



ESA CONTRACT REPORT

Contract Report to the European Space Agency

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

July 2008

Author: Rossana Dragani

Final report for ESA contract 17585-CCN-1:
Technical support for global validation of
ENVISAT data products

European Centre for Medium-Range Weather Forecasts
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**Monitoring and Assimilation of
SCIAMACHY, GOMOS and MIPAS
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Author: Rossana Dragani

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Shinfield Park, Reading, Berkshire, UK

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Abstract

ECMWF is contracted by ESA to provide technical support for the global validation and monitoring of atmospheric data from several instruments on board Envisat (contract 17585-CCN-1, “Technical support for global validation of Envisat data products”). Under this contract, which ran from 1 January 2006 to 31 December 2007, ECMWF monitored near-real time Level 2 data products from SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric CHartography), and GOMOS (Global Ozone Monitoring by Occultation of Stars). Owing to instrumental problem, the dissemination of NRT MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) Level 2 products was stopped in March 2004. The NRT SCIAMACHY total column ozone (TCO) retrieved at ESA were not available during 2007 as the dissemination of this product was also stopped in May 2006. In contrast, the NRT TOSOMI TCO produced at KNMI and distributed via the ESA funded PROMOTE consortium were continuously disseminated during 2007. The TOSOMI product showed stable quality during 2007, and a high level of agreement with the ECMWF ozone analyses. Some inconsistencies were found in the monitoring statistics of the NRT GOMOS temperature for 2007, after these data were fixed to the ECMWF temperature forecasts from surface up to 1 hPa, and to MSIS data in the Mesosphere (GOMOS retrieval scheme v5.0). The monitoring statistics for the NRT GOMOS ozone profiles show that on average the ozone first-guess and analysis departures are within -10 and +30% in most of the stratosphere (for $p < 40$ hPa), but larger in the lower stratosphere and in the mesosphere. Comparisons of one-month worth of data for the four years from 2004 to 2007 showed that the scatter in the ozone data, although still important, was much reduced and their agreement with the ECMWF ozone first-guess and analyses improved since the dissemination started. In January 2007, for the first time since ECMWF have been receiving NRT ENVISAT L2 products, water vapour information retrieved from the GOMOS measurements were made available in the BUFR files. The quality of the GOMOS WV profiles is poor, and on average they exhibit one to four orders of magnitude larger values than their model equivalent in all the stratosphere.

1 Introduction

The present report summarises the results from the global validation and monitoring of ENVISAT atmospheric data products performed at ECMWF under the ESA funded project 17585-CCN-1. These products, usually referred to as the Meteo products, are retrieved at ESA and available to ECMWF on their ftp servers in near-real time (NRT) in BUFR format. As far as the ENVISAT atmospheric instruments are concerned, the products routinely monitored 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 current project continues the work carried out under ESA contracts 14458/00/NL/SF (Dethof, 2003), and 17585/03/I-OL (Dethof, 2004; da Costa Bechtold and Dethof, 2005). The present report discusses the results from the monitoring and assimilation of the ENVISAT L2 atmospheric data products during the period January to December 2007. The results for the period January to December 2006 were given in the 2006 interim report (Dragani, 2006).

The ECMWF deterministic model is a global spectral model. It benefits from a current horizontal resolution truncation of T799, which corresponds to about 25 km grid spacing, and 91 vertical levels with the model top at 0.01 hPa (corresponding to an altitude of about 80 km). The model uses a four-dimensional variational (4D-Var) scheme (Rabier et al., 2000) to assimilate observations at 6- and 12-hourly time windows. The ECMWF assimilation system has two main 6-hour 4D-Var (early-delivery) analysis and forecast cycles for 00 and 12 UTC and two 12-hour 4D-Var analysis and first-guess forecast cycles. The 0000 UTC analysis of the 12-hour 4D-Var analysis uses observations in the time window 2101-0900 UTC, while the 1200 UTC analysis uses observations in the time window 0901-2100 UTC. These analyses are run with a delayed-cut-off time of 14 hours (with respect to the nominal analysis times), in order to use the maximum possible number of observations. The 6-hour 4D-Var analyses have a shorter cut-off time (4 hours) and the analysis observation

windows are 2101-0300 UTC for the 00 UTC analysis and 0901-1500 UTC for the 12 UTC analysis. All the observation monitoring, ENVISAT data monitoring included, is done in the delayed-cut-off analyses (Dethof, 2004) and (Haseler, 2004).

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 the Cariolle and Déqué (1986) scheme (hereafter CD86). Compared with CD86, the ECMWF ozone parameterization includes an additional term which parameterizes the depletion of ozone in the 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 preferred instead.

As far as the ozone model bias is concerned, the ECMWF model still overestimates TCO at high latitudes especially during the spring season (ozone hole) and underestimates it in the tropics. There are also some problems with the vertical ozone structure in particular at high latitudes in the winter hemisphere (Dethof and Hólm, 2004).

During the period January to December 2007, the ECMWF operational model system was upgraded twice to model cycle CY32R1 on 5 June, and to model cycle CY32R3 on 6 November, respectively. Among all the changes introduced in cycle CY32R1, the most relevant change for the validation of ENVISAT data is the change in the term which parameterizes the ozone heterogeneous chemistry. We also acknowledge the active assimilation of IASI radiances and ASCAT wind vectors since 12 June 2007 in cycle CY32R1. The changes introduced with cycle CY32R3 on 6 November included the active assimilation of ozone partial columns retrieved from SBUV/2 on board of NOAA-17 and NOAA-18 satellites, as well as an increase in the number of GPS radio occultation (GPSRO) data from COSMIC actively assimilated¹. In addition, AMSR-E, TMI and SSMIS window channels were also actively assimilated from CY32R3 onwards.

As far as the ozone assimilation is concerned, NRT ozone retrievals from the SBUV/2 (Solar Backscatter Ultra Violet) instrument on the NOAA-16 satellite have been assimilated in the operational ECMWF system since April 2002. As mentioned above starting from 6 November 2007, the ECMWF ozone first-guess and analyses used in the validation of the ENVISAT L2 products also benefited from the active assimilation of ozone partial columns from the SBUV/2 instrument on board of NOAA-17 and NOAA-18. The SBUV/2 data are produced by NOAA and available from NESDIS². They are given as 12 ozone layers and then combined at ECMWF into 6 fixed ozone layers (0.1-1 hPa, 1-2 hPa, 2-4 hPa, 4-8 hPa, 8-16 hPa and 16 hPa-surface) to reduce the observation error correlation. Apart from the SBUV/2 ozone retrievals, NRT SCIAMACHY ozone columns produced by KNMI³ and distributed via the ESA's funded PROMOTE-2 consortium have also been actively assimilated in the ECMWF system since 28 September 2004. SBUV/2 and KNMI SCIAMACHY data are not used at solar zenith angles greater than 84°. Variational quality control and first-guess checks are carried out for all assimilated data. Temperature retrievals are not assimilated at all in the system, although this field is strongly constrained by the assimilation of radiances. The radiance assimilation does not include the assimilation of the ozone band in the infrared.

¹The assimilation of GPSRO data were found to improve and stabilize the stratospheric temperature analyses.

²See <http://orbit-net.nesdis.noaa.gov/crad/sit/ozone/> for more information.

³See either <http://www.temis.nl/products/o3total.html> or <http://www.gse-promote.org/> for further information.

This report presents the results from the monitoring of NRT total column ozone (TCO) retrieved from SCIAMACHY measurements, as well as NRT ozone, water vapour and temperature profiles retrieved from GOMOS observations. Owing to instrumental problems, NRT MIPAS Level 2 retrievals have not been available since 27 March 2004, and so this report does not discuss the monitoring of MIPAS products. It is structured in the following way. Section 2 gives an indication of the “operationability” of ESA and KNMI products during the period 2006 and 2007 (subject to data availability). Section 3 summarizes the 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 Operationability of ESA and KNMI products during the two-year period 2006-2007

This section is meant to provide an indication of the operationability of both ESA and KNMI product at ECMWF.

ENVISAT products (from both ESA and KNMI) are downloaded by ECMWF at a fixed time of three minutes after every half an hour (e.g. 00:03, 00:33, 01:03 and so on). A cross-comparison of the data volume on the local (ECMWF) server and on the remote (ESA and KNMI) servers for a period of about one week⁴ showed that 100% of the data uploaded by ESA and KNMI on their servers is actually downloaded by ECMWF.

To assess the operationability of these products then, we have looked at the data volume received within the analysis cut-off times compared with the total amount of data received. As anticipated above, ECMWF has two main 6-hour 4D-Var analysis and forecast cycles for 00 and 12 UTC (referred to as early-delivery) and two 12-hour 4D-Var analysis and first-guess forecast cycles (referred to as delayed-cut-off). The passive monitoring is performed with a delayed cut-off configuration, while the data actively assimilated - depending on their timely availability - are used in both the delayed-cut-off and early delivery suites. Figures 1 and 2 show the schematics of the delayed cut-off and early delivery configurations respectively.

In the delayed-cut-off, the 00 UTC analysis makes use of all the observations available in the Report Data Base (RDB) within the assimilation window between 2101 and 0900 UTC. These data are extracted in two phases. Data between 2101 and 0300 UTC are extracted from RDB at 1345 UTC; while data between 0301 and 0900 UTC are extracted from RDB at 1400 UTC. The 12 UTC analysis makes use of all the observations available in RDB within the assimilation window between 0901 and 2100 UTC. Data between 0901 and 1500 UTC are extracted from RDB at 0145 UTC; while data between 1501 and 2100 UTC are extracted from RDB at 0200 UTC (Haseler, 2004).

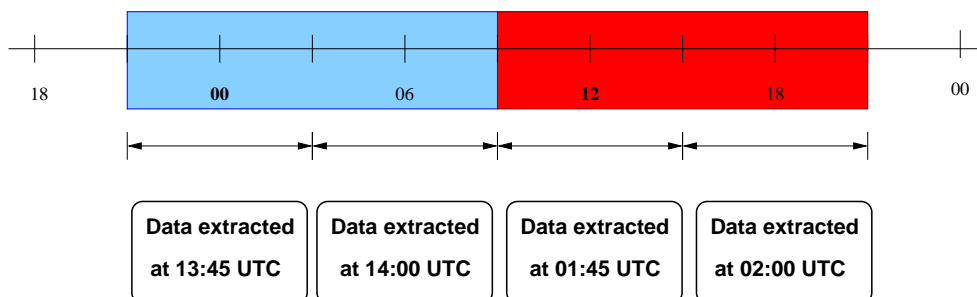


Figure 1: Schematic of the delayed cut-off configuration.

⁴The information on the remote servers is only available for a short period of time.

The early delivery analyses make use of only six-hour observation windows. The 00 UTC analyses are obtained by assimilating all data within the assimilation window between 2101 and 0300 UTC that are available in RDB by 0400 UTC. The 12 UTC analyses are obtained by assimilating all data within the assimilation window between 0901 and 1500 UTC that are available in RDB by 1600 UTC. All the observations that fall into a given observation window but are not available in the RDB by the early delivery cut-off times can still be used in the delayed-cut-off analyses. We also note that the information from the data that cannot be actively assimilated in the early delivery system (but arrive in time for the delayed-cut-off) still indirectly affects the (early delivery) analyses as the first guess used in the assimilation are the three-hour forecasts from the delayed-cut-off.

