ESA Contract Report

Contract Report to the European Space Agency

Monitoring of retrievals from the MIPAS and SCIAMACHY instruments on board ENVISAT

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Final report for ESA contract 14458/00/NL/SF: Technical Support for global validation of ENVISAT data products

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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 14458/00/NL/SF (Technical support for global validation of ENVISAT data products), which ran from 1.4.2000 to 30.9.2003, ECMWF monitored near-real-time Level 2 data products from SCIAMACHY, MIPAS and GOMOS. During the first part of the contract, a monitoring framework for these ENVISAT data was developed at ECMWF. During the second part of the contract, the tools that had been developed were used to monitor and validate the ENVISAT data. This paper is the final report for ESA contract 14458/00/NL/SF and describes results from the monitoring statistics of MIPAS and SCIAMACHY data.

1 Introduction

ESA's ENVISAT (Environmental Satellite) was launched on 1 March 2002. On board are several instruments that allow the retrieval of profiles or total column values of various atmospheric constituents. One of these instruments is SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY), a spectrometer that measures backscattered, reflected, transmitted or emitted radiation from the atmosphere and the Earth's surface in the wavelength region 240-2380 nm at moderate spectral resolution (0.2 nm - 1.5 nm). The instrument has three viewing modes: limb, nadir and occultation, and its prime objective is to provide global measurements of various trace gases in the troposphere and stratosphere (including O_3, NO_2, BrO, OClO, SO_2 and H_2CO), as well as the determination of aerosols and clouds. The second instrument is MIPAS (Michelson Interferometer for Passive Atmospheric Sounding), 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. 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. The third instrument is GOMOS (Global Ozone Monitoring by Occultation of Stars) that 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.

ECMWF is contracted by ESA (project 14458/00/NL/SF) 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 GOMOS (GOM_RR__2P), as well as SCIAMACHY total column ozone data from from nadir measurements (SCI_RV__2P).

The ECMWF model is a global spectral model with a horizontal truncation of T511 (about 40 km grid spacing). The model has 60 levels in the vertical and the model top is at 0.1 hPa (corresponding to about 65 km). The operational model uses a 4-dimensional variational analysis scheme (Rabier et al. 2000), to assimilate observations at 12 hourly intervals. The 4D-Var data assimilation works in the following way: A first-guess trajectory is calculated by running the model for 12 hours. During this forecast the differences between the model and the observations are being recorded. A minimization run is then carried out with the tangent linear and adjoint models. During this minimization the differences between model and observations are transported back in time to the start of the forecast in order to derive a corrected state for a model run within the time window. From this improved state a new forecast is run. At ECMWF two trajectory runs and two minimizations are carried out in each assimilation cycle. The first minimization uses a simplified parameterization of the physical processes in the atmosphere and is run at the lower resolution of T95, the second one uses a more comprehensive physics package and is run at the resolution of T159.

Because ozone is fully integrated into the ECMWF forecast model and analysis system (Dethof and Hólm 2003) as an additional three-dimensional model and analysis variable, the ECMWF model can be used to monitor ozone retrievals from the ENVISAT instruments in addition to temperature and water vapour. The forecast model includes a simple ozone parameterization, which is an updated version of Cariolle and Déqué (1986). The ECMWF ozone parameterization includes an additional term which parameterizes the depletion of ozone in polar regions by heterogeneous reactions. At present, ozone is included uni-variately in the ECMWF data assimilation system. This means that there are no ozone increments from the analysis of the dynamical fields, even though the assimilation of ozone observations will modify the wind field in 4D-Var through the adjoint calculations. The univariate treatment was chosen to minimize the effect of ozone on the rest of the analysis system. For the same reason, the model's ozone field is not used in the radiation scheme, where an ozone climatology (Fortuin and Langematz 1995) is used instead.

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. Between April 2002 and June 2003, total column ozone retrievals from the GOME (Global Ozone Monitoring Experiment) instrument on ERS-2 were also assimilated operationally. The GOME retrievals were the NRT total column data produced by KNMI's fast delivery service, version FD 3.1 (Valks et al. 2003). The ozone data are used in the following way. GOME data are only used at solar zenith angles less than 80° and at latitudes between 40°N and 50°S. This conservative approach was chosen because the bias between the GOME data and the model can be large outside this latitude band, and we wanted to minimize the impact of the ozone assimilation on the rest of the assimilation system. The SBUV/2 data are not used at solar zenith angles greater than 84°. Variational quality control and first-guess checks are carried out for both datasets.

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 to avoid an unrealistically drying of the stratosphere in the ECMWF model (Simmons pers. comm.). 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.

Satellite data can be monitored with the help of a data assimilation system by looking at the differences between the observations and collocated model fields. The model fields are interpolated in time and space to the location of the observations, statistical analyses of the differences between the model's first-guess or analysed fields and the observations are calculated, and their time evolution is monitored. The differences between the observations and the model fields are called departures. We distinguish between first-guess departures (observations minus first-guess field) and analysis departures (observations minus analysed field). If the model fields are stable the departures normally show a relatively smooth behaviour from day to day. A sudden jump on a global scale, which is larger than the instrument noise, is an indication of possible problems in the data or the model. Long term monitoring of the departures can disclose errors and biases in the satellite data products, as well as errors or biases in the model. It enables us to carry out a continuous quality assessment of the ENVISAT data. Such long term monitoring statistics can also detect biases between the different ENVISAT products (e.g. between ozone retrievals from different instruments) and allows us to monitor instrument and algorithm stability. The advantage of using an assimilation system to monitor satellite data is that it provides continuous global coverage and that it allows one to build up statistics quickly. Furthermore, it gives a framework in which to compare the satellite data with other sources of information, for instance radiosondes or ozone sondes, and it also helps to characterize the error statistics of the observations if the model error characteristics are known.

Even though ENVISAT was launched on 1 March 2002, ECMWF did not receive any data until August 2002, and even then there were problems with the data flow. During the first weeks, only parts of orbits were received. Because of problems with the delivery of the Meteo products in BUFR format, ENVISAT data in PDS form were used and converted into BUFR format at ECMWF. Further problems with the data delivery meant that no ENVISAT data were monitored in January 2003 and the first half of February 2003. From the middle of February 2003 onwards the data flow improved and the monitoring could continue. The quality of the NRT ESA GOMOS retrievals has been poor up to now, and we are waiting for an algorithm update before monitoring the data. Hence, GOMOS data are not discussed in this report.

At the beginning ENVISAT data were used only passively in the ECMWF assimilation system. This means the data were fed into the system, first-guess statistics were calculated, but the data were not assimilated into the ECMWF model. The assimilation of MIPAS ozone retrievals was tested in research experiments and was found to have a positive impact on the ECMWF ozone field (Dethof 2003). It underwent pre-operational testing from June to October 2003 (in the CY26R3 e-suite) and has been included in the operational ECMWF system since October 2003.

The monitoring statistics shown in this paper cover the period 17 February to 5 October. They are split into two parts. From 17 February to 31 May 2001 ENVISAT data were monitored in off-line experiments which used 3-dimensional variational analysis (Courtier et al. 1998) and which were run at a horizontal truncation of T159, using CY25R4 of the ECMWF model. All ENVISAT data were passive in these experiments. From 1 June to 5 October 2003, ENVISAT data were monitored in the pre-operational CY26R3 e-suite using the full T511, 12-hour 4D-Var system. MIPAS ozone profiles were actively assimilated in CY26R3, while the other ENVISAT data were monitored passively.

This paper describes the monitoring of SCIAMACHY and MIPAS data at ECMWF. It is structured in the following way. Section 2 summarizes the results of the monitoring of SCIAMACHY total column ozone data, Section 3 the results of the monitoring of MIPAS temperature, water vapour and ozone retrievals, and Section 4 gives the conclusions.

2 Monitoring of NRT retrievals from SCIAMACHY (SCI_RV__2P)

At ECMWF SCIAMACHY total column ozone data from nadir measurements in the UV/VIS (SCI_RV__2P) are monitored. Unfortunately, these NRT Level 2 SCIAMACHY data do not include geolocation information like solar zenith angle or field of view 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 1 shows timeseries of zonal mean total column ozone values (averaged over 6-hourly analysis cycles) from SCIAMACHY in Dobson Units (DU) from 17 February to 30 May (top panel) and from 1 June to 5 October 2003 (bottom panel). The timeseries shows the periods when no data were available. It also illustrates that SCIAMACHY ozone values lie within a realistic range and reproduce well the seasonal cycle of total column ozone (e.g. high values in the NH during spring, the development of the Antarctic ozone hole between

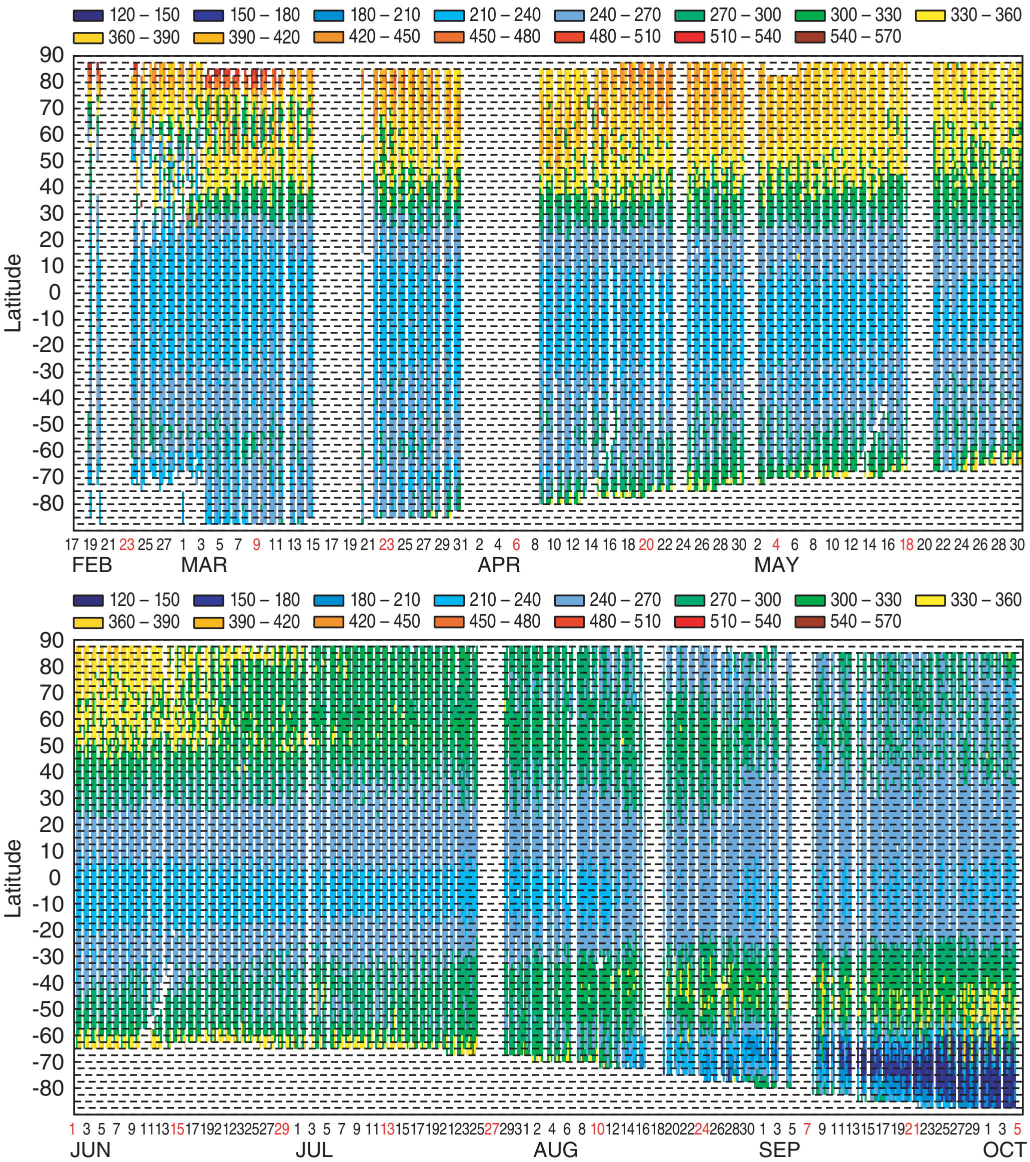

Figure 1: Timeseries of zonal mean SCIAMACHY total column ozone values in DU from 17 February to 30 May 2003 (top) and from 1 June to 5 October 2003 (bottom).

