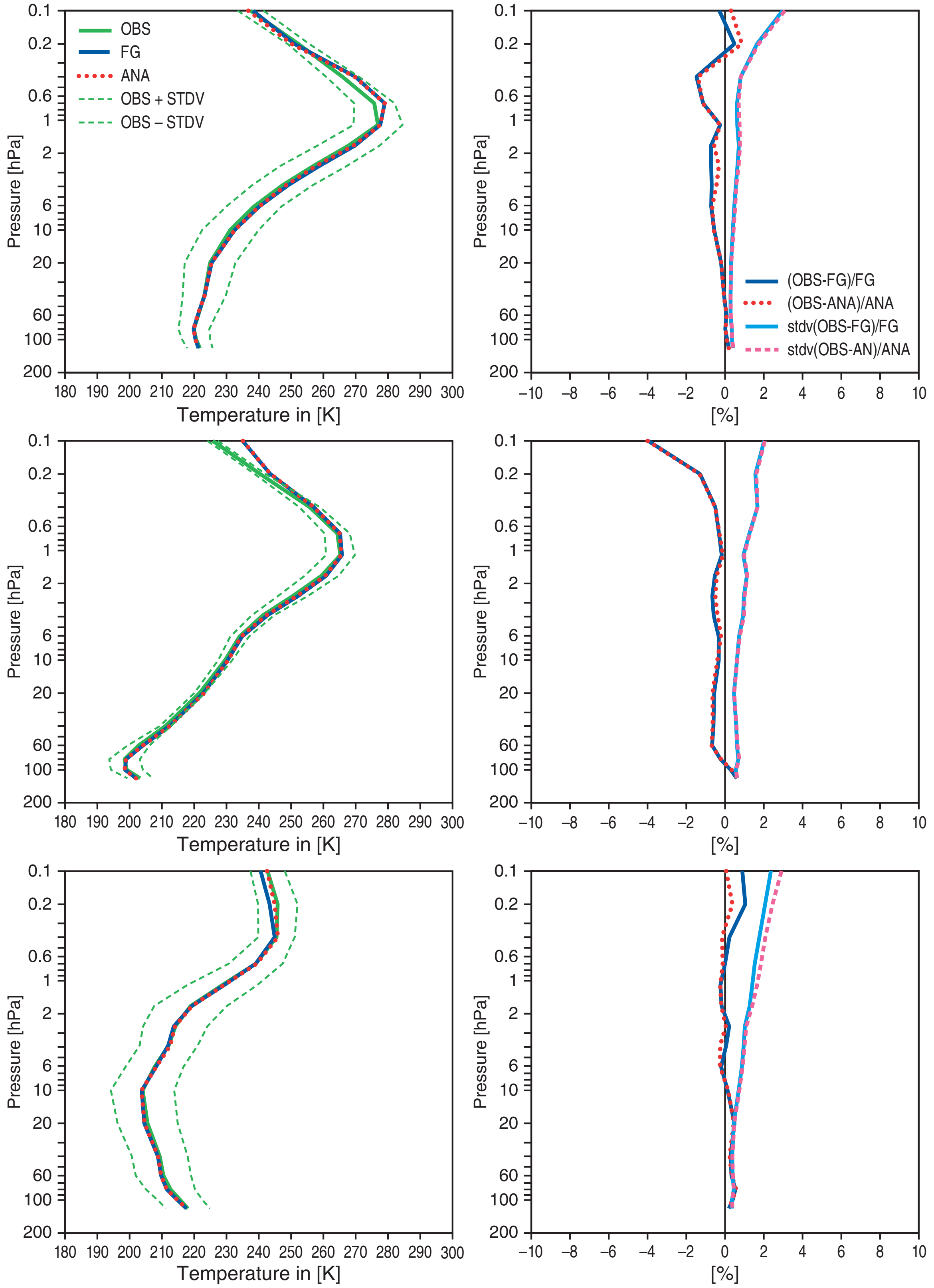


Figure 33: Profiles of time and area averaged GOMOS and ECMWF temperatures in K (left) and GOMOS departures in % (right) for the areas 90-60° N (top), 30° N-30° S (middle), and 60-90° S (bottom). Averaging period is 1 April to 30 June 2004.