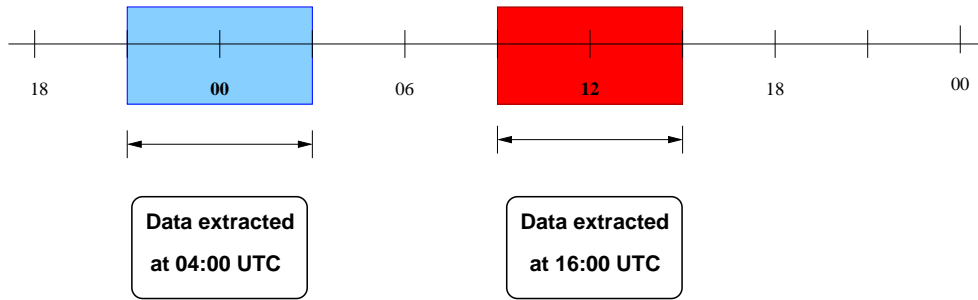


Figure 2: Schematic of the early delivery configuration.

Figures 3 and 4 show the data volume received by ECMWF within the analysis delayed-cut-off times given above relative to the total amount of data downloaded. Values of 100% correspond to the total amount of data received within the analysis cut-off times. In contrast, 0% values mean that either there was an instrument unavailability or the total data volume was received after the cut-off times. It should be noted that because the information on the uploading times is only available on the remote (ESA and KNMI) servers for a short period (up to one week), it is not possible to cross-compare the uploading and downloading times for long periods. Therefore, delays in the data acquisition (values that are less than 100% in plots 3 and 4) could be related either to delays in the data processing, or to server access problems. Table 1 gives the annual mean percentage of data volume received in time for the delayed-cut-off analyses. (Note that the mean for ESA SCIA was computed using only the data between 1 January and 8 May 2006.)

Year	GOMOS	ESA SCIA	TOSOMI
2006	96.1%	90.7%	89.0%
2007	94.7%	NA	83.1%

Table 1: Annual mean of the data volume received by ECMWF within the delayed cut-off times relative to the total amount of data delivered. Periods of total data unavailability (such as during instrument unavailability) were not included in the annual mean.

As far as the SCIAMACHY instrument is concerned, almost 91% of the total amount of data received from ESA arrived within the delayed cut-off analysis times, at least for the just over four-month worth of data available in 2006⁵. By contrast, a smaller percentage of data was acquired within the delayed-cut-off times from KNMI. By comparing the middle and bottom panels of figure 3, it also appears that the timeliness of the TOSOMI product was higher in 2006 than that in 2007. Overall, about 89% of the TOSOMI data was delivered on time in 2006, and just over 83% in 2007.

The best timeliness was found to be that of GOMOS products that was about 95% during 2006 and 2007. As already noted for the TOSOMI data, also the timeliness of the GOMOS products was better in 2006 (about 96%) than in 2007 (just below 95%).

⁵The dissemination of the SCLRV_2P products was stopped on 8 May 2006.

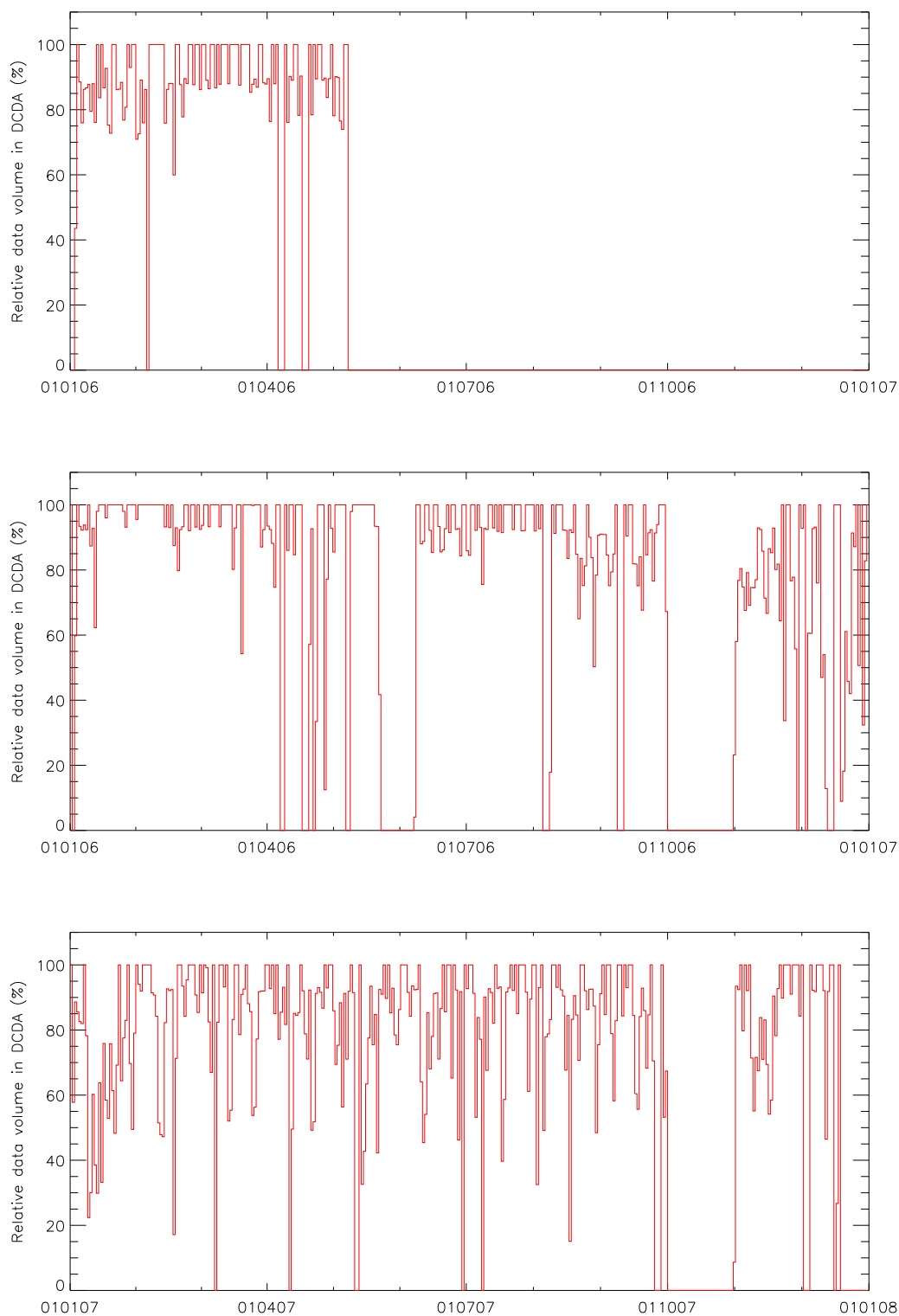


Figure 3: Time series of the daily data volume received in time for the delayed-cut-off relative to the total daily data volume received. The top panel refers to the ESA SCI_RV_2P product during 2006 (top); the middle and bottom panels refer to the TOSOMI total column ozone during 2006 and 2007 respectively. Values are in %.

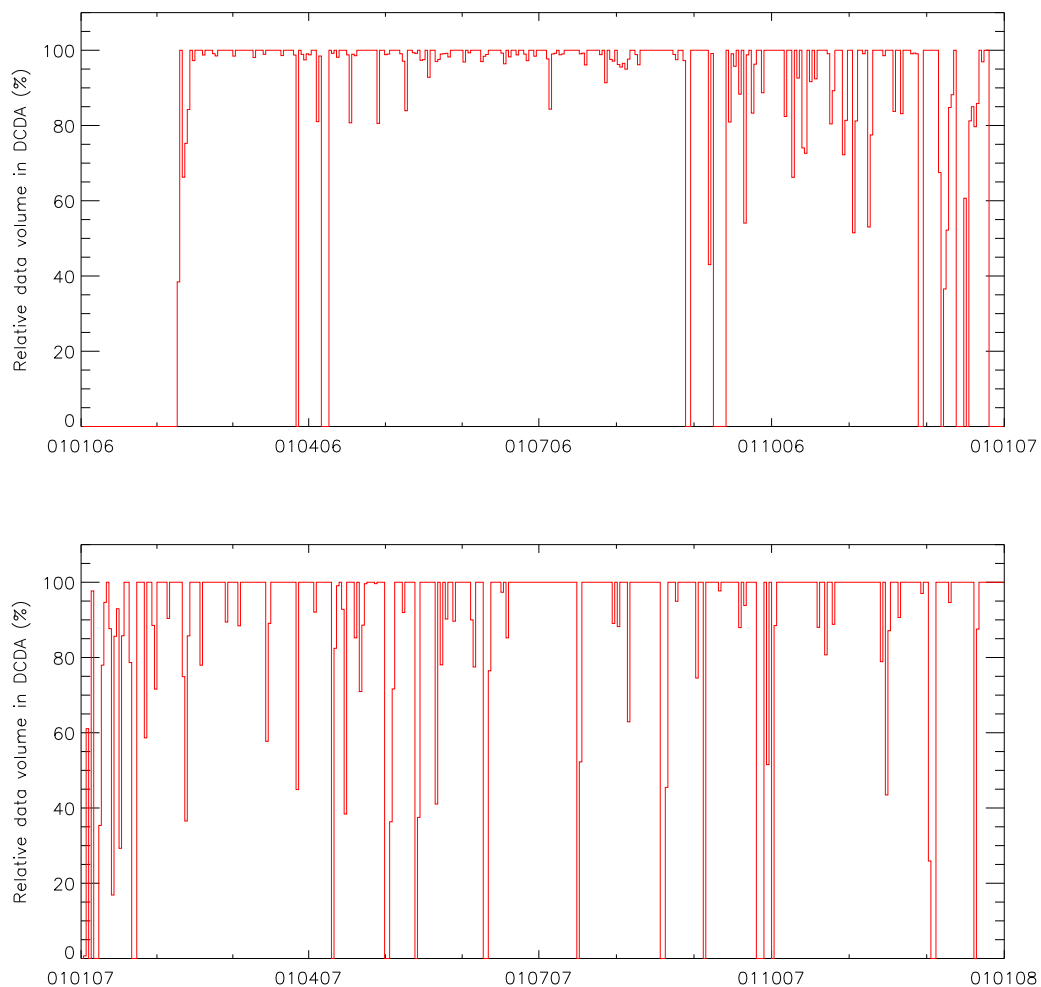


Figure 4: Like in figure 3, but for GOMOS during 2006 (top) and 2007 (bottom).

Finally, we note that the information used to calculate these statistics are only stored for a period of about two years. Therefore, the MIPAS product records are no longer available as they were disseminated only until March 2004.

3 Monitoring and assimilation of SCIAMACHY NRT total column ozone retrievals

SCIAMACHY (Burrows et al., 1988) measures sunlight, transmitted, reflected and scattered by the Earth's atmosphere or surface in the ultraviolet, visible and near infrared 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 measurements are performed in three viewing modes: nadir, limb and occultation. Depending on the type of measurement mode, global coverage is achieved within 3 to 6 days, e.g. nadir measurements yield global coverage in about 6 days.

NRT total column ozone retrievals from the nadir measurements in the UV/VIS (SCI_RV_2P) were produced operationally by ESA until May 2006. These retrievals were monitored passively⁶ at ECMWF in the operational suite from February 2003 until 8 May 2006, when the dissemination of the Level 2 products was stopped. The results from the monitoring of ESA SCIAMACHY TCO for the period 1 January to 8 May 2006 were discussed by Dragani (2006).