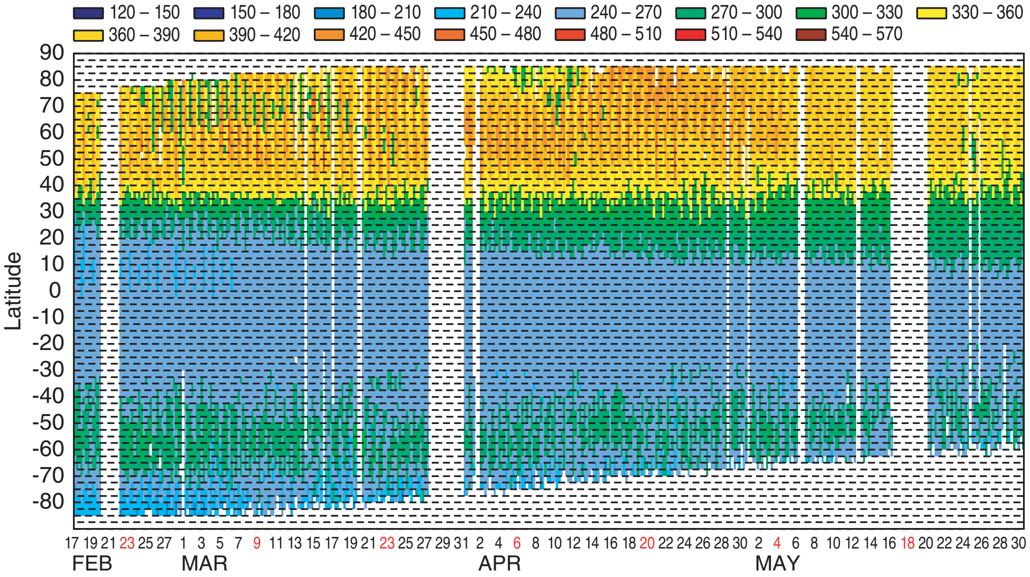

Figure 2: Timeseries of zonal mean GOME total column ozone data in DU from 17 February to 30 May 2003.

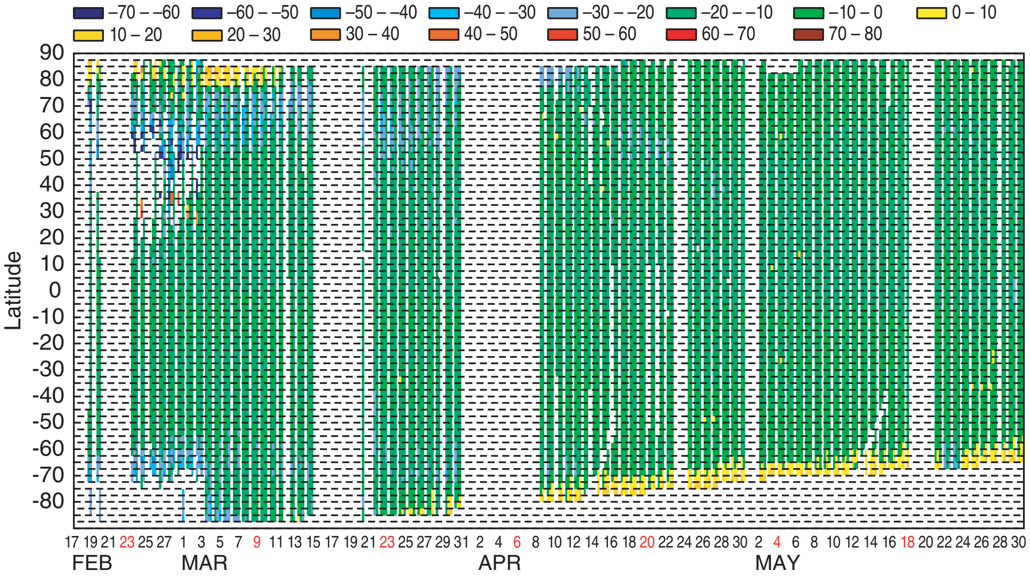

Figure 3: Timeseries of zonal mean SCIAMACHY first-guess departures in DU from 17 February to 30 May 2003.

August and October). However, compared to GOME total column ozone retrievals (Figure 2) SCIAMACHY data show a negative bias of about 30 DU over much of the globe. The same bias can be seen when comparing SCIAMACHY data with the ECMWF first-guess ozone field. Figure 3 shows a timeseries of zonal mean first-guess departures in % for SCIAMACHY. The SCIAMACHY data are 10-20% lower than the first-guess over most of the globe. At the beginning of the timeseries during February and March, the negative departures are even larger. Positive departures are seen at the northern end of the orbits in February and March, and at the southern end of the orbits from the end of March onwards. It is possible that there are problems with SCIAMACHY retrievals at high solar zenith angles, but this can not be further investigated because there is no information about solar zenith angle in the NRT SCIAMACHY data.

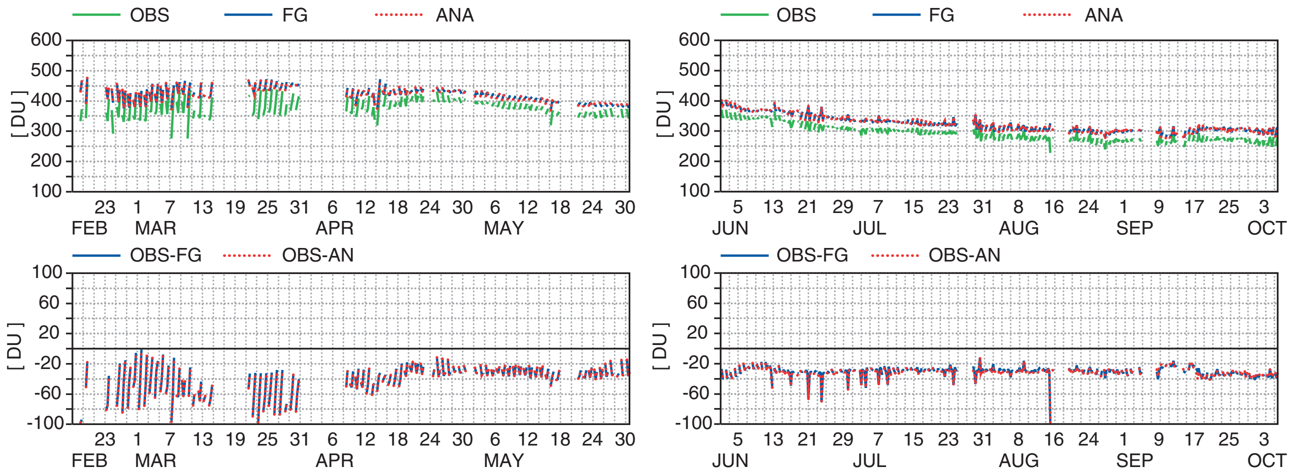

Figure 4: Timeseries of data averaged over 90-65° N covering the periods 17 February to 30 May (left) and 1 June to 5 October 2003 (right). The top panels show SCIAMACHY observations, first-guess and analysis values, the second panels first-guess and analysis departures. All ozone values are in DU.

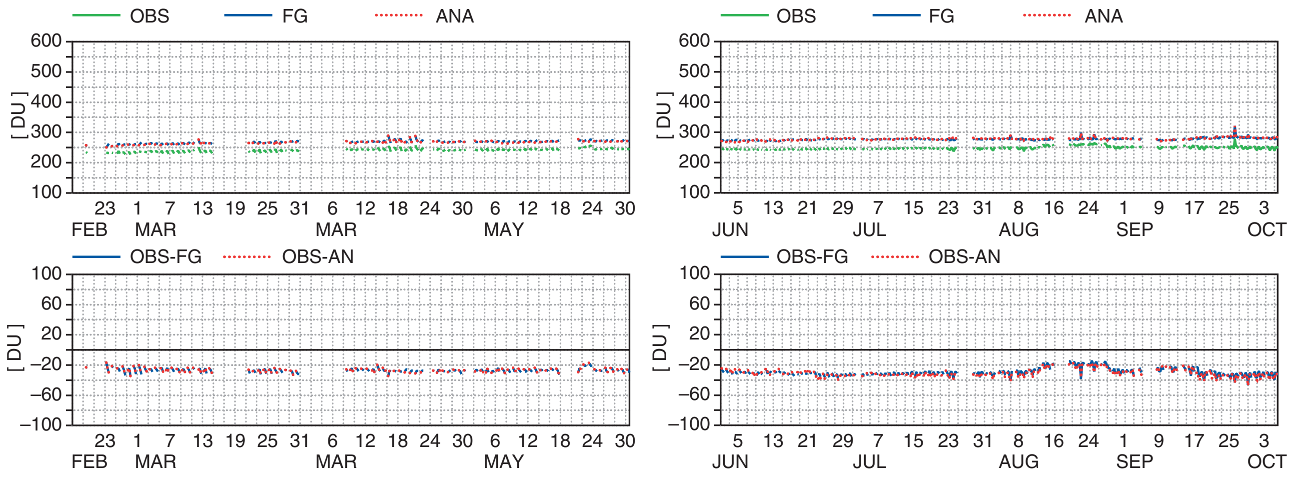

Figure 5: Like Figure 4 but for 30° N-30° S.