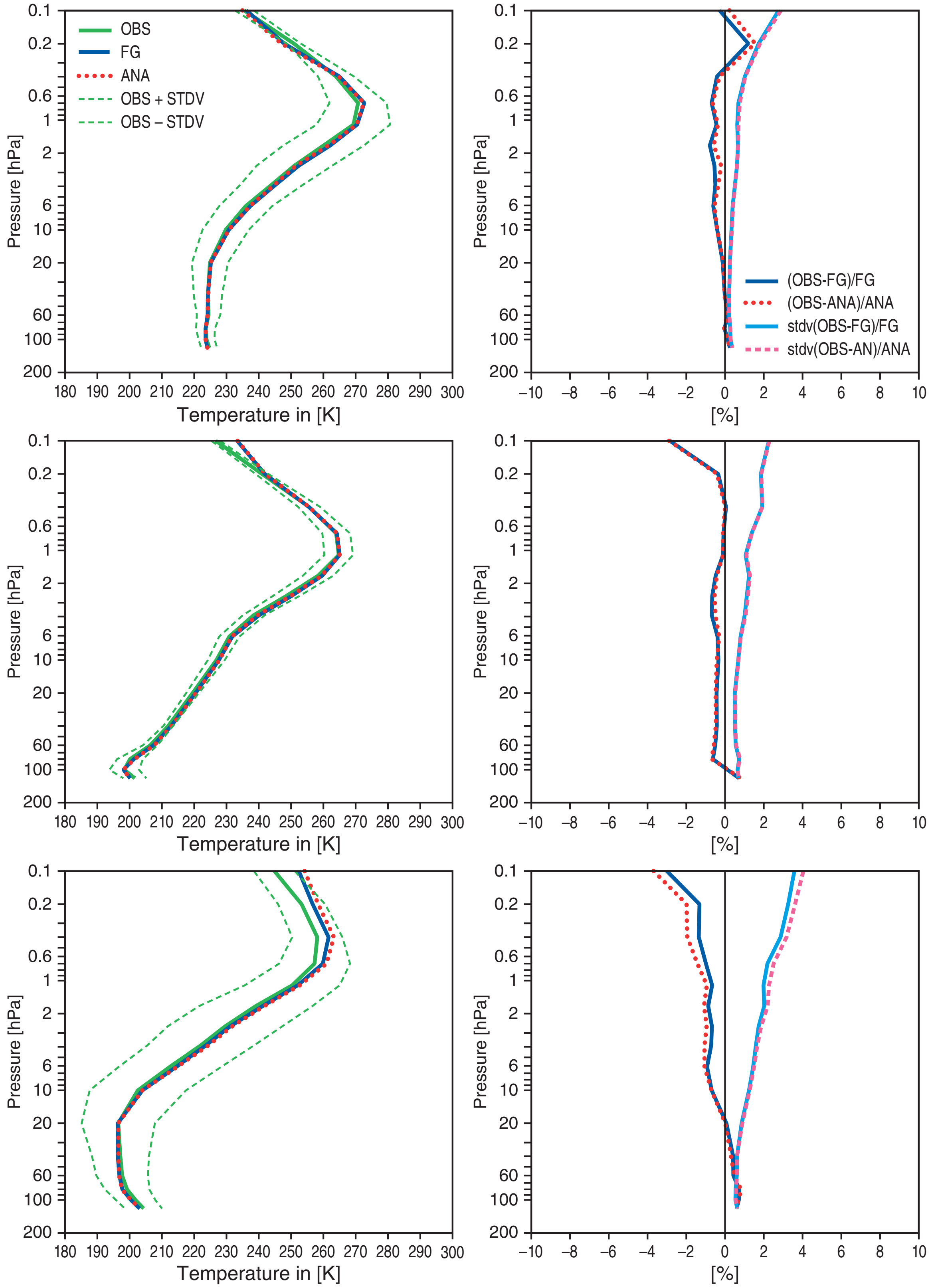


Figure 34: Like Figure 33 but for averaging period 1 July to 30 September 2004.