In addition to the NRT ESA TCO, ECMWF has also been receiving NRT total column ozone data retrieved by KNMI from the nadir measurements in the UV/VIS spectral range and distributed via the ESA funded PROMOTE 2 consortium (the so-called TOSOMI product) since March 2004. In contrast with the former product, the TOSOMI data are retrieved using the Ozone Monitoring Instrument (OMI) Differential Optical Absorption Spectroscopy (DOAS) algorithm (Veefkind and de Haan, 2002). Given the unavailability of the NRT ESA SCIAMACHY TCO retrievals, it was agreed that the TOSOMI product should be regarded as the operational ESA Level 2 total column ozone retrieval from SCIAMACHY (Minute of the ENVISAT progress meeting held at ECMWF on 6 December 2006). The interim results from the monitoring and assimilation of the TOSOMI data in 2006 were discussed by Dragani (2006). Section 3.1 focusses on the results from the TOSOMI monitoring and assimilation during 2007.

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

NRT total column ozone retrieved from SCIAMACHY measurements at KNMI (the TOSOMI product) was passively monitored at ECMWF from March 2004 to 27 September 2004. Based on the positive impact that these data could make on the ECMWF ozone analyses, especially in the Antarctic polar vortex region (Dethof, 2004), this product was actively assimilated since 28 September 2004, when the model was updated to cycle CY28R3.

SCIAMACHY nadir measurements have a typical horizontal resolution of 30 km (along track) x 60 km (across track). In the ECMWF assimilation system, the KNMI SCIAMACHY retrievals are pre-thinned to a horizontal resolution of $1^\circ \times 1^\circ$ before the assimilation.

The quality of the TOSOMI retrievals was generally stable during all 2007, and consistent with that reported in 2006. The TOSOMI data dissemination continued during 2007 without major disruptions.

Figure 5 presents the timeseries of globally averaged NRT KNMI SCIAMACHY ozone data, its averaged departures, standard deviations, and number of data actively assimilated with respect to the number of available observations for the periods January to June (l.h.s. panels), and July to December (r.h.s. panels), respectively. The timeseries in figure 5 show a generally stable behaviour of the data. The first-guess and analysis departures (blue and red lines in the mid panels) were well within $\pm 5\text{DU}$ during the whole year. A few episodes characterized by larger first-guess and analysis departures were registered during the year. In some cases, like for example on 10 October, the large difference between the TOSOMI data and their model equivalent (about 15DU) is due to the lack of SCIAMACHY observations during the three days before. When such an unavailability occurs, the system partly loses memory of the contribution provided by previously assimilated observations. In other cases, the large differences are associated to episodes of large ozone variations in the data (only partly captured by the first guess) associated with smaller than average standard deviations. When situations like this occur, the 4D-Var assimilation scheme is likely to give a large weight to the observations which can lead to large changes in the analyses. An example is the episode on 26 March 2007.

⁶ Data go into the system, statistics are calculated e.g. statistical analyses of the differences between the model's first-guess or analysed fields and the observations, the so-called departures, but the data is not assimilated into the ECMWF model.

The standard deviation of the observations (green line in bottom panels) during the second half of the year shows slightly smaller mean value, as well as a smaller variability than that seen during the first six months. Also the standard deviations of the first-guess and analysis departures (blue and red lines in bottom panels respectively) are slightly smaller than those during the first part of 2007. In the latter case, the reduction, although apparently small (typically 1 to 2 DU smaller), still represents about 10-20% of the annually mean value.

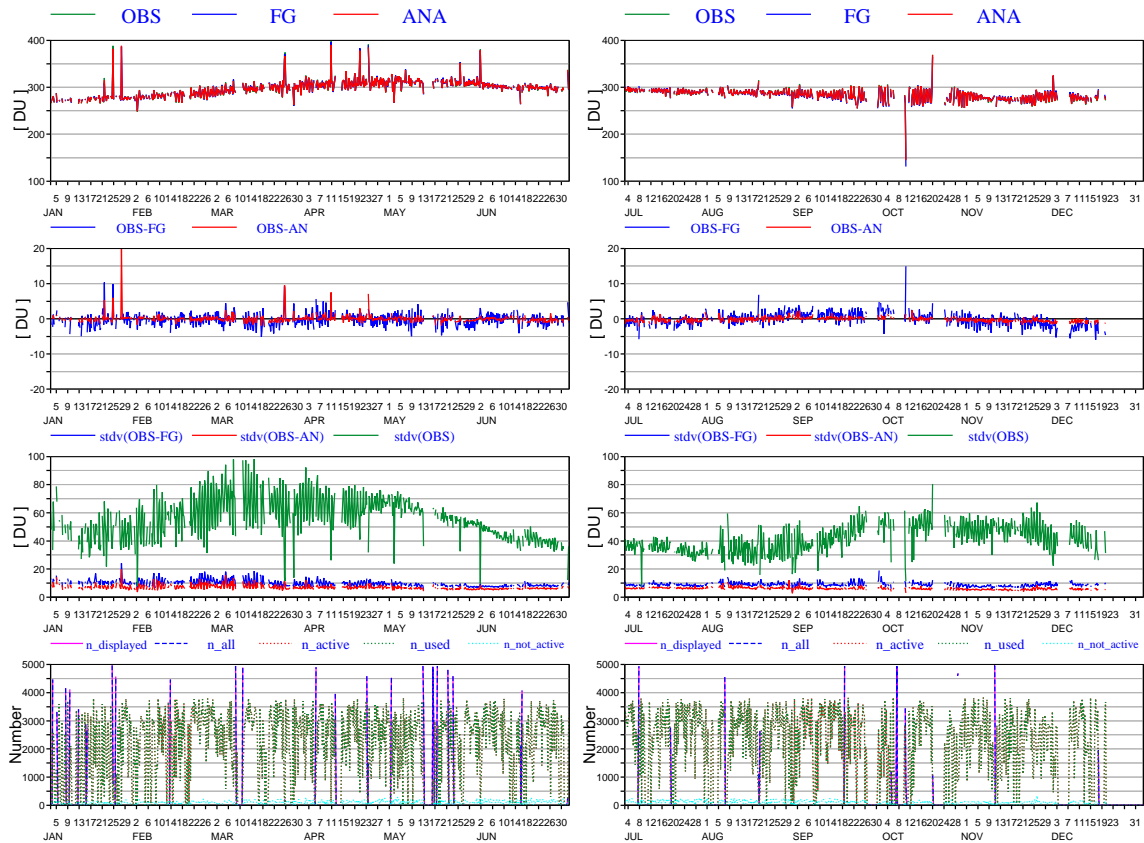


Figure 5: Timeseries of globally averaged data covering the periods 1 January to 30 June (left panel), and 1 July to 31 December 2007 (right panel). The top panels of each figure show TOSOMI SCIAMACHY NRT total ozone observations, first-guess and analysis values, the middle panels first-guess and analysis departures and the bottom panels the standard deviations of SCIAMACHY and of first-guess and analysis departures. All ozone values are in DU.

The generally good behaviour of the TOSOMI data can also be seen in the timeseries of the zonal mean first guess departures shown in figure 6. On average the first-guess departures (top panel in figure 6) are only a few Dobson Unit at most latitudes. However, a lower level of agreement between the model and the observations near the end of the orbits is observed especially in the winter hemisphere.

This reflects in the observation standard deviations (bottom panel in figure 6) which exhibit higher values than average near the end of the orbits in the winter hemisphere. Here, the observation standard deviation can reach values of 50 to 70 DU. In the tropics the observation standard deviation exhibits smaller values, typically around 10DU⁷.

Comparisons with independent data also show the high quality of these observations. Figure 7, in particular, shows the comparison between the time series of the zonal mean SCIAMACHY total column ozone (top panel)

⁷This is consistent with what was found in the 2005 and 2006 studies (da Costa Bechtold and Dethof, 2005; Dragani, 2006).

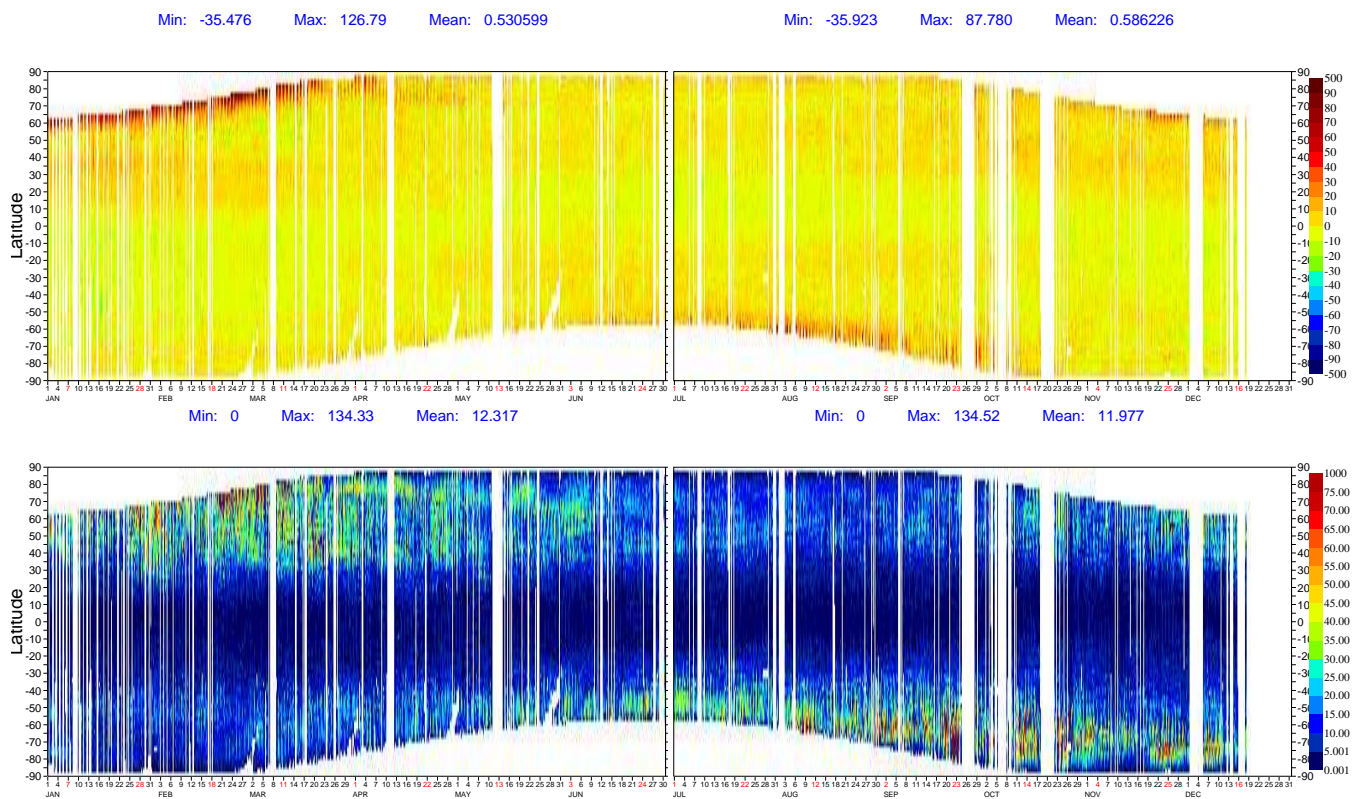


Figure 6: Time series of the zonal mean NRT SCIAMACHY first-guess departures (top panel) and of the zonal mean NRT SCIAMACHY standard deviation (bottom panel) during 2007. All ozone values are in DU.

and of the zonal mean OMI total column ozone⁸ (bottom panel) for the whole 2007. The OMI data used in the comparisons are the TOMS-like⁹ gridded total column ozone data available on-line from NASA. On average, figure 7 shows a good level of agreement between SCIAMACHY and OMI total column ozone. Some differences can be found in the tropics, where SCIAMACHY usually exhibits lower values than OMI throughout the year, and at high latitudes where the OMI ozone values are lower than those for SCIAMACHY. It should be noted that sensors like OMI and SCIAMACHY¹⁰ are prone to provide less precise measurements near the end of the orbits, as noted in the bottom panel of figure 6, and therefore the large differences at these latitudes should be of a less concern.