The negative bias of the SCIAMACHY data becomes even clearer when looking at timeseries of area averaged SCIAMACHY and analysis values, as well as timeseries of departures. Figure 4 shows a timeseries of data averaged over the area between 90-65° N. The observation values are systematically lower than the first-guess and analysis values. The departures are larger during February and March, and the departures as well as the observations show a larger standard deviation then. From about 24 April onwards the standard deviation of the

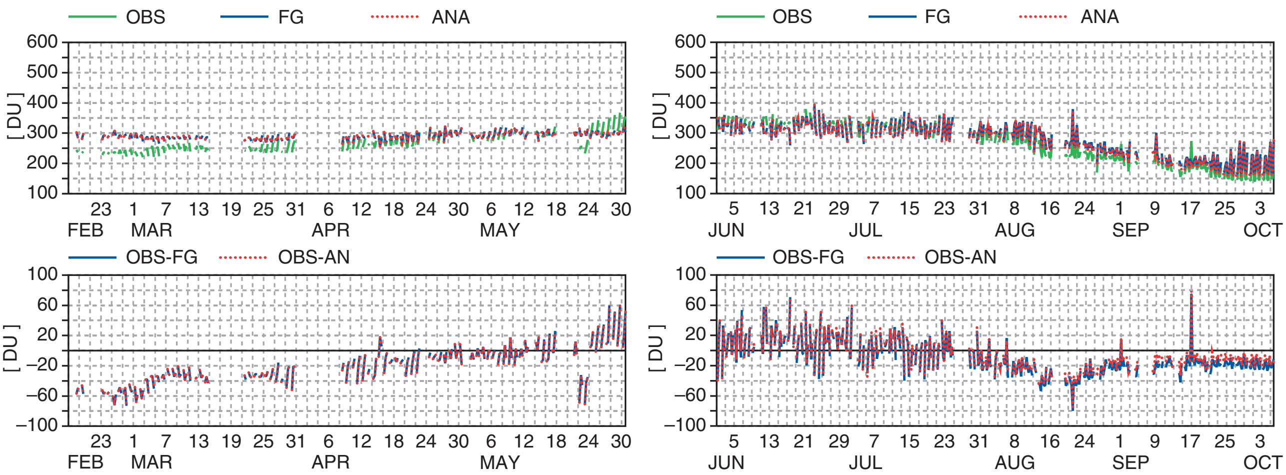

Figure 6: Like Figure 4 but for 65-90° S.

observations and departures is smaller and more stable, and SCIAMACHY data are around 30 DU lower than the ECMWF first-guess and analysis values.

Between 30° N-30° S (Figure 5) the observation values and the departures are more stable, with a negative bias of 25-30 DU for the whole period from February to October 2003. There is an offset during August when SCIAMACHY values are higher than normal and departures are smaller (around 20 DU). The reason for this change is not clear. Another offset in the departures can be seen from 6-17 September, when the analysis values are slightly lower than outside this period, again leading to smaller departures around 20 DU. This change is a result of an offset in MIPAS ozone retrievals assimilated at that time, which affected the ozone analysis (see Section 3 for more details).

Between 65-90° S (Figure 6) the area averaged departures are less stable. The largest negative departures are seen in February and March. From May to July departures are small or even slightly positive, and from August onwards they are negative again. It is likely that the reason for these changes is the varying data coverage of the area between 65-90° S from February to October, with only few data going into the average between May and August.

The negative bias of the SCIAMACHY data seen in the timeseries plots is also apparent when plotting a histogram of SCIAMACHY first-guess departures (Figure 7). The mean bias over the period 17 February to 30 May 2003 is -30.7 DU, with a standard deviation of 16.8 DU. This figure illustrates that the bias of the SCIAMACHY data is the main problem, and that otherwise the data seem to be well characterized with normally distributed departures. SCIAMACHY data might be suitable for assimilation if the bias can be removed, ideally by improving the retrieval algorithm, or otherwise by implementing a bias correction scheme for SCIAMACHY data at ECMWF to remove the bias before the data are assimilated.

More information about the SCIAMACHY data can be gained by looking at scatter diagrams of the data and the departures. Figure 8 shows scatter plots for the period 17 February to 30 May 2003 of GOME data (top left), SCIAMACHY data (top right) and SCIAMACHY first-guess departures (bottom). The most noticeable features are unrealistically large SCIAMACHY values north of 70° N and between 30-40° N. The large values north of 70° N all occurred between February and the middle of April, suggesting that there is a problem with retrievals at high solar zenith angles. The high values between 30-40° N all occurred from 17 February to 2 March 2003. They are an artefact resulting from an error in matching ozone and geolocation information in the conversion from PDS to BUFR format, and disappeared after this problem had been corrected. Between 0 and 30° S SCIAMACHY data show a relatively large scatter with some unrealistically low and some too

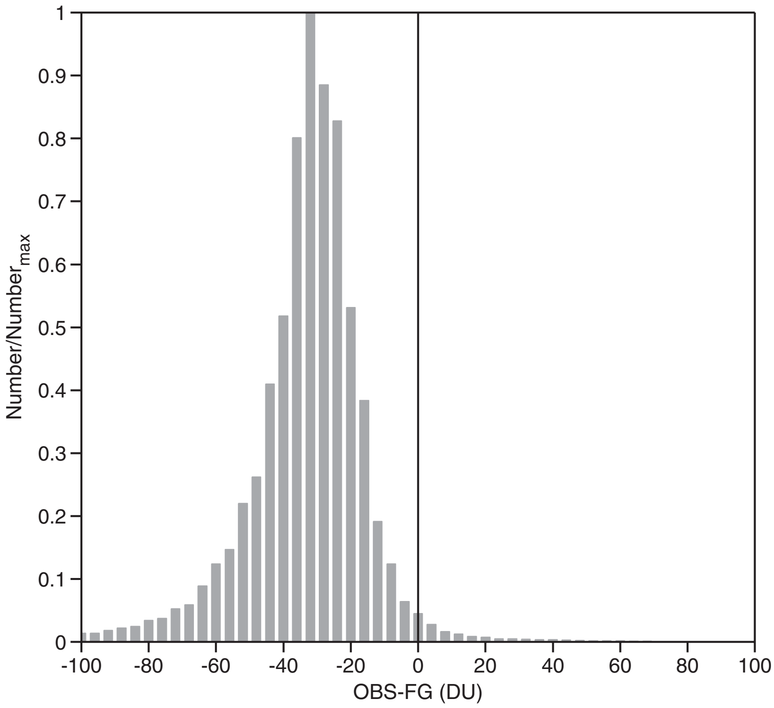

Figure 7: Frequency distribution of SCIAMACHY first-guess departures in DU for the period 17 February to 30 May 2003.

high ozone values. This might be a sign of cloud contamination, but because there is no information about cloud cover or cloud top height in the NRT SCIAMACHY data this can not be investigated further. The scatter diagram of GOME data for the same period does not show such a large scatter between 0 and 30°S nor does it show unrealistically large values north of 70°N. Comparing the scatter diagrams of GOME and SCIAMACHY data again shows the negative bias of the SCIAMACHY data, which is also apparent in the scatter plot of SCIAMACHY first-guess departures.

Figure 9 shows scatter plots of SCIAMACHY data (left) and first-guess departure (right) for 1 June to 5 October 2003. The unrealistically large values north of 70°N are not seen any more, but there is still a large scatter between 0-30°S. The plot of the departures shows again a mean negative bias of 25-30 DU over most latitudes, but larger departures are seen at hight latitudes in both hemispheres.

In summary it can be said that there are still too many problems with the NRT SCIAMACHY data to allow their assimilation in the ECMWF system. The main problem is the negative bias of the data which has been observed and reported to ESA ever since the first data became available. A further problem is the lack of geolocation information in the NRT SCIAMACHY data, such as solar zenith angle, field of view, cloud top height, or cloud cover information. This makes it impossible to attribute problems to certain parameters (e.g. cloud contamination, problems with observations at hight solar zenith angle) and makes a thorough analysis of the data difficult. It also makes it impossible to use a subset of the data screened according to certain criteria, for instance, to only use data below a solar zenith angle threshold actively in the assimilation.

SCIAMACHY retrievals produced by KNMI are currently being tested at ECMWF. First studies show these retrievals to be of better quality than the ESA NRT SCIAMACHY products. The KNMI retrievals do not show a negative bias, and agree better with the ECMWF total ozone field. Furthermore, they do include geolocation information. The assimilation of the KNMI SCIAMACHY retrievals will be tested in research experiments.

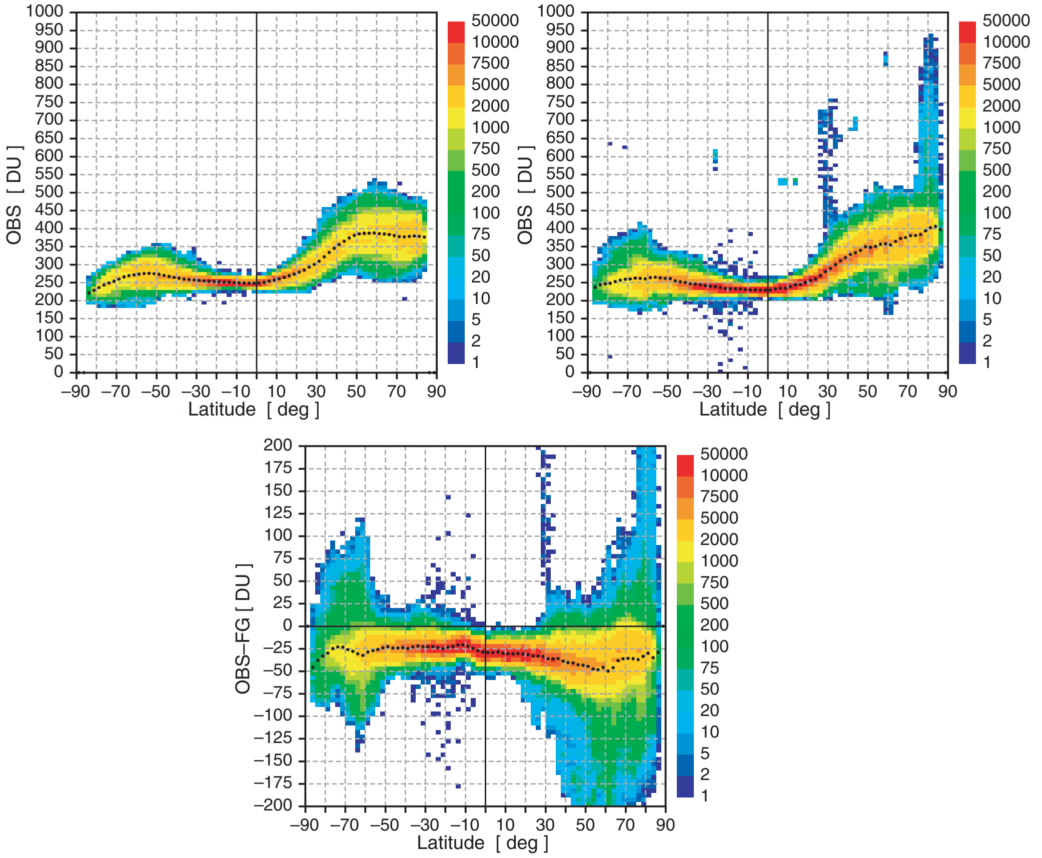

Figure 8: Scatterplots for the period 17 February to 30 May 2003 of GOME total ozone (top left), SCIAMACHY total ozone (top right), and SCIAMACHY first-guess departures (bottom). Ozone values are in DU.

3 Monitoring of NRT temperature, water vapour and ozone retrievals from MIPAS (MIP_NLE_2P)

This section describes on the monitoring of NRT temperature, water vapour and ozone retrievals from the MIPAS instrument (MIP_NLE_2P) at ECMWF.

3.1 NRT temperature retrievals from MIPAS

Figure 10 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 17 February to 30 May 2003. The right panels show the corresponding MIPAS departures. On the whole, MIPAS temperature profiles are of good quality, and the differences between MIPAS and ECMWF temperatures are less than 2% (less than 4 K) for most levels. Larger departures are seen near 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. This leads to relatively small mean departures in 90-65°N and 65-90°S for the whole averaging period, but departures can be large for shorter periods, as illustrated by the large standard deviations of the departures near the model top. MIPAS temperatures are usually lower than ECMWF temperature at 0.1 hPa, with the exception of the winter pole, where the ECMWF model has a cold bias of up to 20K at the model top.