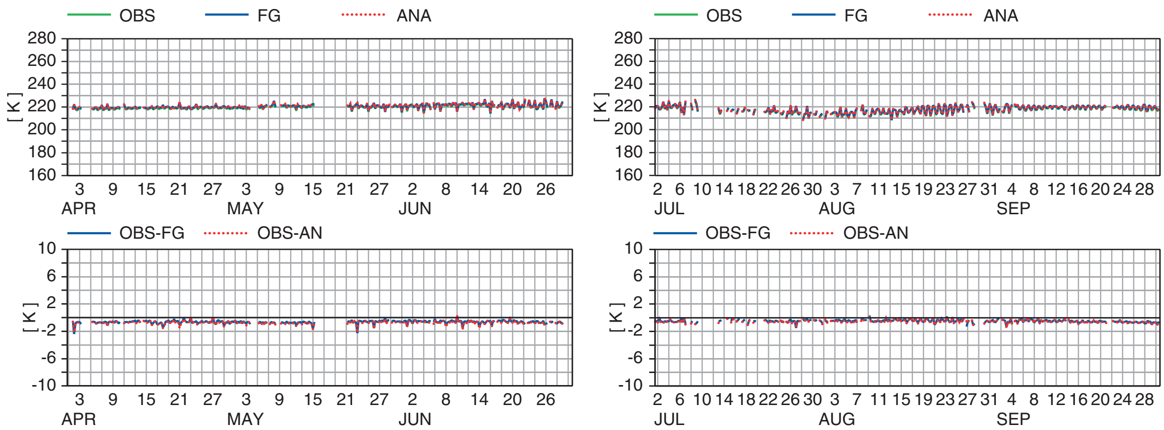


Figure 35: Timeseries of globally averaged temperature data at 20 hPa covering the periods 1 April to 30 June 2004 (left) and 1 July to 30 September 2004 (right). The top panels show GOMOS temperatures, first-guess and analysis values, the second panels first-guess and analysis departures. All temperature values are in K.

4.3 Summary GOMOS

While ECMWF and GOMOS temperatures agree well, there are large differences between ECMWF and GOMOS ozone profiles. The GOMOS ozone data show a large scatter and unrealistically large as well as unrealistically low ozone values. Water vapour information is not included in the GOMOS NRT files at the moment.

5 Conclusions

Under ESA contract 17585/03/I-OL (Technical support for global validation of Envisat data products (ENVISAT II)) NRT retrievals from MIPAS (MIP_NLE_2P), SCIAMACHY (SCI_RV__2P) and from GOMOS (GOM_RR__2P) are monitored at ECMWF using the operational analysis system. Ozone retrievals from MIPAS were actively assimilated in the operational ECMWF system between October 2003 and March 2004, and total column ozone retrievals from SCIAMACHY (produced by KNMI) have been assimilated in the operational system since the end of September 2004.

The monitoring statistics have shown MIPAS NRT temperatures to be of reasonable quality. They agree with the ECMWF analysis to within 1% in most regions. Larger departures are found at the model top (0.1 hPa).

MIPAS water vapour values are larger than ECMWF values almost everywhere. The departures are greater than 20% over much of the stratosphere. While the ECMWF model is known to have a dry bias, this bias should not be larger than 10-15%, and is hence not large enough to explain all of the departures. MIPAS water vapour values in the stratosphere are too high.

Because MIPAS ozone retrievals were actively assimilated in the ECMWF system (from 7 October 2003 until the L2 data delivery stopped on 26 March 2004), the comparison with the ECMWF ozone analysis does not give an independent validation any more, and other independent data have to be used for validation instead. The monitoring statistics show that the analysis is drawing to the MIPAS data. The resulting analysis ozone profiles agree well with profiles from ozone sondes. However, the total column ozone analysis is 5-10% larger than TOMS data in the zonal mean. These differences are larger than they would be if no MIPAS ozone data are assimilated. This result is surprising because it was not seen in MIPAS ozone assimilation experiments that were carried out prior to the operational assimilation of MIPAS ozone data.