Also the monthly mean geographical distributions of the TOSOMI TCO show a good level of agreement with OMI TCO. An example is shown in figure 8 for April 2007. Top and middle panels show the geographical distribution of TOSOMI and OMI, respectively. Bottom panel shows their difference. Figure 8 confirms that the large differences between OMI and TOSOMI can be found near the end of the orbits. In the tropical region, TOSOMI total column ozone values are up to 20DU lower than those of OMI.

⁸Data obtained from the NASA ftp server at <ftp://toms.gsfc.nasa.gov/pub/omi/data/ozone/Y2007/>.

⁹As opposite to the OMI DOAS TCO which is retrieved with a retrieval scheme similar to that used for TOSOMI data.

¹⁰The SCIAMACHY data used are those produced from the nadir measurements only.

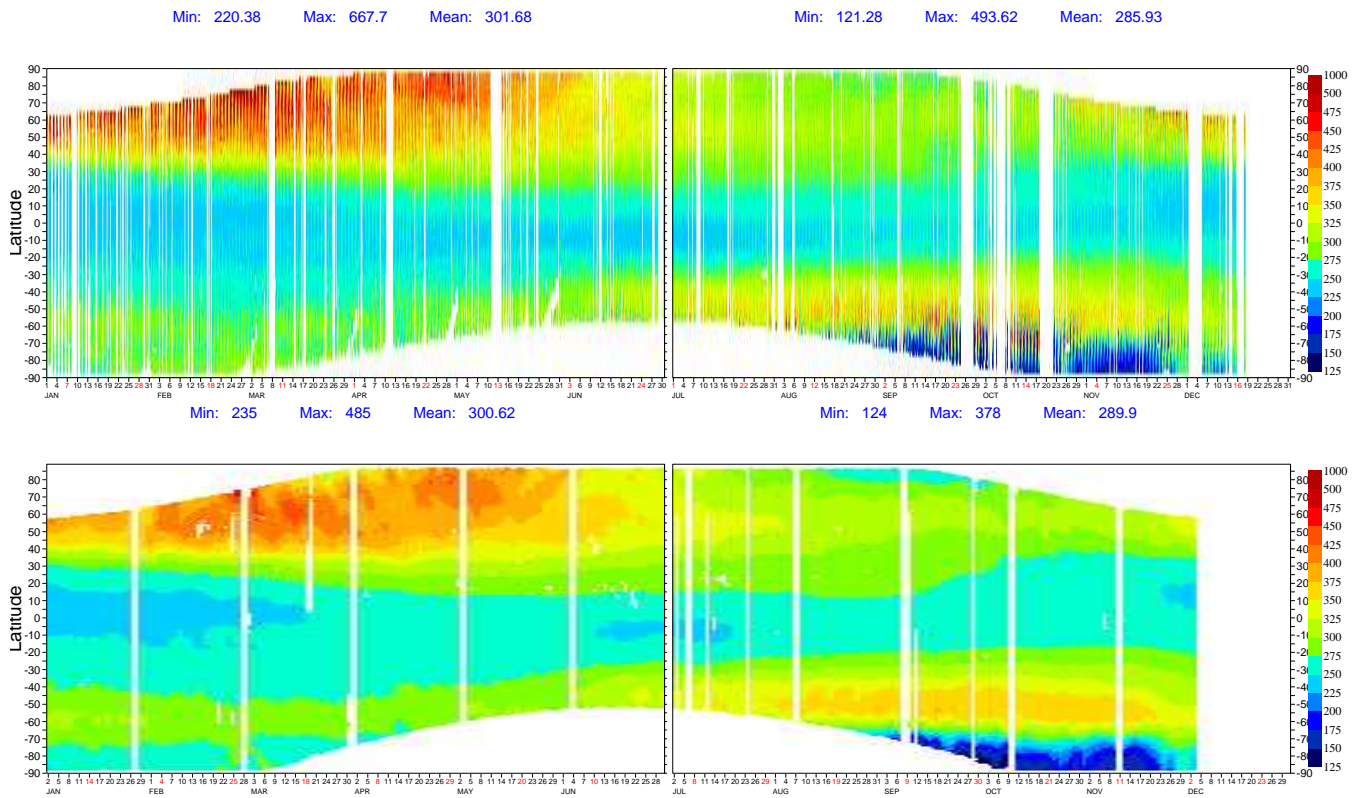


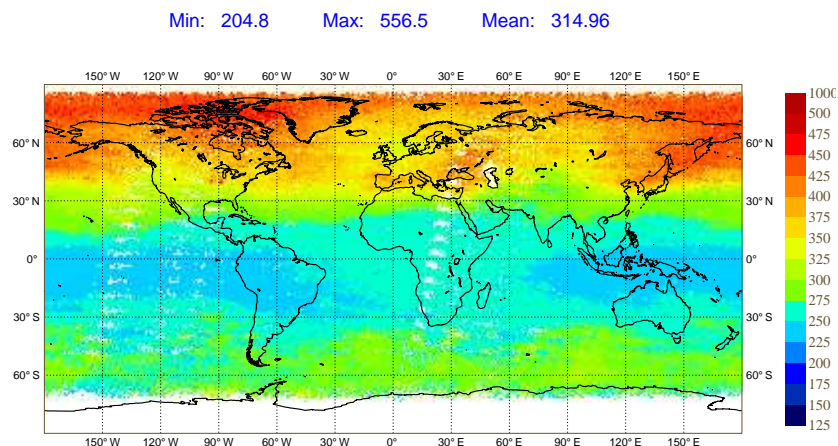
Figure 7: Time series of the zonal mean NRT SCIAMACHY ozone (top panel) and OMI total column ozone (bottom panel) for 2007. All ozone values are in DU.

3.2 Summary of the NRT SCIAMACHY monitoring and assimilation

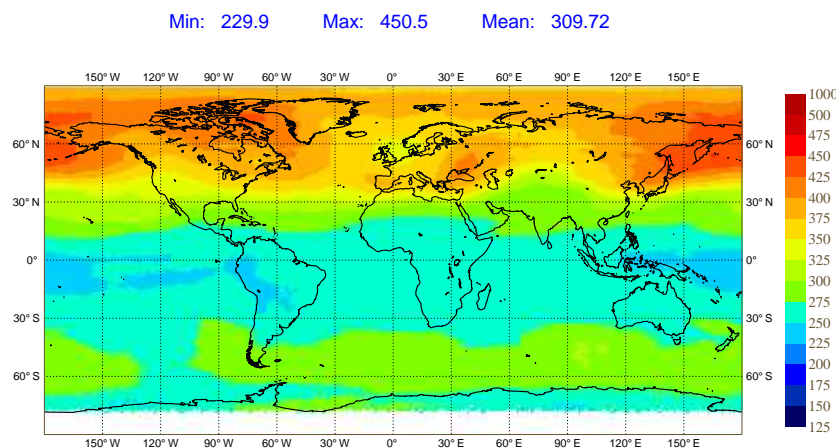
During the time frame covered by the ESA contract 17585-CCN-1 (January 2006 - December 2007), the NRT SCIAMACHY ozone columns produced by ESA (SCI_RV_2P) were only available from 1 January to 8 May 2006. During these months, the quality of the ESA NRT SCIAMACHY data was found improved compared with that reported on previous years. However, the retrieval procedure was found less reliable than for example the KNMI’s retrieval scheme when anomalies occurred on the satellite (e.g. during April 2006). Full account of the results from the monitoring statistics for the ESA NRT SCIAMACHY TCO was given by Dragani (2006).

The availability of the NRT TOSOMI TCO was generally continuous during the whole 2007. The quality of these data was found stable and consistent with that reported e.g. by da Costa Bechtold and Dethof (2005); Dragani (2006). The monitoring statistics show a good level of agreement between the SCIAMACHY TCO and the ECMWF TCO both in the global mean and area average. In particular, the global mean first-guess and analysis departures for NRT SCIAMACHY TCO were found to be well within ± 5 DU.

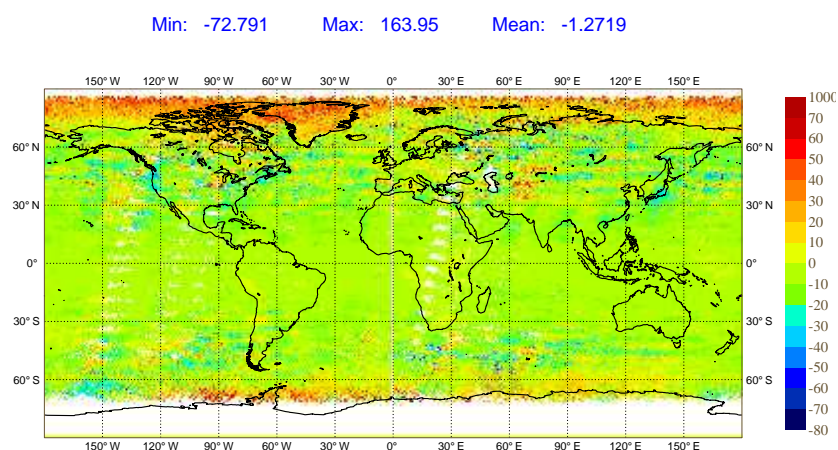
The generally good quality of the SCIAMACHY TCO was also confirmed by comparisons with independent total column ozone observations retrieved from the OMI measurements. Results from these comparisons showed that the regions characterized by the largest differences in TCO between OMI and SCIAMACHY were near the end of the orbits and the tropics.



(a)



(b)



(c)

Figure 8: Geographical distribution of monthly mean SCIAMACHY TCO (top), monthly mean OMI TCO (middle), and their difference (bottom) for April 2007. Values are in DU.

4 Monitoring of GOMOS data

GOMOS makes use of the occultation measurement principle by tracking stars as they set behind the atmosphere. GOMOS has an ultra violet-visible and a near-infrared spectrometer, covering the wavelength region between 250 and 950 nm. It allows the retrieval of atmospheric trace gas profiles in the altitude range 100–15 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 , $OCIO$, H_2O and temperature (fixed to the ECMWF temperature forecasts in v5.00).

A subset of these retrieved products that is available in NRT (GOM_RR_2P) is routinely and passively monitored at ECMWF. This subset includes temperature, water vapour and ozone profiles.

The data availability was generally continuous during the whole 2007. From the beginning of the year until 17 January, the ozone and temperature retrievals were unusable for monitoring. This was the consequence of changes in the settings of the **local air density** and of the **local temperature**¹¹ introduced in the Level 2 processor on August 2006. Following these changes, the ozone and temperature retrievals were forced to be set to “MISSING” in the BUFR files, and therefore unusable. To overcome this problem, ESA suggested to extract the information on density and temperature from the “Tangent Point Density from External Model”, and “Tangent Point Temperature from External Model” in the Geolocation Annotation Dataset (GAD), respectively. An updated version of the PDS2BUFR converter, which accounted for these changes, was provided by ECMWF in October 2006, and implemented in operations on 17 January 2007, when the dissemination of the data with corrected values restarted. The BUFR files distributed since 17 January 2007 for the first time also included NRT GOMOS water vapour profiles.