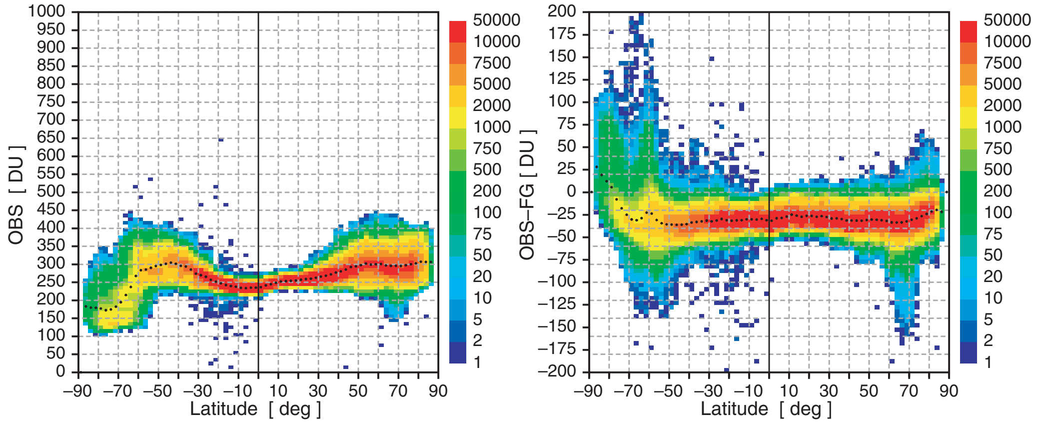

Figure 9: Scatterplots for the period 1 June to 5 October 2003 of SCIAMACHY total ozone (left), and SCIAMACHY first-guess departures (right). Ozone values are in DU.

Figure 11 shows MIPAS temperature profiles and departures averaged over the period from 1 June to 5 October 2003, based on results from the CY26R3 e-suite. In CY26R3 radiances from the AIRS instrument on Aqua are assimilated, which has an impact on the ECMWF temperatures in the stratosphere and mesosphere. The profile plots show a good agreement between MIPAS and ECMWF temperatures over most of the stratosphere in 90-65°N and 0-20°S, with departures of less than 2%. MIPAS temperatures are again larger than ECMWF values in the stratosphere and lower near the model top. In 65-90°S, there are some unrealistic structures in the ECMWF temperature profiles in the upper stratosphere and lower mesosphere. The ECMWF model has a strong cold bias over the winter pole, and problems arise when AIRS radiances are assimilated in the presence of this bias. The AIRS data warm the model top, but the background error formulation has temperature errors that have anti-correlations in the vertical, and this leads to unrealistic oscillations further down the profiles when trying to fit the AIRS radiances. These problems are an artefact of the assimilation system and not a problem in the data. They are currently addressed by blacklisting the upper stratospheric AIRS channels. In the long term the model's cold bias will have to be reduced. MIPAS data were a useful independent data set to identify these problems.

Figures 12 to 14 show timeseries of area averaged temperatures and departures at 20 hPa for the areas 90-65°N, 0-20°S, and 65-90°S, respectively. The figures illustrate that MIPAS data delivery is better from June onwards, and that there are several data gaps between February and May 2003. The timeseries show that the area averaged MIPAS temperatures at 20 hPa in the tropics are relative constant around 225 K throughout the monitoring period. In the other two areas there is a pronounced seasonal cycle. In 90-65°N, temperatures increase from values around 215-220 K in February and March, to values around 230K in April and then remain are between 230-235 K until the beginning of September, when they begin too decrease to values of 215 K by the beginning of October. In 65-90°S, temperatures at 20 hPa reach minimum values of 175 K in July during the polar night and then increase again to values around 235 K at the beginning of October. Figure14 shows that temperatures over the South Pole are low enough for the formation of polar stratospheric clouds (PSCs) from June to September.

MIPAS temperatures are slightly higher than ECMWF temperatures in all three areas, but departures are less than 2 K for most of the timeseries. The departures usually show a stable behaviour from day to day, but there are some periods (23 February to 1 March, 20/21 March, 21 May to 10 June, 6 to 17 September) when MIPAS temperatures are 3-8 K higher than normal. These discontinuities occurred after payload or instrument switch-offs. For example, when the operation of MIPAS was resumed on 6 September, the ice deposition conditions were different to what they had been before the cooler switch-off. However, pre-switch-off gain calibrations

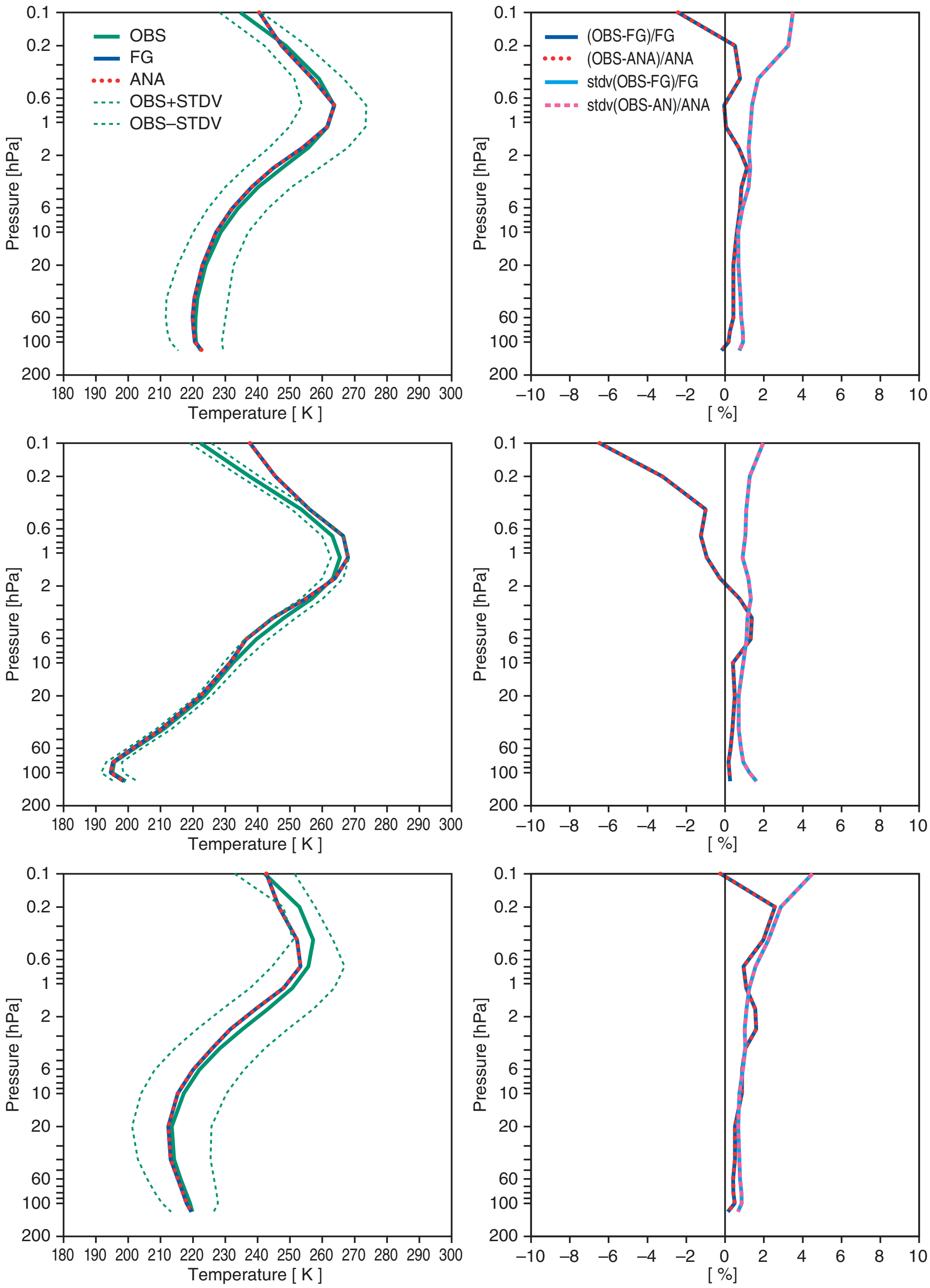

Figure 10: Profiles of time and area averaged MIPAS and ECMWF temperatures in K (left) and MIPAS departures in % (right) for the areas 90-65°N (top), 0-20°S (middle), and 65-90°S (bottom). Averaging period is 17 February to 30 May 2003.

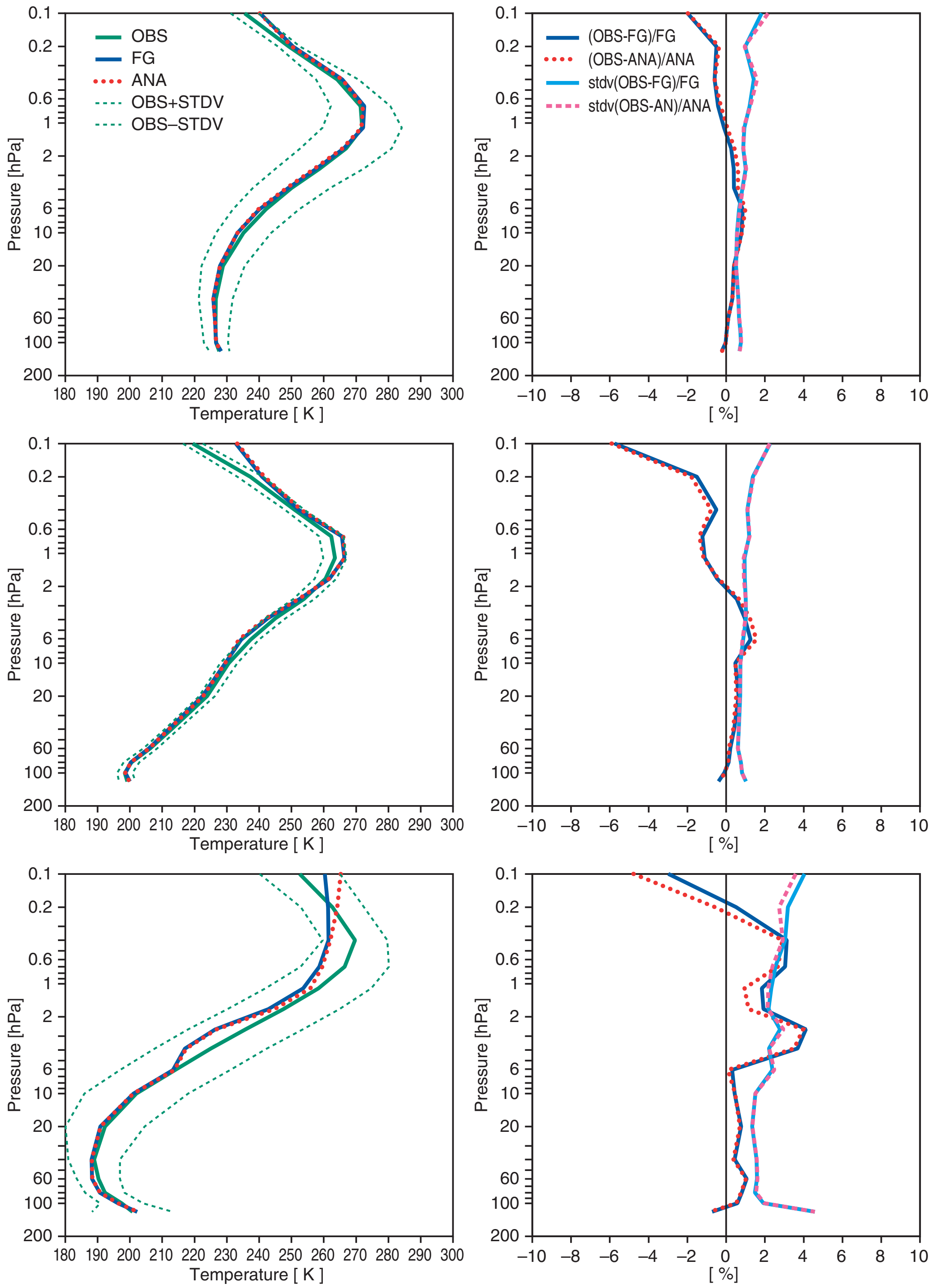

Figure 11: Like Figure 10 but for 1 June to 5 October 2003.