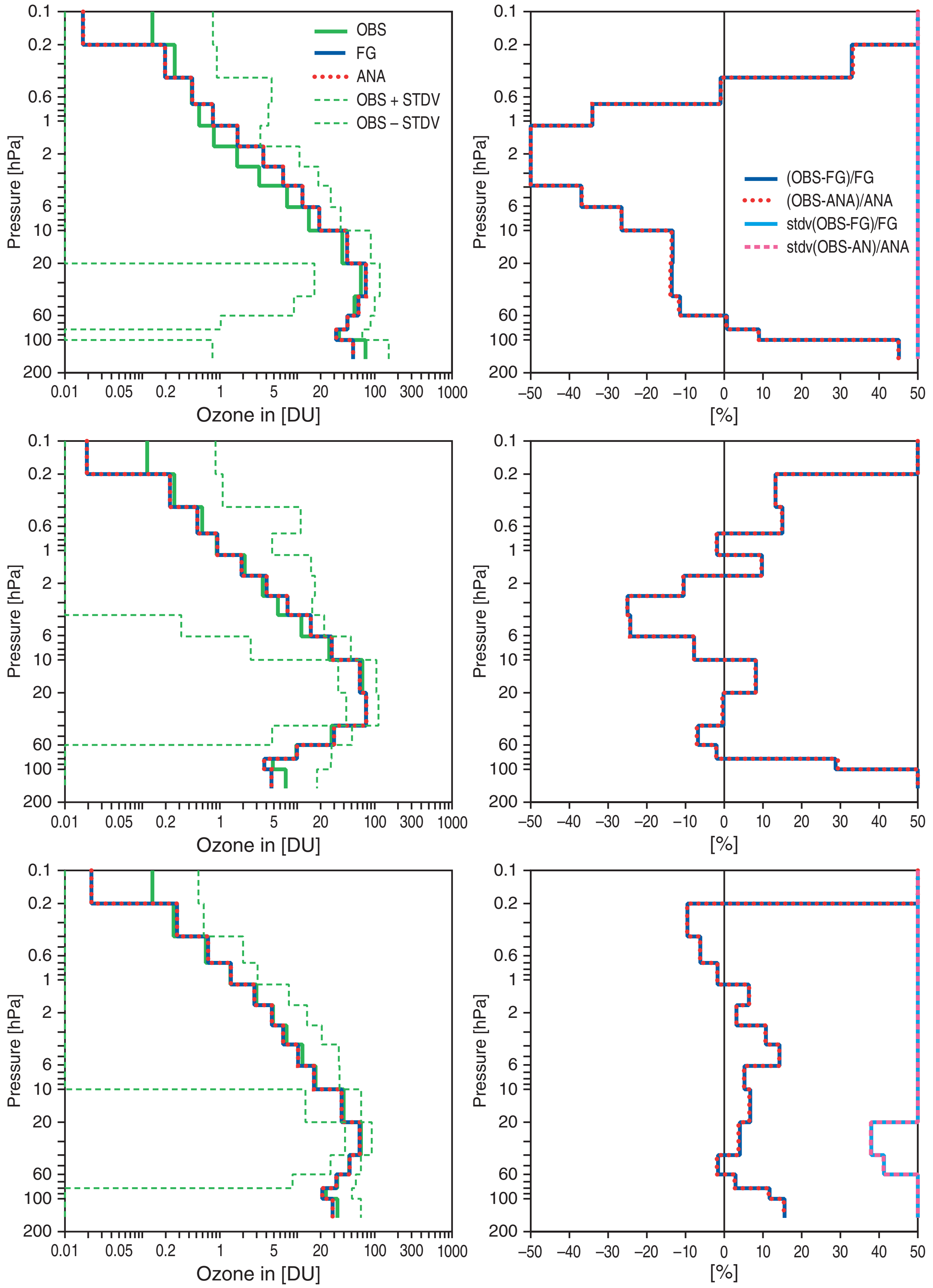


Figure 36: Profiles of time and area averaged GOMOS and ECMWF ozone in K (left) and GOMOS departures in % (right) for the areas 90-60°N (top), 30°N-30°S (middle), and 60-90°S (bottom). Averaging period is 1 April to 30 June 2004.