An important change was introduced in operations on 21 May 2007 by ESA. Following instructions provided by the GOMOS QWG team, a new PDS2BUFR converter was implemented to filter out the GOMOS data sampled in bright, twilight or straylight limb conditions, and retain only those retrieved from full dark limb measurements. Meijer et al. (2004) showed that the quality of GOMOS observations strongly depends on the illumination of the limb through which the star is observed, and according to the GOMOS quality disclaimer¹², only the data sampled in dark limb conditions have good quality for scientific applications. With the implementation of this new converter, the global number of observations reduced to about half of their initial number. Figure 9 shows the time series of the global number of GOMOS temperature observations during 2007 as an example. In particular, it was noticed that all data at mid and high latitudes in the NH were filtered out from the BUFR files as they did not fulfil the condition of being sampled in dark limb conditions, which confirms the dependence of the illumination condition on the position. Figure 10 shows the time series of the zonal mean GOMOS temperature during 2007 as an illustration. Therefore, the monitoring statistics for the period after this change could only be performed for the tropics and SH. As the satellite orbits started to shift northward at the end of 2007, a few observations retrieved from measurements sampled in full dark limb conditions became available at midlatitudes in the NH.

4.1 Monitoring of GOMOS temperature data

The quality of the temperature profiles in the BUFR files was stable during 2007, and consistent with the temperature data retrieved in 2006. The results from the monitoring statistics for 2006 were discussed by Dragani (2006).

¹¹In the Level 2 processor (IFP 5.0), which was switched on 8 August 2006, both the local air density and the local temperature were set equal to zero.

¹²See <http://envisat.esa.int/dataproducts/availability/disclaimers/> for more information.

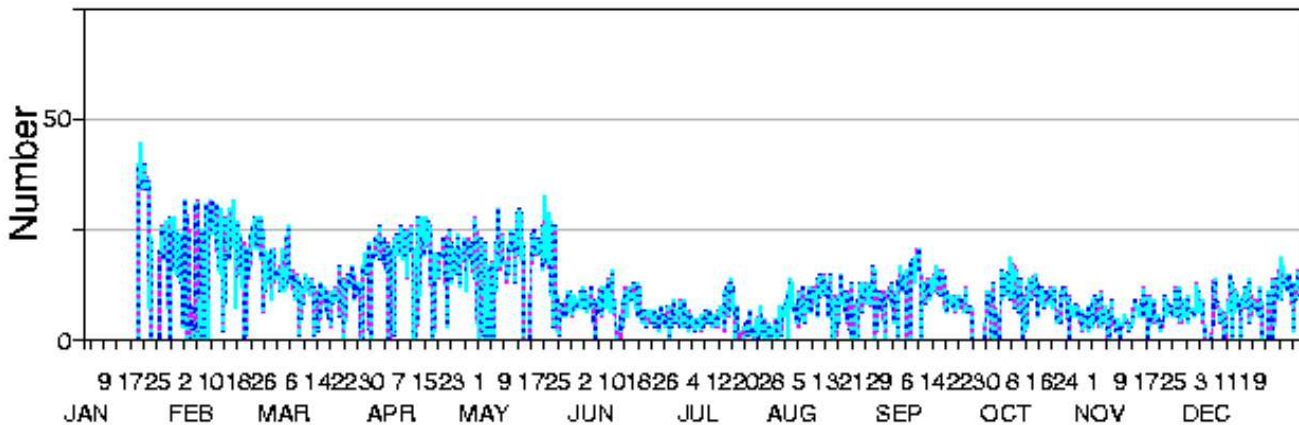


Figure 9: Time series of the global number of GOMOS temperature observations during 2007.

Min: 203.2 Max: 289.1 Mean: 248.58

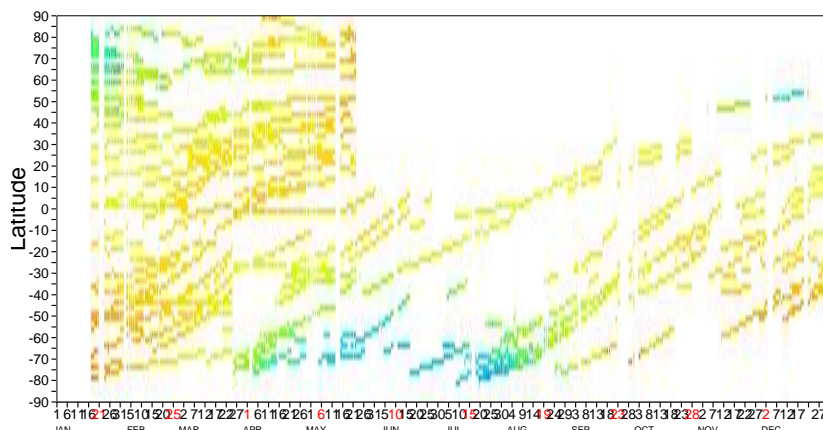


Figure 10: Time series of the zonal mean GOMOS temperature observations during 2007.

Figures 11 and 12 show the comparisons between area averaged GOMOS and ECMWF temperature profiles (left panel) and GOMOS temperature departures (right panel) for the periods 1 April to 30 June (AMJ) and 1 September to 30 November 2007 (SON), respectively. In figure 11, the top panels refer to the high latitudes in the NH ($[90^{\circ}\text{-}60^{\circ}\text{N}]$), the middle panels refer to the tropical band ($[30^{\circ}\text{N}\text{-}30^{\circ}\text{S}]$), and the bottom panels refer to the high latitudes in the SH ($[60^{\circ}\text{-}90^{\circ}\text{S}]$). As anticipated above, because after applying the converter on 21 May 2007, all data at mid and high latitudes in the NH were filtered out from the BUFR files, the top panels in figure 12 refer to the tropical band, the middle panels refer to the midlatitudes in the SH ($[30^{\circ}\text{-}60^{\circ}\text{S}]$), and the bottom panels refer to the high latitudes in the SH.

Both figures 11 and 12 show that, in general, the temperature profiles in the BUFR files are lower than their model equivalent. In particular, the first guess and analysis departures were typically up to about -1% (-2 K) in all the stratosphere in the tropics, and within $\pm 1\%$ at the other latitudinal bands in the stratosphere. Larger first guess and analysis departures were found in the mesosphere, with differences up to about -3% (-6 K) between 0.2 and 0.4hPa.

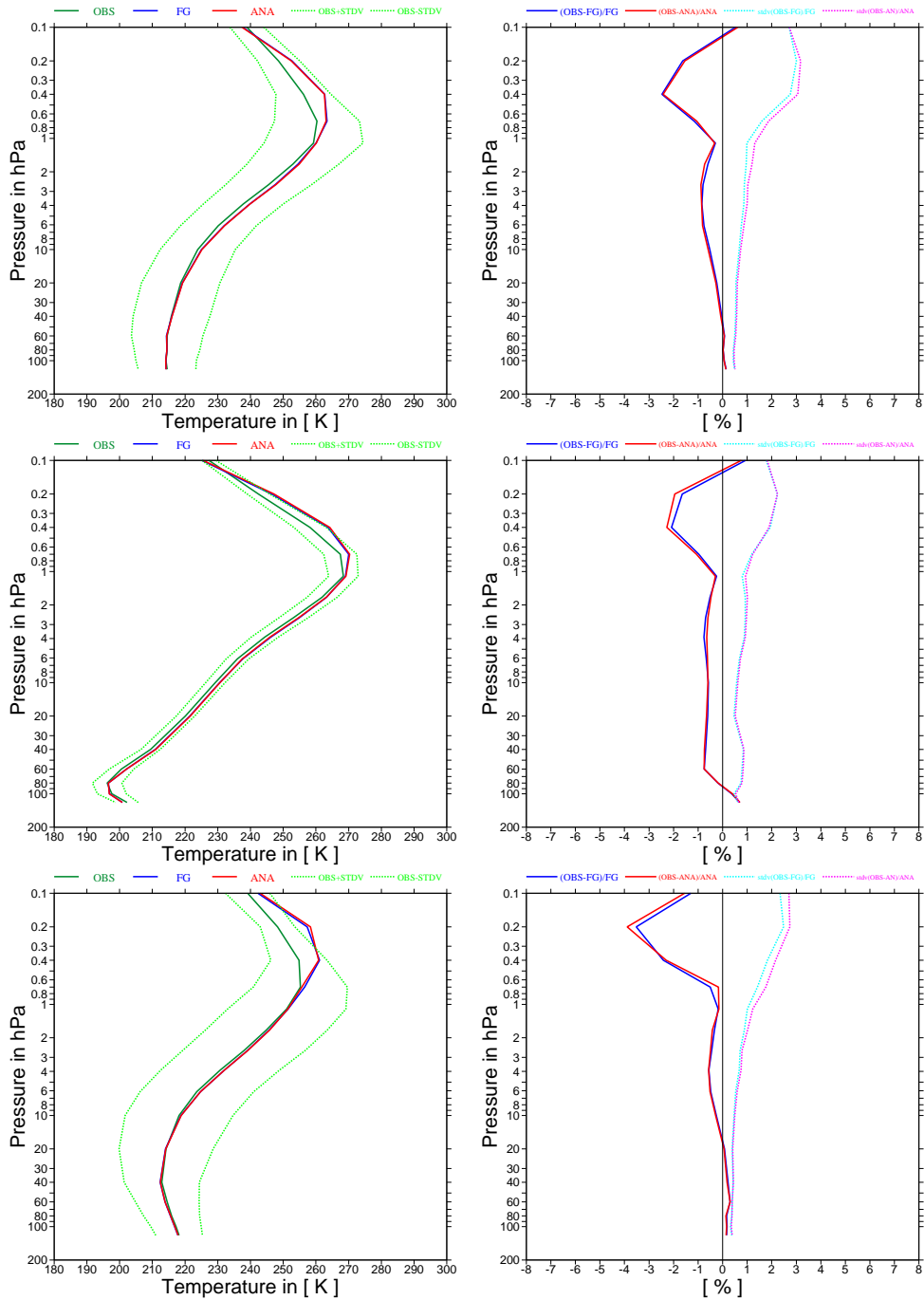


Figure 11: Comparisons between the area averaged temperature extracted from the GOMOS files and the area averaged ECMWF temperature first-guess and analysis. Right panels refer to the profile comparisons, left panels show the relative first-guess and analysis departures. The averaging period is between April and June 2007. Panels [a] (top) refer to the latitudinal band 90°-60°N, panels [b] refer to the tropical band ([30°N-30°S]), and panels [c] refers to the latitudinal band between 60° and 90°S. Temperature values are in K, departures are in %.