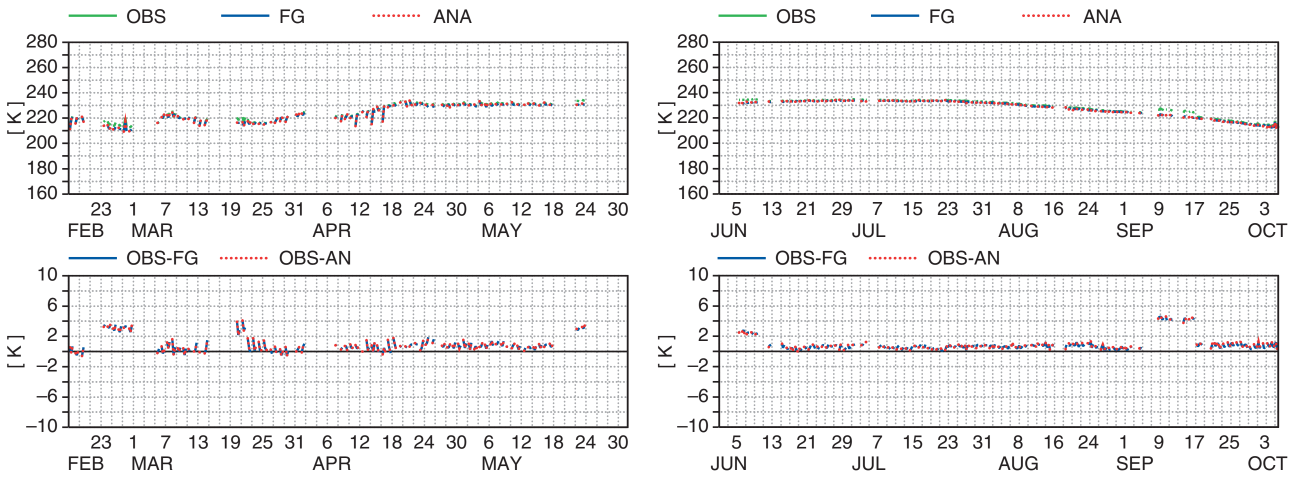

Figure 12: Timeseries of temperature data averaged over 90-65°N covering the periods 17 February to 30 May (left) and 1 June to 5 October 2003 (right). The top panels show MIPAS temperatures, first-guess and analysis values, the second panels first-guess and analysis departures. All temperature values are in K.

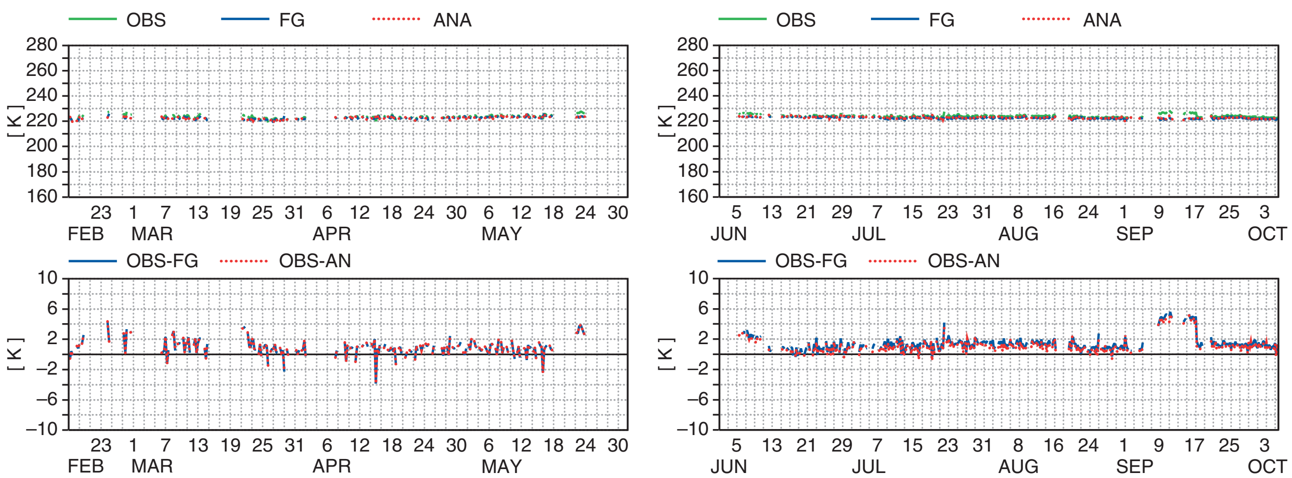

Figure 13: Like Figure 12 but for 0-20°S.

were applied to the post-switch-off data. After new gain calibrations had been performed, MIPAS values went back to pre-switch-off levels. The offsets in the temperature retrievals propagated into the trace retrievals and can be seen in the monitoring timeseries for MIPAS water vapour (Figures 17 to 19) and ozone retrievals (Figures 22 to 24). These timeseries illustrate the power of an assimilation system for monitoring satellite data. It allows ECMWF to quickly identify and quantify problems and give ESA feedback.

3.2 NRT water vapour retrievals from MIPAS

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 profiles and departures for the areas 90-65°N, 0-20°S, and 65-90°S are shown in Figure 15 averaged over the periods 17 February to 30 May (left) and 1 June to 5 October

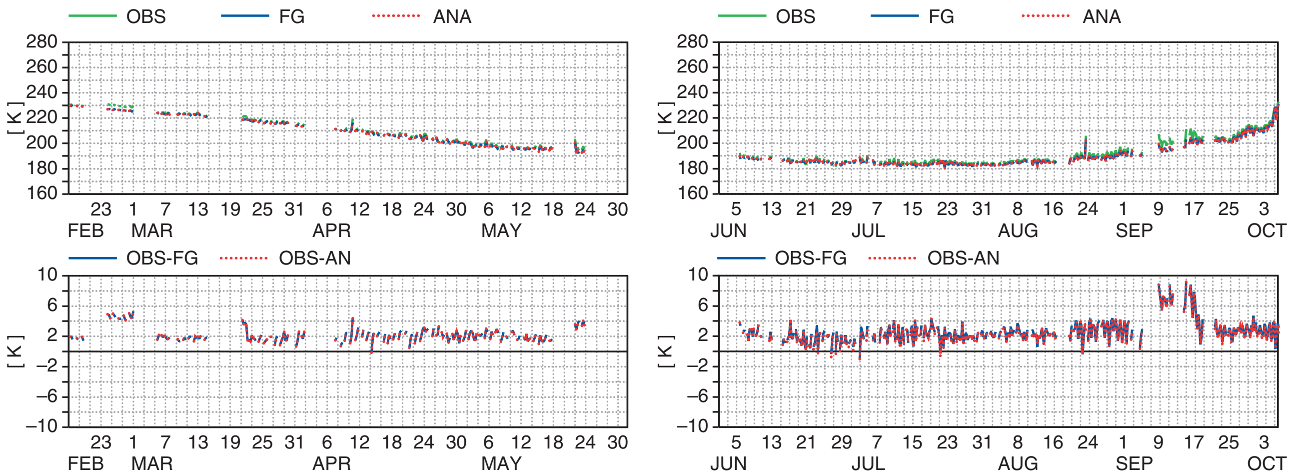

Figure 14: Like Figure 12 but for 65-90° S.

2003 (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 that the ECMWF model shows compared to UARS data in the stratosphere. 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, and below 20 hPa in 65-90°S between 1 June and 5 October, when time and area averaged MIPAS water vapour data are about 5 times higher than 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. Figure 16 shows a scatter plot of MIPAS water vapour data for July 2003 for a layer between 80-100 hPa and illustrates the problem more clearly. While the mean water vapour values for this layer lie between 400-600 mg/m^2, there are outliers with values up to 2000 mg/m^2 in the tropics and over the South Pole. These values are much above the saturation values. In the tropics high altitude clouds can cause a problem for the MIPAS retrieval up to about 60 hPa, while contamination by PSCs over the South Pole can be a problem at even higher altitudes, up to 20 hPa. Cloud contamination is also a problem for the ozone retrievals in the tropics and over the South Pole (see Section 3.3). Even though a cloud clearing algorithm was implemented on 23 July 2003, it is not flagging the cloudy data properly and unrealistically large water vapour and ozone values continue to be seen in the MIPAS data in the tropics and over the South Pole after July.

Figures 17 to 19 show timeseries of area averaged MIPAS water vapour values and departures for a layer between 20-40 hPa for the areas 90-65°N, 0-20°S, and 65-90°S, respectively. All three 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 all areas. In 90-65°N (Figure 17) MIPAS values and departures are relatively stable from the second half of April on. During February and March there is more variability, and data and departures have larger standard deviations (not shown). The periods that showed problems with the temperature retrievals (see Section 3.1) show up in the water vapour timeseries as periods when MIPAS water vapour values are about 100 mg/m^2 lower than during the rest of the timeseries. At these times they agree considerably better with ECMWF values.