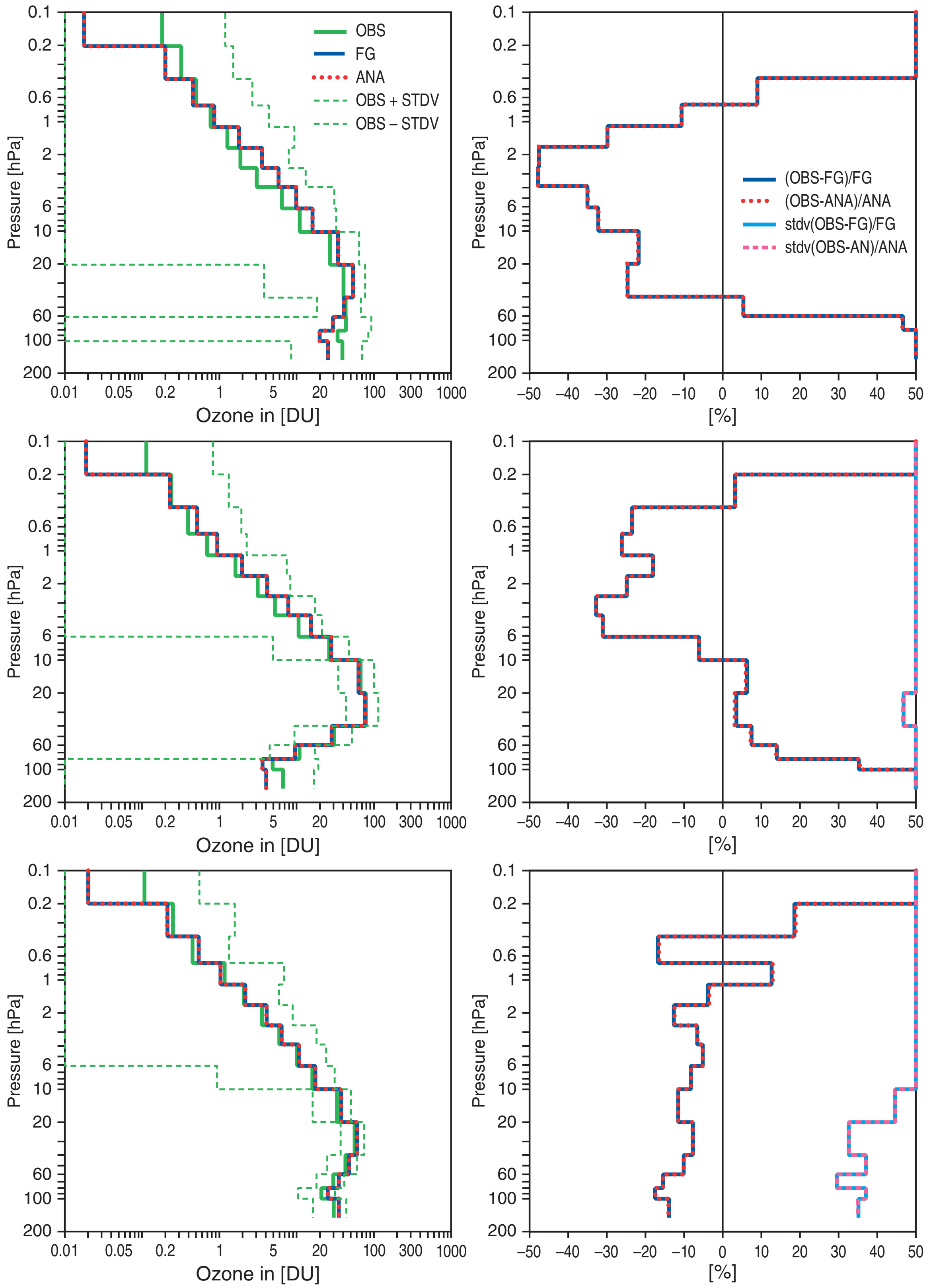


Figure 37: Like Figure 36 but for averaging period 1 July to 30 September 2004.