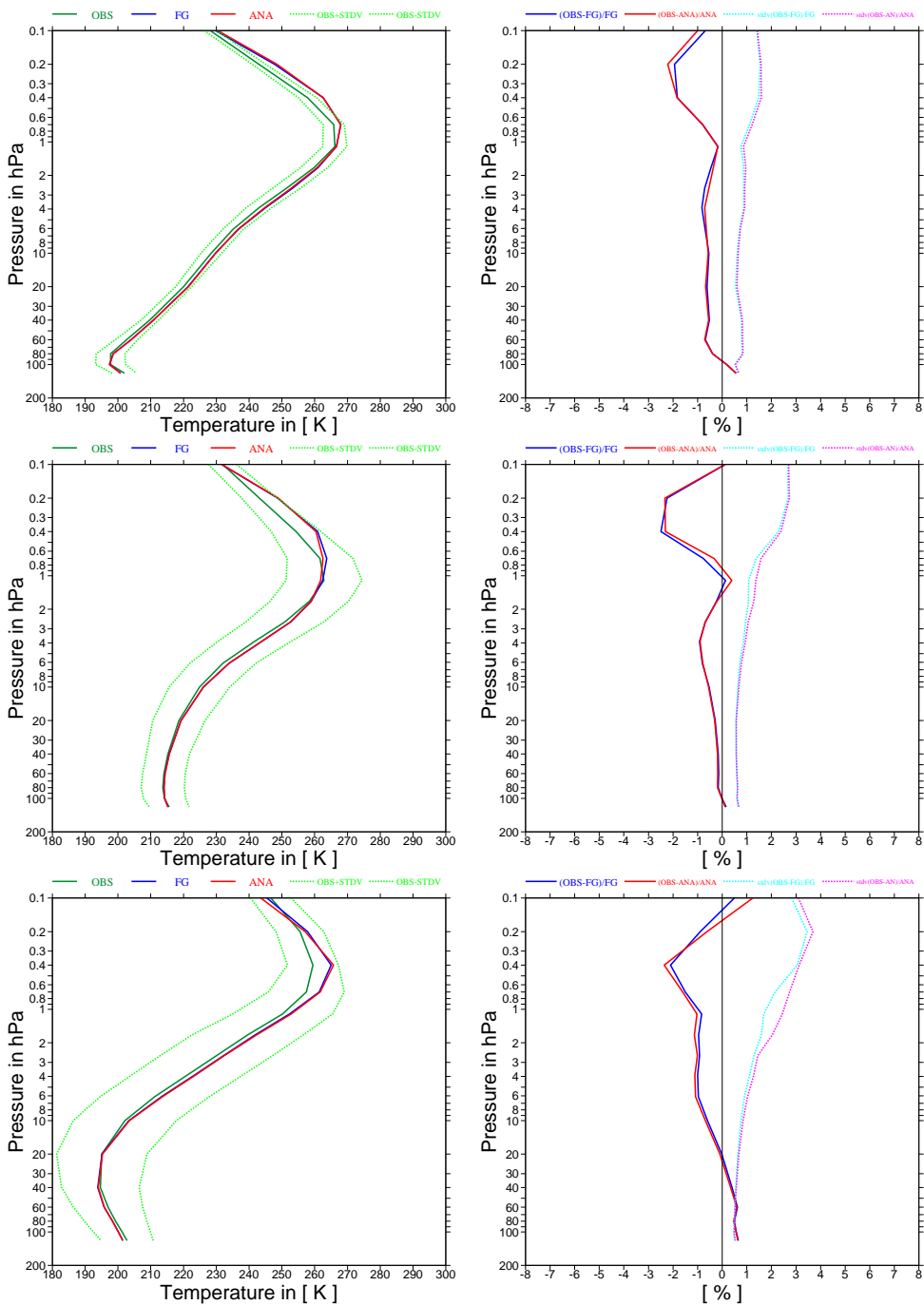


Figure 12: Like in figure 11, but the averaging period is between 1 September and 30 November 2007. Top panels refer to the tropical band ($[30^{\circ}N-30^{\circ}S]$), panels [b] refer to the midlatitudes in the SH ($[30^{\circ}-60^{\circ}S]$), and panels [c] refers to the high latitudes in the SH ($[60^{\circ}-90^{\circ}S]$).

Despite the stability of the temperature profile quality and their consistency with the 2006 results, the monitoring statistics seemed to highlight some inconsistency regarding the actual nature of the data presented as GOMOS temperature profiles in the BUFR files. As mentioned in section 4, to overcome the problem of having the temperature and ozone data set to “MISSING VALUE” in the BUFR files that followed the implementation of IFP 5.0 on August 2006, it was advised to extract the temperature information as the “Tangent Point Temperature from External Model” stored in the GAD. This means that the *temperature profile is obtained by the combination of the ECMWF data in the lower part of the profile¹³ and of the MSIS90 data in the upper part of the profile (smooth transition altitude range around the pressure level 1hPa)* (ESA, 2007). ESA (2007) also clarified that the ECMWF data to be used are the 24-hour temperature forecasts.

The mean departure between the temperature profiles in the GOMOS files and the ECMWF temperature analyses (differences up to 2K in the Stratosphere) seem to exceed the expected mean departures between the ECMWF 24-hour temperature forecasts and the ECMWF temperature analyses themselves.

As an example, figure 13 shows the global mean analysis departures (left panels) and relative analysis departures (right panels) computed for the temperature in the GOMOS files¹⁴ (the dashed line), and the corresponding global mean profiles obtained by using the ECMWF 24-hour temperature forecasts interpolated at the GOMOS locations instead of the GOMOS temperature (the solid line). In the top panel plots, the profiles are averaged over the period August 2007; in the bottom panel plots, the profiles are averaged over the period September 2007. From the plots in figure 13, it follows that the expected global mean difference between the 24-hour temperature forecasts and temperature analyses are within $\pm 0.3^\circ$, about one order of magnitude smaller than what given by the monitoring statistics.

Unless a more complicated processing is used to derive the temperature field in the GOMOS files¹⁵, namely the local temperature from the external model, the comparison between the global mean monthly mean profiles presented in figure 13 seems to indicate some problems (e.g. interpolation problems), and that the temperature profiles retrieved from the GOMOS BUFR files (up to 1hPa) differ from the ECMWF 24-hour temperature forecasts at the GOMOS locations. This should be taken into account especially if such a temperature is used in the GOMOS retrieval process to infer information about other fields.

4.2 Monitoring of GOMOS ozone data

This section discusses the results from the monitoring of the NRT GOMOS Level 2 ozone profiles in 2007.

Figure 14 presents the comparisons between the global mean GOMOS ozone profiles and the global mean ECMWF ozone first-guess and analysis, averaged over the whole 2007. In the global average, the agreement between the GOMOS ozone observations and their model equivalent is better than the GOMOS one standard deviation limit at all vertical levels. The first-guess and analysis departures are within -5 and +10% in most of the stratosphere (for pressure values smaller than 40hPa), but larger departures were found on average, in the lower stratosphere (for pressure values larger than 40hPa), and in the mesosphere. The standard deviations of the departures were found to be larger than 50% at most vertical layers.

¹³The ECMWF forecasts and analyses were only available up to 1 hPa.

¹⁴This is directly provided by the satellite monitoring package.

¹⁵In this case, mention should probably be made in the ESA (2007), as the current definition could be misleading.

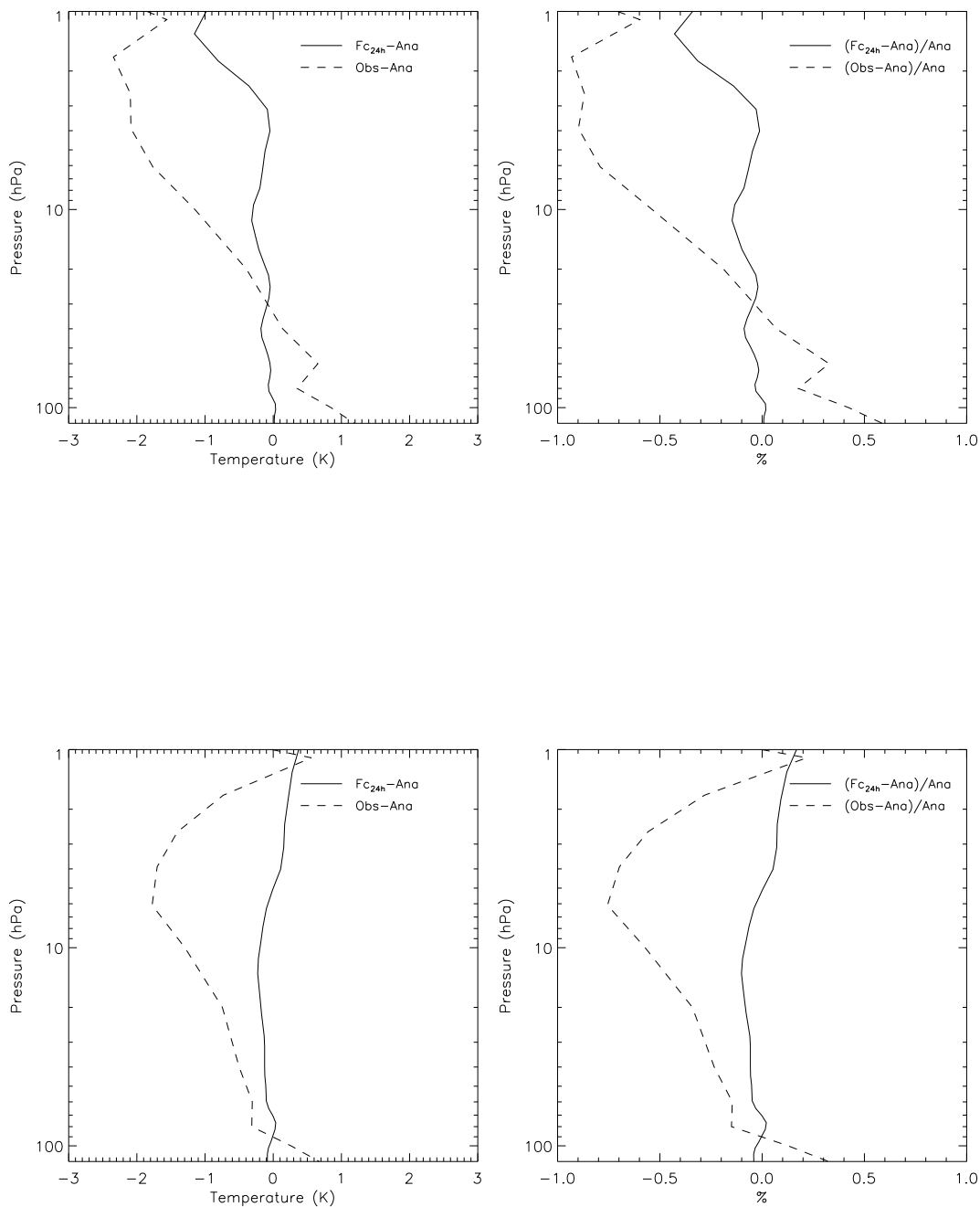


Figure 13: Monthly mean the analysis departures (left panels) and relative analysis departures (right panels) from the 24-hour temperature forecasts (solid) and temperature in the GOMOS files (dashed). Top panels refer to August 2007; bottom panels refer to September 2007.

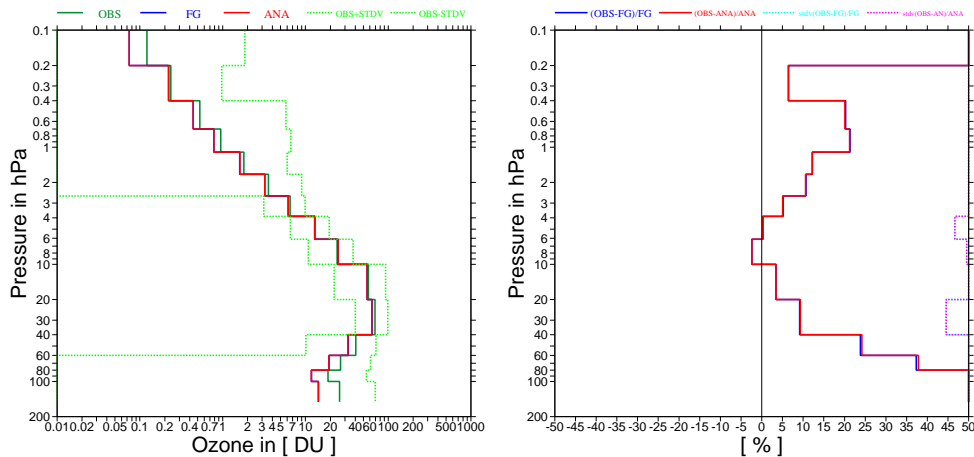


Figure 14: Comparisons between the annual mean global mean GOMOS ozone profiles and the area averaged ECMWF ozone first-guess and analysis. Right panels refer to the profile comparisons, left panels show the relative first-guess and analysis departures. Ozone values are in DU, departures are in %.