In 65-90°S (Figure 19) we see a pronounced difference for the two parts of the timeseries. From 17 February to 30 May, MIPAS water vapour values and departures are relatively stable with a small seasonal increase. Between June and October, however, the area averaged MIPAS water vapour values are very noisy and show

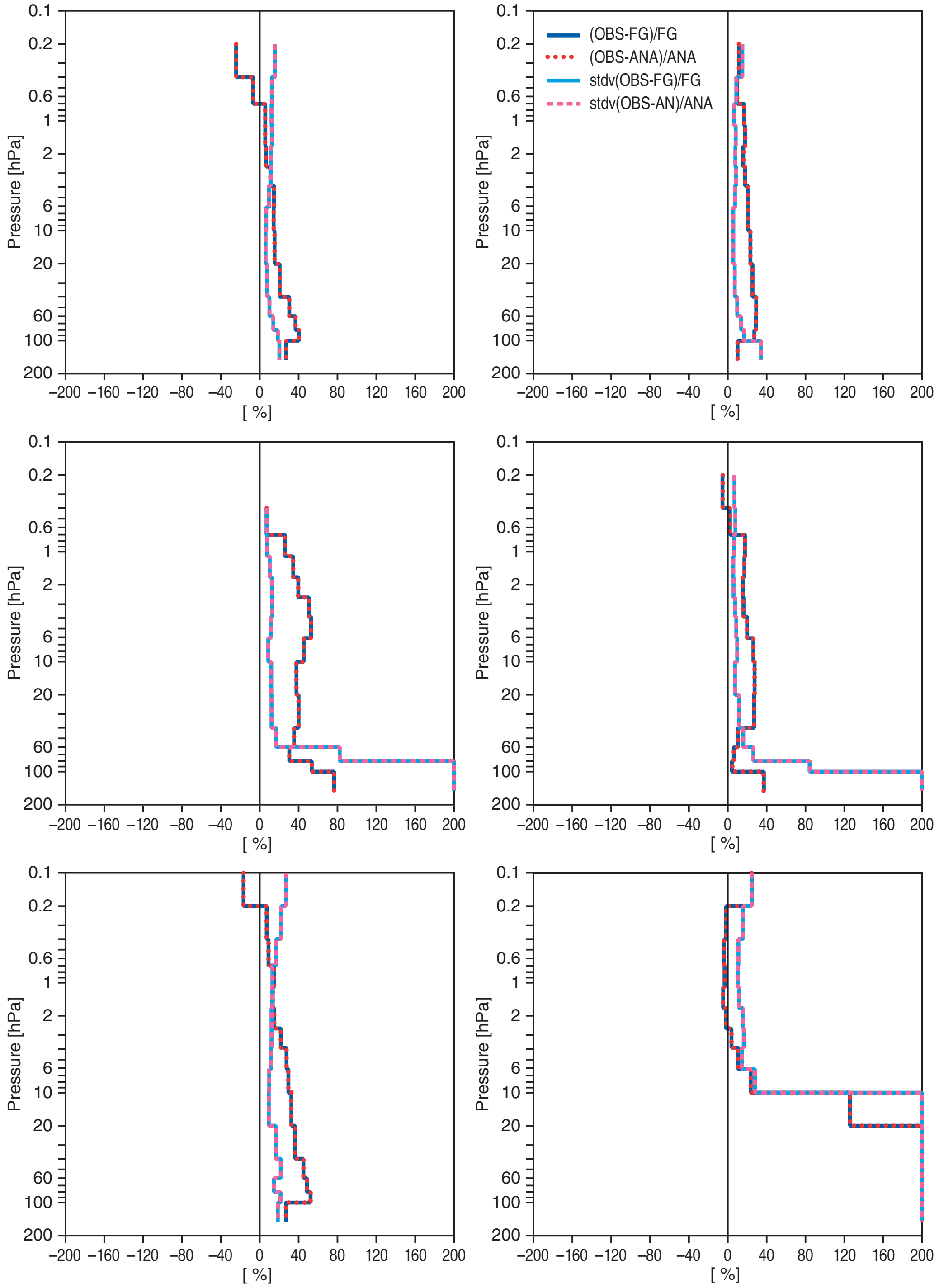

Figure 15: Profiles of time and area averaged MIPAS water vapour departures in % for the areas 90-65°N (top), 0-20°S (middle), and 65-90°S (bottom). Averaging periods are 17 February to 30 May 2003 (left) and 1 June to 5 October 2003 (right).

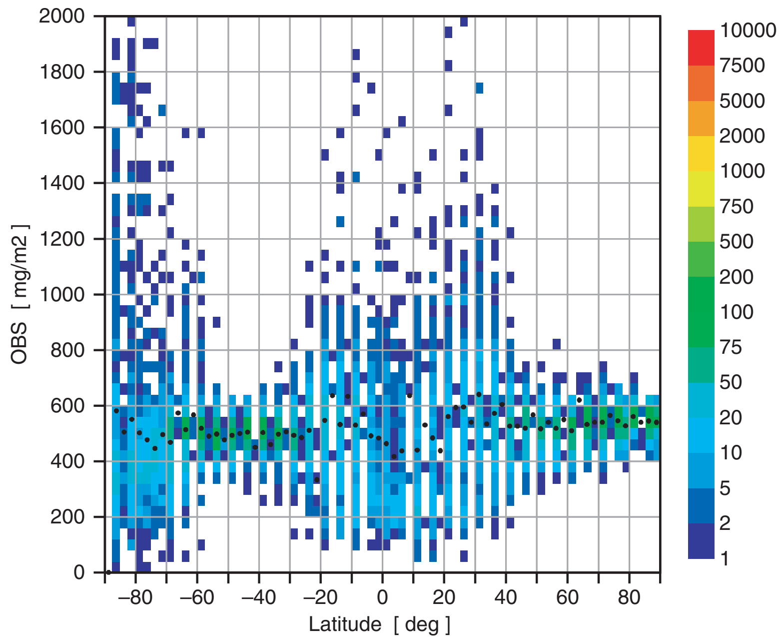

Figure 16: Scatter plot of MIPAS water vapour values in mg/m2 in a layer between 80-100 hPa in July 2003.

large standard deviations. This illustrates again the problem of cloud contamination by PSCs over the South Pole, which leads to unrealistically large water vapour values over the South Pole. While the ECMWF water vapour values show a seasonal dehydration at 20-40 hPa over the South Pole, this behaviour is masked in the MIPAS data because of unrealistically large water vapour values that go into the area average.

3.3 Monitoring of NRT ozone retrievals from MIPAS

The ECMWF assimilation system uses ozone layers or partial columns (unit kg/m^2 or DU) not ozone profile points. Like for water vapour these partial layers are calculated for MIPAS data during the conversion from PDS to BUFR format. At first, MIPAS ozone profiles were monitored passively with the help of the ECMWF assimilation system. Later, assimilation experiments were run to establish the impact of the assimilation of MIPAS ozone profiles on the ECMWF ozone analysis. The experiments showed that the assimilation of MIPAS ozone retrievals improved the ECMWF ozone field while having a neutral impact on the forecast scores and the meteorological fields. Results from these experiments are described in a separate paper (Dethof 2003). Because of the positive impact on the ozone analysis it was decided to include the assimilation of MIPAS ozone profiles in the operational system, even though the MIPAS data were still being validated and not completely stable yet, and the operational assimilation of MIPAS ozone profiles began in October 2003. This subsection discusses results from the monitoring of MIPAS ozone profiles. From 17 February to 30 May 2003 MIPAS ozone data were monitored passively, while they were actively assimilated from 1 June to 5 October 2003 onwards.

Figure 20 shows time and area averaged ozone departures in % for the areas 90-65°N (top), 0-20°S (middle), and 65-90°S (bottom) for the averaging periods 17 February to 30 May 2003 (left) and 1 June to 5 October 2003 (right). MIPAS ozone values are lower than ECMWF values at high latitudes in both hemispheres throughout the stratosphere and part of the mesosphere. Between 90-65°N, MIPAS values averaged from 17 February to 30 May 2003 are 5-10% lower than ECMWF values, between 65-90°S the differences are larger and MIPAS values are up to 30% lower at 2 hPa. The ECMWF model is known to have a positive bias at high latitudes in both hemispheres (Dethof and Hólm 2003) which agrees with the differences seen between ECMWF and MIPAS

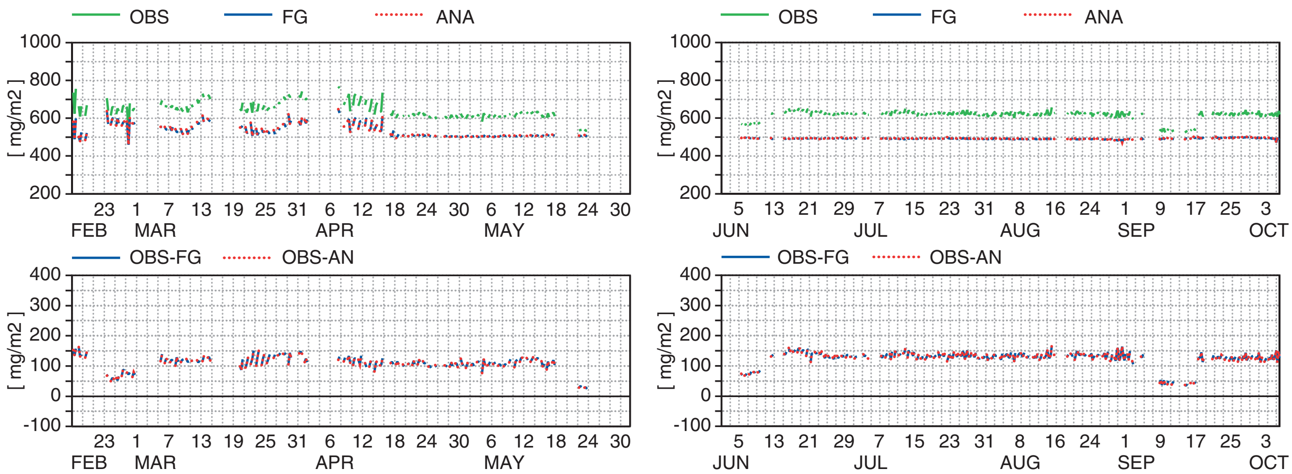

Figure 17: Timeseries of water vapour data averaged over 90-65° N covering the periods 17 February to 30 May (left) and 1 June to 5 October 2003 (right). The top panels show MIPAS water vapour data, first-guess and analysis values, the second panels first-guess and analysis departures. All water vapour values in mg/m^2.

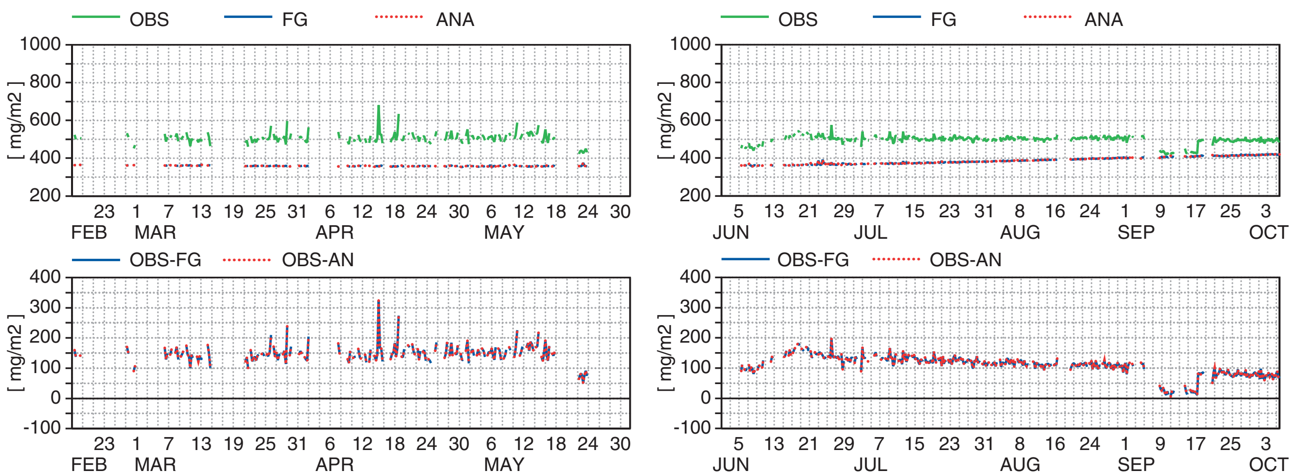

Figure 18: Like Figure 17 but for 0-20° S.

ozone values. In the tropics the situation is different. Here MIPAS ozone values are larger than ECMWF values below 10 hPa, with the biggest differences in the lower stratosphere and upper troposphere, where the time and area averaged MIPAS values are up to five times larger than ECMWF ozone values. The same problem was seen in MIPAS water vapour retrievals and is likely to be a sign of contamination by high altitude clouds. A scatter plot of MIPAS ozone values for July 2003 (Figure 21) for a layer between 80-100 hPa shows that while mean ozone values between 80-100 hPa lie around 5 DU in the tropics, there are outliers with values up to 100 DU. A similar problem is seen over the South Pole where contamination by polar stratospheric clouds is a problem for the retrieval.