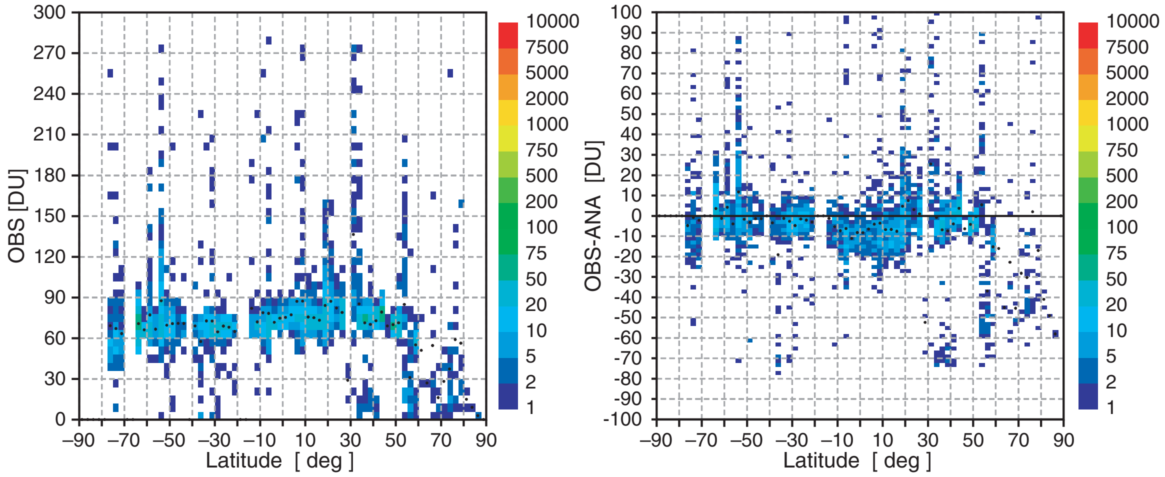


Figure 38: Scatter plots for June 2004 of GOMOS ozone (left) and GOMOS analysis departures (right) in DU in a layer between 20-40 hPa plotted against latitude. The colours give the number of observations per bin, and the black dots the mean per bin.

No MIPAS data have been available since 26 March 2004. If MIPAS operations resume MIPAS ozone data will at first be monitored passively in the ECMWF system, to establish the data quality of the new data. Also, the impact of assimilating MIPAS ozone profiles on the total column ozone analysis will have to be carefully studied.

The monitoring of SCIAMACHY total column ozone data shows a low bias of the NRT SCI_RV__2P data prior to 27 April 2004, and also reveals several problems with the SCI_RV__2P data, particularly during March 2004. Since 27 April 2004 the situation is much improved, and SCI_RV__2P are more stable and agree better with the ECMWF analysis.

NRT SCIAMACHY retrievals produced by KNMI are also monitored at ECMWF. These data were found to be more stable than the SCI_RV__2P, they did not suffer from problems in March 2004, and they did not have a large negative bias relative to the ECMWF ozone analysis prior to April 2004. The assimilation of the KNMI SCIAMACHY data was tested in research experiments, and was included in the operational ECMWF model in early September 2004.

NRT data from GOMOS (GOM_RR__2P) are also monitored in the operational ECMWF system. While GOMOS temperatures show a good agreement with ECMWF temperatures, the differences between GOMOS and ECMWF ozone values are large. GOMOS ozone values show a large scatter and unrealistically low as well as unrealistically large ozone values. At present, there is no information about water vapour in the NRT GOMOS BUFR files.

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