Figure 15 shows the 2007 global mean time series of the observations and their model equivalent (top panel), of the first-guess and analysis departures (middle panel), and of their standard deviations (bottom panel) for the vertical layer between 20 and 40 hPa, which corresponds roughly to the layer where ozone peaks. From the time series in figure 15, GOMOS observations exhibit higher ozone values than the ECMWF ozone analyses, with differences in that layer of about 6 DU during the first five months of 2007, and about 4 DU afterwards. Large standard deviations up to 20 DU were found in the data, corresponding to just below 25% of the annual mean ozone value in this layer.

When averaging over latitudinal bands, the level of agreement just discussed is usually confirmed. Figures 16 and 17 show the area averaged GOMOS ozone profiles (left hand side panels) and GOMOS departures (right hand side panels) for the period under consideration computed for three latitudinal bands and averaged over the period April to June (AMJ), and September to November 2007 (SON), respectively. In figure 16, the top panels refer to the high latitudes in the NH ($[90^{\circ}-60^{\circ}]N$), the middle panels refer to the tropical band ($[30^{\circ}N-30^{\circ}S]$), and the bottom panels refer to the high latitudes in the SH ($[60^{\circ}-90^{\circ}]S$). In figure 17, the top panels refer to the tropical band, the middle panels refer to the midlatitudes in the SH ($[30^{\circ}-60^{\circ}]S$), and the bottom panels refer to the high latitudes in the SH.

In both periods, the agreement between the GOMOS ozone observations and their model equivalent is better than the GOMOS one standard deviation at all vertical levels and latitudinal bands. The largest differences are found in the lower stratosphere, typically for pressure values larger than 40 hPa, and in the upper mesosphere where the first-guess and analysis departures can be larger than 20%. Also the first-guess and analysis departure standard deviations are very large with values larger than 50% in places indicative of a lot of noise in the ozone retrievals, especially during the period AMJ. During the period SON, improvements were seen in the tropics (top panels of figure 17) at mesospheric levels compared with the same latitudinal band during AMJ (middle panels of figure 16). Particularly noticeable is the standard deviations of the departures which is also reduced at all vertical levels in the tropical band. Also a good level of agreement between GOMOS ozone profiles and their model equivalent was found at high latitudes in the NH during spring months, consistent with that obtained for the autumn period. In the SH, while the level of agreement between observations and model is reasonably good in autumn, larger first-guess and analysis departures (within -20 and +40% in the stratosphere) were observed in spring.

The presence of large noise in the data is also illustrated by the scatter plots of GOMOS ozone data and its

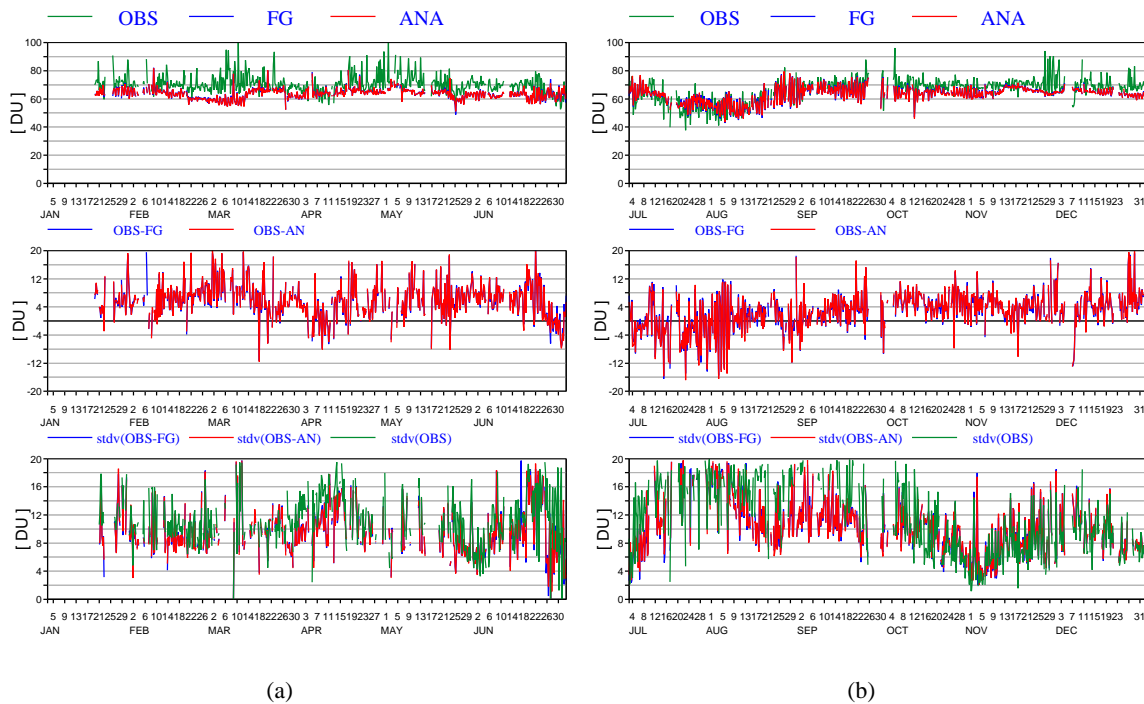


Figure 15: Timeseries of globally averaged data covering the periods (a) 1 January to 30 June, and (b) 1 July to 31 December 2007 at 20-40 hPa. The top panels of each figure show GOMOS NRT partial column ozone, first-guess and analysis values, the middle panels first-guess and analysis departures and the bottom panels the standard deviations of GOMOS ozone data and of first-guess and analysis departures. All ozone values are in DU.

first-guess departures for the layer 20-40 hPa (figure 18). Figure 18(a) refers to the period from 1 to 30 April 2007, while figure 18(b) refers to the period from 1 to 31 October 2007. The panels on the left show the scatter plots of the observations versus latitude, those on the right show the scatter plots of the first-guess departures versus latitude. The relatively large scatter in the observations against the latitudes leads to a large scatter in the first-guess departures as well, with variability within -20 and 40 DU in April, and between -20 and 20 DU in October. The smaller scatter presented in October compared with that in April is due to the fact that only high quality observations (i.e. those retrieved from measurements sampled in full dark limb illumination conditions) were used.

It should be acknowledged that the GOMOS ozone product has continuously improved during the years. As an account, figure 19 shows the scatter plots of NRT GOMOS ozone first-guess departures in the ozone layer (20-40hPa) for July 2004 (top left panel), July 2005 (top right panel), July 2006 (bottom left panel), and finally July 2007 (bottom right panel). Data in July 2005 were only available for the period between 17 and 31, as the GOMOS operations were suspended due to an anomaly in the telescope elevation drive from 25 January 2005 until 17 July 2005 (da Costa Bechtold and Dethof, 2005). Also in July 2007, the data sampled in the NH were discarded as they did not fulfil the full dark illumination conditions. Regardless of the partial lack of data, the quality of the ozone retrievals has been improved over the last four years, and the scatter in the first-guess departures has been reduced.

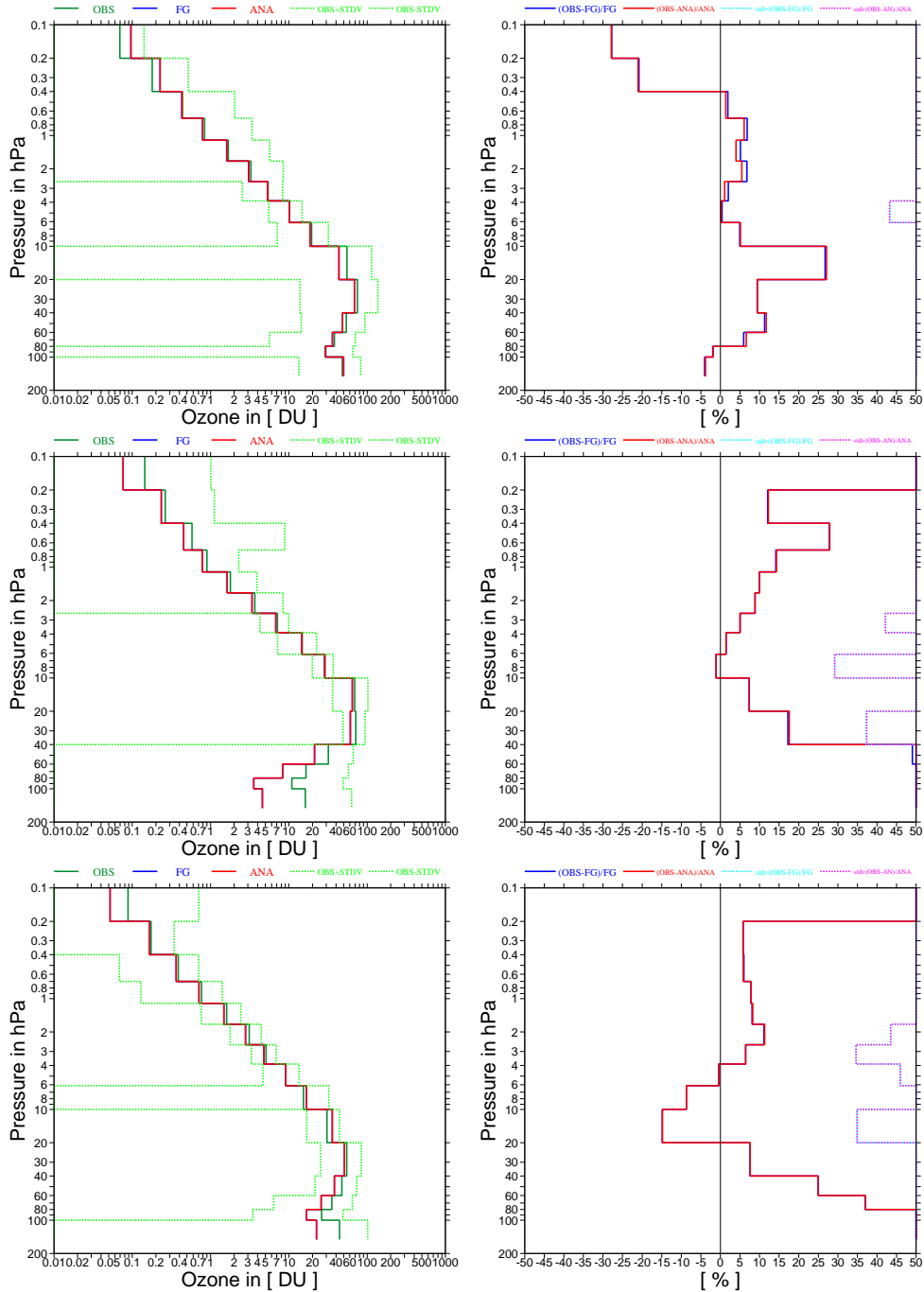


Figure 16: Comparisons between the area averaged GOMOS ozone profiles and the area averaged ECMWF ozone first-guess and analysis. Right panels refer to the profile comparisons, left panels show the relative first-guess and analysis departures. The averaging period is between April and June 2007. Top panels refer to the latitudinal band 90°-60°N, middle panels refer to the tropical band (30°N-30°S), and bottom panels refer to the latitudinal band between 60° and 90° S. Ozone values are in DU, departures are in %.