The right plots of Figure 20 show ozone profiles and departures for the period from 1 June and 5 October 2003 from the CY26R3 e-suite when MIPAS ozone profiles were actively assimilated in the ECMWF system. Now an independent validation of MIPAS ozone values against ECMWF data is not possible any more. For further information about the assimilation of MIPAS ozone retrievals see Dethof (2003) where independent data are used to assess the impact of the assimilation of MIPAS ozone profiles on the ozone analysis. The signs of the departures are the same as seen for the period 17 February to 30 May (left panels in Figure 20), negative at

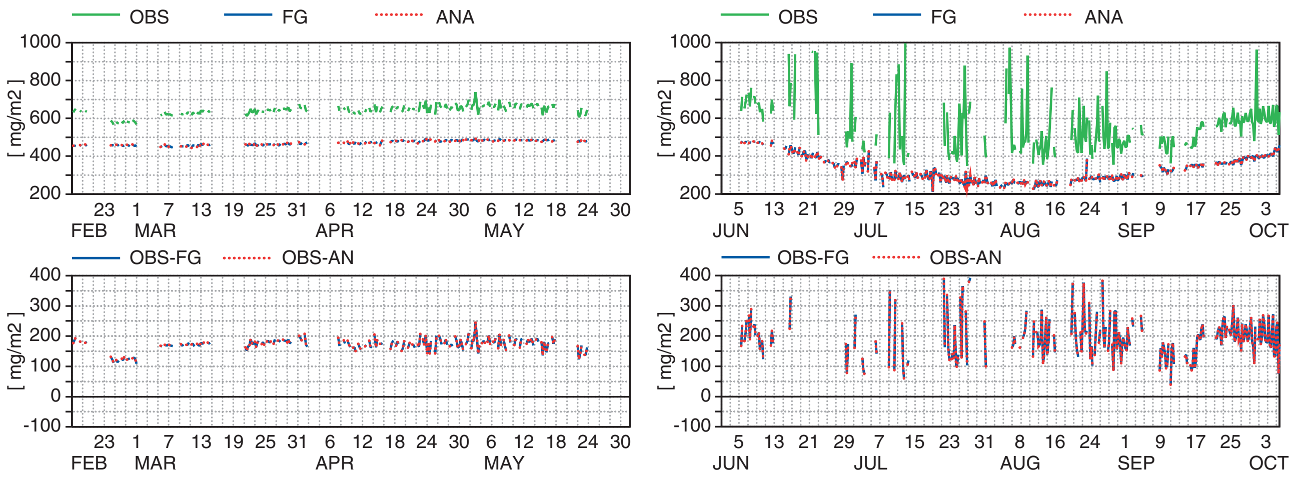

Figure 19: Like Figure 17 but for 65-90° S.

high latitudes and positive in the tropics. It can be seen that the analysis is drawing to the MIPAS data (analysis departures are smaller than first-guess departures), particularly over the South Pole and between 10-60 hPa in the tropics. The quality control checks implemented for the ozone analysis ensure that the unrealistically large MIPAS ozone values seen over the South Pole and below 60 hPa in the tropics are rejected and not used in the analysis. At high northern latitudes the differences between analysis and first-guess departures are small. Here, the ECMWF model bias is smaller at this time of year than in spring, MIPAS data and model agree better, and the analysis correction is smaller than in the SH or in the tropics.

Figures 22 to 24 show timeseries of area averaged ozone values and departures for a layer between 20-40 hPa for 90-65° N, 0-20° S, and 65-90° S, respectively. The timeseries for the area 90-65° N (Figure 22) shows negative departures between 17 February and 20 April 2003. This was already seen in the profile plots and is in agreement with the ECMWF model bias at this time of year. From 20 April onwards the departures are smaller and so are the standard deviations of observations and departures (not shown). From June to October the timeseries shows small departures because the model bias is smaller and the analysis is drawing to the MIPAS data.

The departures in 0-20° S (Figure 23) are larger than in 90-65° N and positive. The second part of the timeseries (1 June to 5 October 2003) shows that the analysis is drawing to the MIPAS data, and that departures are much reduced when MIPAS ozone data are assimilated. The timeseries also show a discontinuity and lower MIPAS ozone values and smaller departures at the end of May and from 6 to 17 September, a result of the discontinuities in the temperature retrievals (see Section 3.1) that propagated into the ozone retrievals. Because MIPAS ozone profiles are actively assimilated in September, this discontinuity affects the ECMWF ozone analysis and is seen in the monitoring statistics for SCIAMACHY data (Figures 4 to 6). This offset illustrates the importance of having stable data products for the analysis.

In 65-90° S (Figure 24) MIPAS data are lower than ECMWF data, which again agrees with the known model bias. The second part of the timeseries shows more noisy MIPAS observations and departures during June and July than during the rest of the period. The reason for this is cloud contamination by PSCs that affects ozone retrievals up to 20 hPa over the South Pole, and means that unrealistically large ozone values go into the area average. Despite, the implementation of a cloud check for MIPAS retrievals by ESA on 23 July 2003, unrealistically large ozone (and water vapour) values remain in the retrievals, particularly in the tropics. Over the South Pole the number of unrealistically large ozone values is reduced after 23 July, but this could simply be a seasonal effect, because temperatures over the South Pole rise, and contamination by PSCs should be less

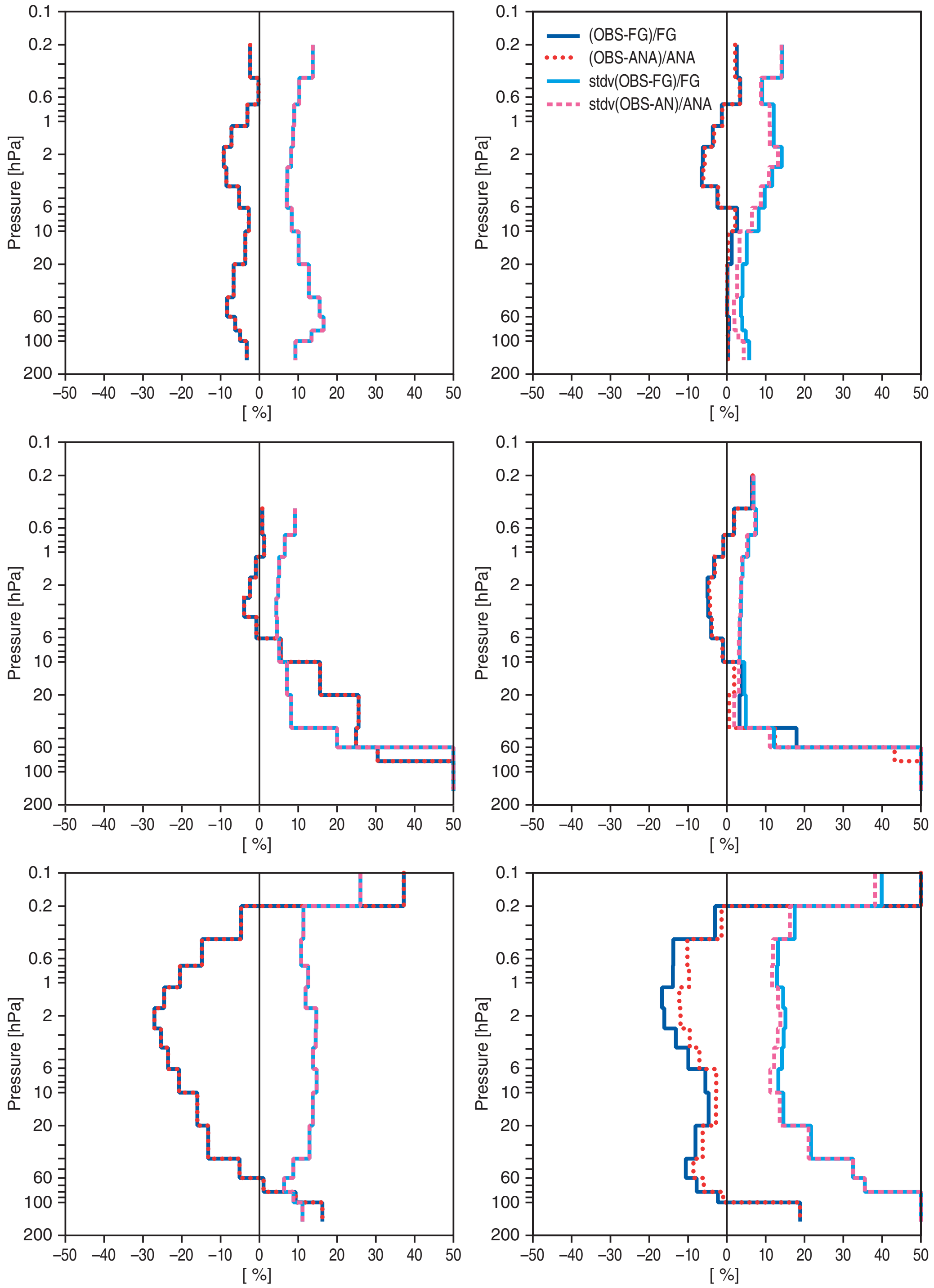

Figure 20: Profiles of time and area averaged MIPAS ozone departures in % for the areas 90-65°N (top), 0-20°S (middle), and 65-90°S (bottom). Averaging periods are 17 February to 30 May 2003 (left) and 1 June to 5 October 2003 (right).

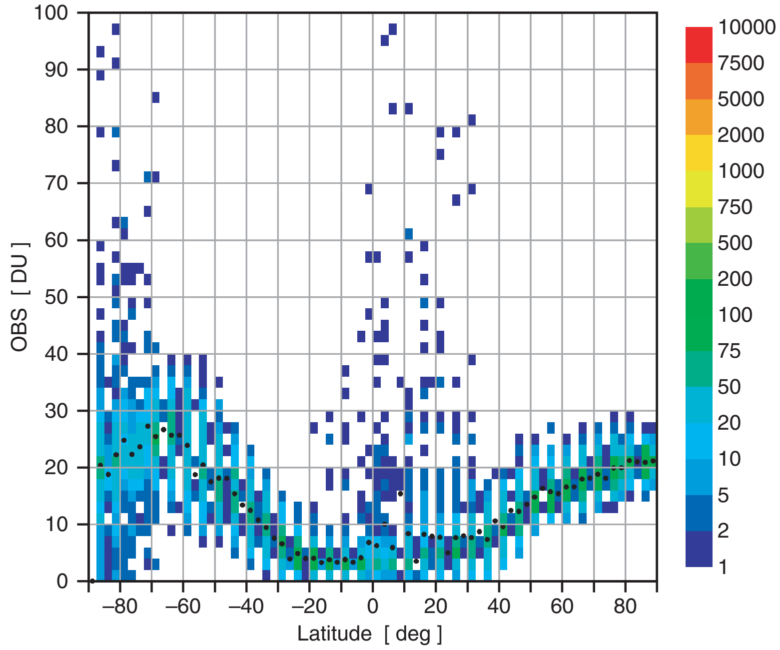

Figure 21: Scatter plot of MIPAS ozone values in DU in a layer between 80-100 hPa in July 2003.

of a problem after July.

4 Conclusions

Under ESA contract 14458/00/NL/SF a technical framework was developed at ECMWF to monitor NRT retrievals from SCIAMACHY, MIPAS and GOMOS, and the monitoring of these data is now included in the operational ECMWF system. Total column ozone retrievals from SCIAMACHY, and temperature and water vapour profiles from MIPAS are now monitored passively at ECMWF. Ozone retrievals from MIPAS have been actively assimilated in the operational ECMWF system since October 2003. The statistics for GOMOS NRT data are not analysed at the moment because the data quality is not good enough.

The monitoring statistics have shown SCIAMACHY NRT total column ozone data to have a negative bias of 25-30 DU over much of the globe. This bias makes it impossible to actively assimilate the data in the ECMWF system at present. A further problem with the NRT SCIAMACHY data is the lack of geolocation information (e.g. solar zenith angles, field of view) which makes a thorough analysis of the data difficult. It also stops us from using a sub-set of the data screened or bias corrected according to geolocation parameters, for instance below a solar zenith angle threshold.

MIPAS NRT retrievals are of reasonable quality, and the temperature retrievals agree with the ECMWF analysis to within 2% in most regions. The departures of MIPAS ozone and water vapour retrievals are larger, but some of these differences can be attributed to deficiencies of the ECMWF ozone or water vapour fields.

MIPAS temperature values are larger than ECMWF temperatures in the stratosphere, but departures are smaller than 2%. Larger departures can be seen at the model top where the ECMWF model has a cold bias over the winter pole. MIPAS data show up these model problems, and they also served as a useful independent data set to identify problems in the ECMWF temperature analysis which came from the assimilation of AIRS radiances. However, even though MIPAS temperature retrievals are relatively stable over most of the monitoring period,

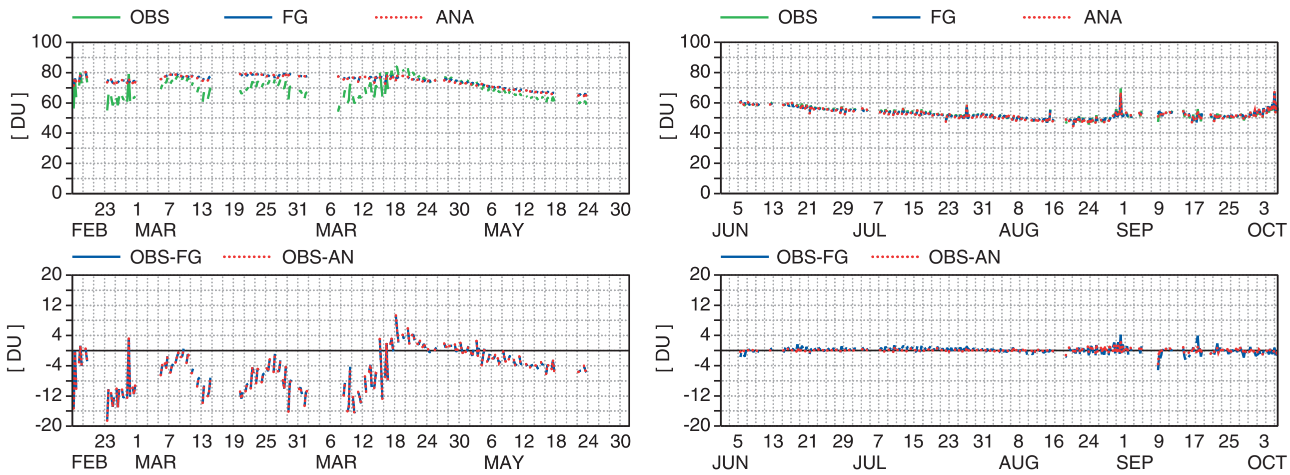

Figure 22: Timeseries of ozone data averaged over 90-65°N covering the periods 17 February to 30 May (left) and 1 June to 5 October 2003 (right). The top panels show MIPAS ozone data, first-guess and analysis values, the second panels first-guess and analysis departures. All ozone values in DU.

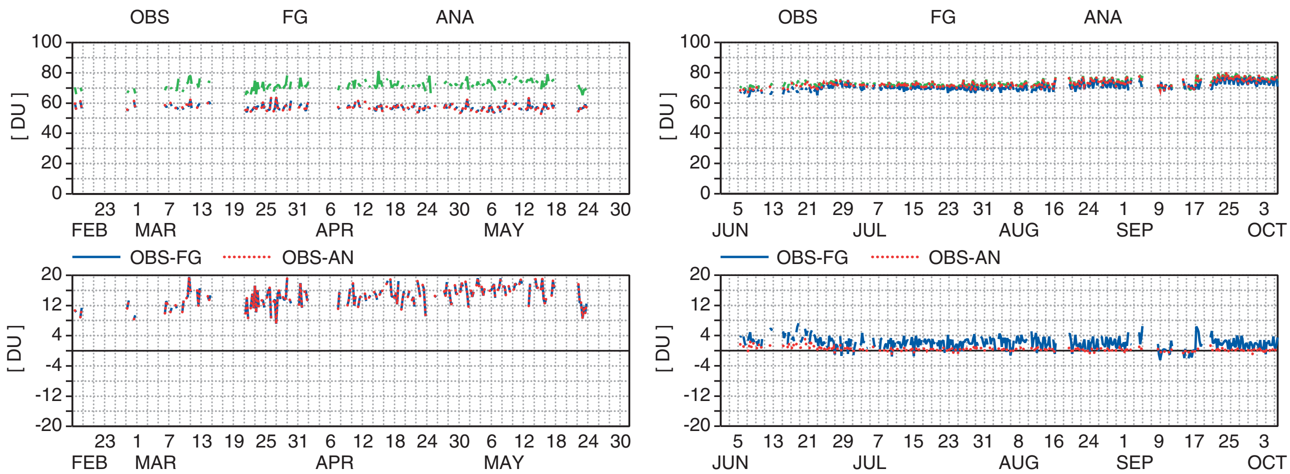

Figure 23: Like Figure 22 but for 0-20°S.

there are discontinuities after unplanned payload switch-offs if no gain calibration is performed when MIPAS operations resume. This leads to changes of up to 8K in area averaged temperature retrievals. These errors propagate into the mixing ratio retrievals and lead to discontinuities in MIPAS water vapour and ozone fields. When MIPAS ozone profiles are actively assimilated, these discontinuities affect the ECMWF ozone analysis and can be seen in timeseries of SCIAMACHY departures.

MIPAS ozone values are lower than ECMWF values over most of the stratosphere in the extratopics of both hemispheres. These differences reflect a known bias of the ECMWF ozone field. When MIPAS data are assimilated (Dethof 2003) the resulting ozone analysis agrees much better with independent ozone sondes and TOMS data in the extratropics. The improvement is particularly pronounced in the NH during spring and in the SH during the ozone hole season, i.e. at times when the systematic error of the model is largest. In the tropics, MIPAS ozone values are larger than ECMWF values around the ozone maximum. Comparisons with ozone sondes and TOMS data (Dethof 2003) show that the fit to the independent data is slightly degraded when MIPAS ozone profiles are assimilated, suggesting that MIPAS ozone values in the tropics are too high around the ozone maximum.

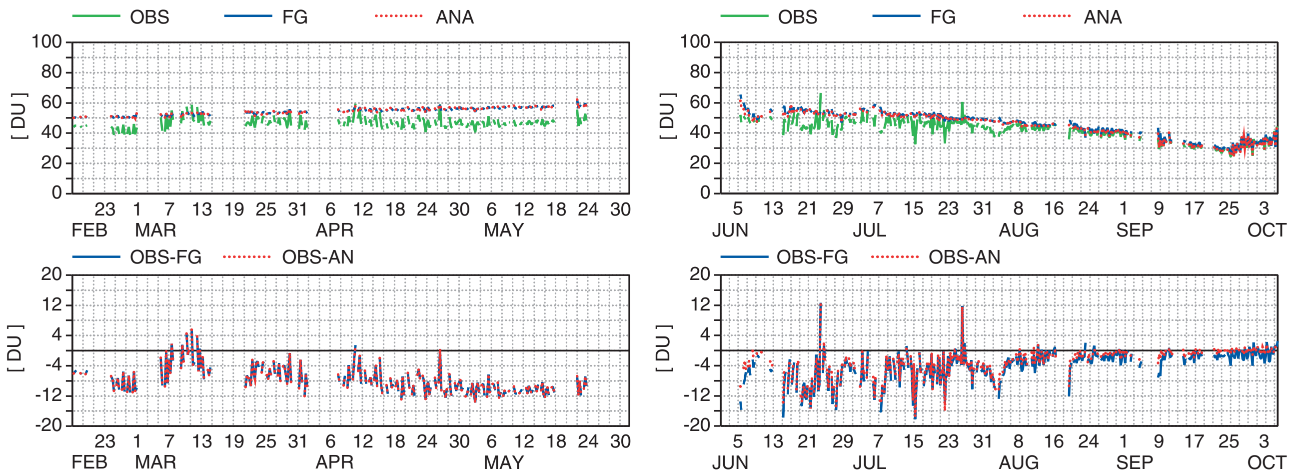

Figure 24: Like Figure 22 but for 65-90° S.

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.

Cloud contamination is a problem for MIPAS ozone and water vapour retrievals in the tropics, and also over the South Pole where PSCs affect the retrieval from June to September. This results in unrealistically large MIPAS ozone and water vapour values. Even though a cloud clearing algorithm was implemented on 23 July 2003, it seems to have little effect and unrealistically large values continue to be seen after 23 July.

The monitoring of SCIAMACHY and MIPAS data will continue at ECMWF, and so will the assimilation of MIPAS ozone retrievals. The assimilation of MIPAS water vapour retrievals will be tested when the new ECMWF humidity analysis is completed. If SCIAMACHY data quality improves, the assimilation of SCIAMACHY data will be tested. Also, GOMOS monitoring statistics will be analysed if an algorithm update leads to improved data quality.

5 Acknowledgements

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References

Cariolle, D. and M. Déqué (1986). Southern hemisphere medium-scale waves and total ozone disturbances is a spectral general circulation model. *J. Geophys. Res.*, 91. 10825–10846.

Courtier E., Andersson P., Heckley W., Pailleux J., Vasiljevic D., Hamrud M., Hollingsworth A., Rabier F. and Fisher M. (1998). The ECMWF implementation of three dimensional variational assimilation (3D-Var). Part I: Formulation. *Quart. J. Roy. Meteor. Soc.*, 124. 1783–1808.

Dethof, A., and Hólm, E.V. (2003). Ozone assimilation at ECMWF. *Quart. J. Roy. Meteor. Soc.*, 128. submitted.

Dethof, A. (2003). Assimilation of ozone retrievals from the MIPAS instrument on ENVISAT. *ECMWF Technical Memorandum 428*.

Fortuin, J.P.F. and U. Langematz (1995). An update on the global ozone climatology and on concurrent ozone and temperature trends. *SPIE Proceedings Series*, Vol. 2311, ”Atmospheric Sensing and Modeling”, pp 207-216.

Rabier F., Järvinen H., Klinker E., Mahfouf J-F. and Simmons A. (2000). The ECMWF operational implementation of four-dimensional variational assimilation. I: Experimental results with simplified physics. *Quart. J. Roy. Meteor. Soc.*, 126. 1143–1170.

Valks, P. J. M., Piters, A. J. M., Lambert, J. C., Zehner, C., and Kelder, H. (2003). A Fast Delivery System for the retrieval of near-real time ozone columns from GOME data. *Int. J. Rem. Sens.*, 24. 423–436.