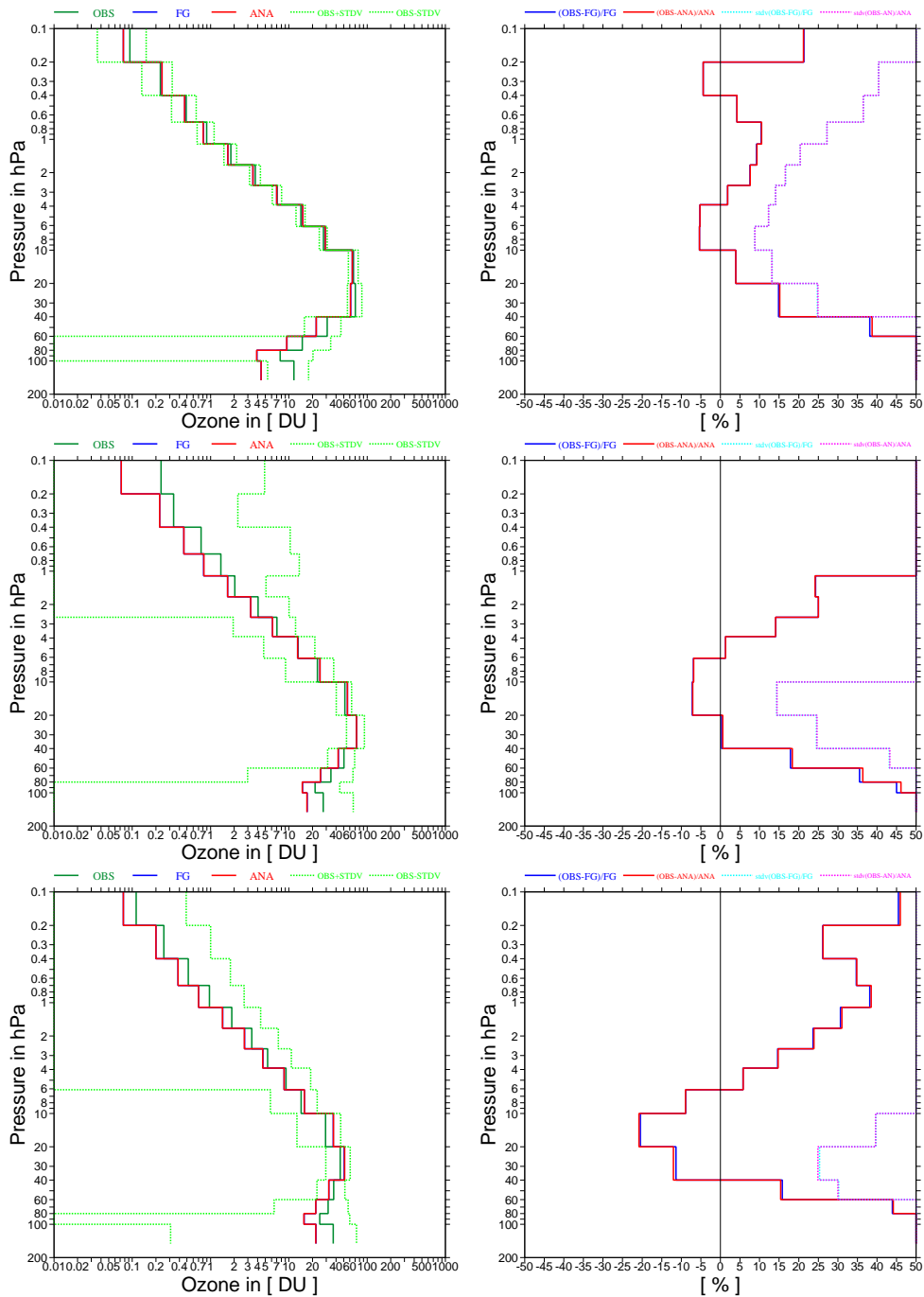
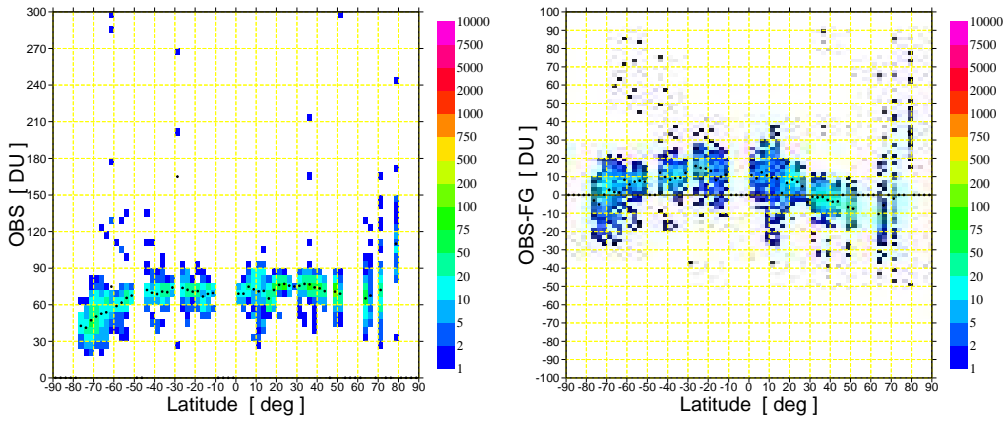
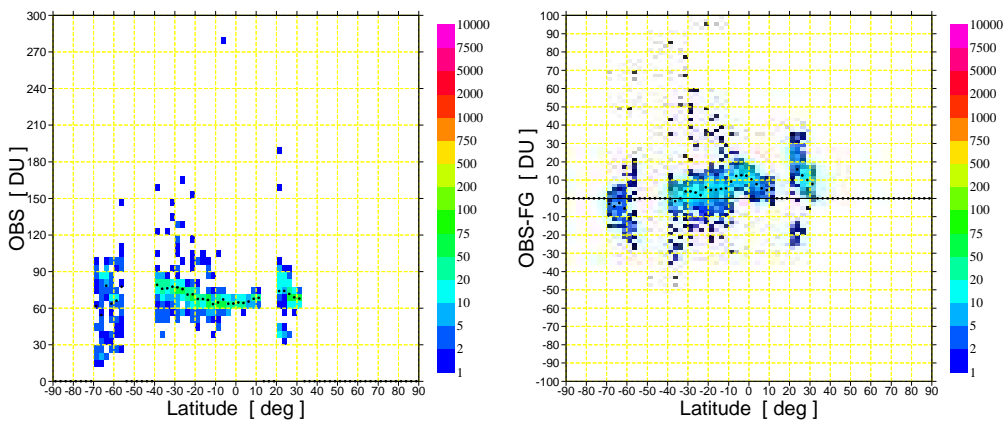


Figure 17: Like in figure 16, but the averaging period is between 1 September and 30 November 2007. Top panels refer to the tropical band ($[30^{\circ}\text{N}-30^{\circ}\text{S}]$), middle panels refer to the midlatitudes in the SH ($[30^{\circ}-60^{\circ}\text{S}]$), and bottom panels refer to the high latitudes in the SH ($[60^{\circ}-90^{\circ}\text{S}]$).



(a)



(b)

Figure 18: Scatter plots of NRT GOMOS ozone (left) and of NRT GOMOS ozone first-guess departures (right) in the layer 20-40 hPa plotted against latitude, for the periods April 2007 (panels [a]) and October 2007 (panels [b]). The colours give the number of observations per bin, and the black dots the mean per bin. All ozone values are in DU.

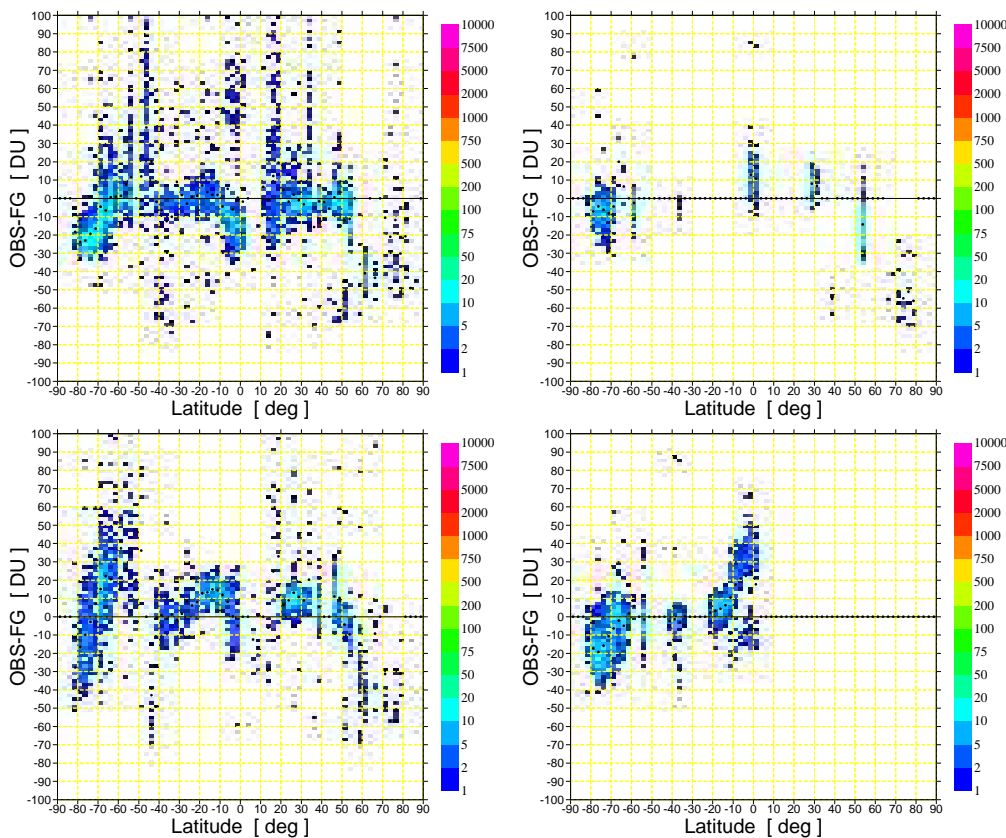


Figure 19: Scatter plots of NRT GOMOS ozone first-guess departures in the layer 20-40 hPa plotted against latitude, for the periods July 2004 (top left), July 2005 (top right), July 2006 (bottom left), and July 2007 (bottom right). The colours give the number of observations per bin, and the black dots the mean per bin. Values are in DU.

4.3 Monitoring of GOMOS water vapour data

On 17 January 2007, for the first time since the beginning of the dissemination of the NRT GOMOS data, information on water vapour was made available in the GOM_RR_2P BUFR files and continuously provided for the whole of 2007. However, the quality of the water vapour data is poor.

Figures 20 and 21 show two examples of comparisons between the monthly mean area averaged GOMOS water vapour profiles (the green lines) with their model equivalent at three latitudinal bands during September and December 2007, respectively (see figure captions for details). These profile plots show that the GOMOS water vapour values were from one to four orders of magnitude larger than those given by the model at all stratospheric levels. The largest differences were found in the upper stratosphere, where not only did the GOMOS observations exhibit on average values of four order of magnitudes larger than their model equivalent, they also were larger than the mean GOMOS tropospheric observation. A slightly higher level of agreement was found at midlatitudes in the NH in December (panel [c] in figure 21). Here the GOMOS WV observations still exhibited higher values than their model equivalent, but the departures were considerably smaller than those seen in the other latitudinal bands. In addition, the WV content decreases with height as expected.

The poor level of agreement between the GOMOS water vapour profiles and their model equivalent is also shown in the scatter plots presented in figure 22 for the integrated layer between 1 and 100 hPa. The two panels show the scatter plot for April and October 2007, respectively.

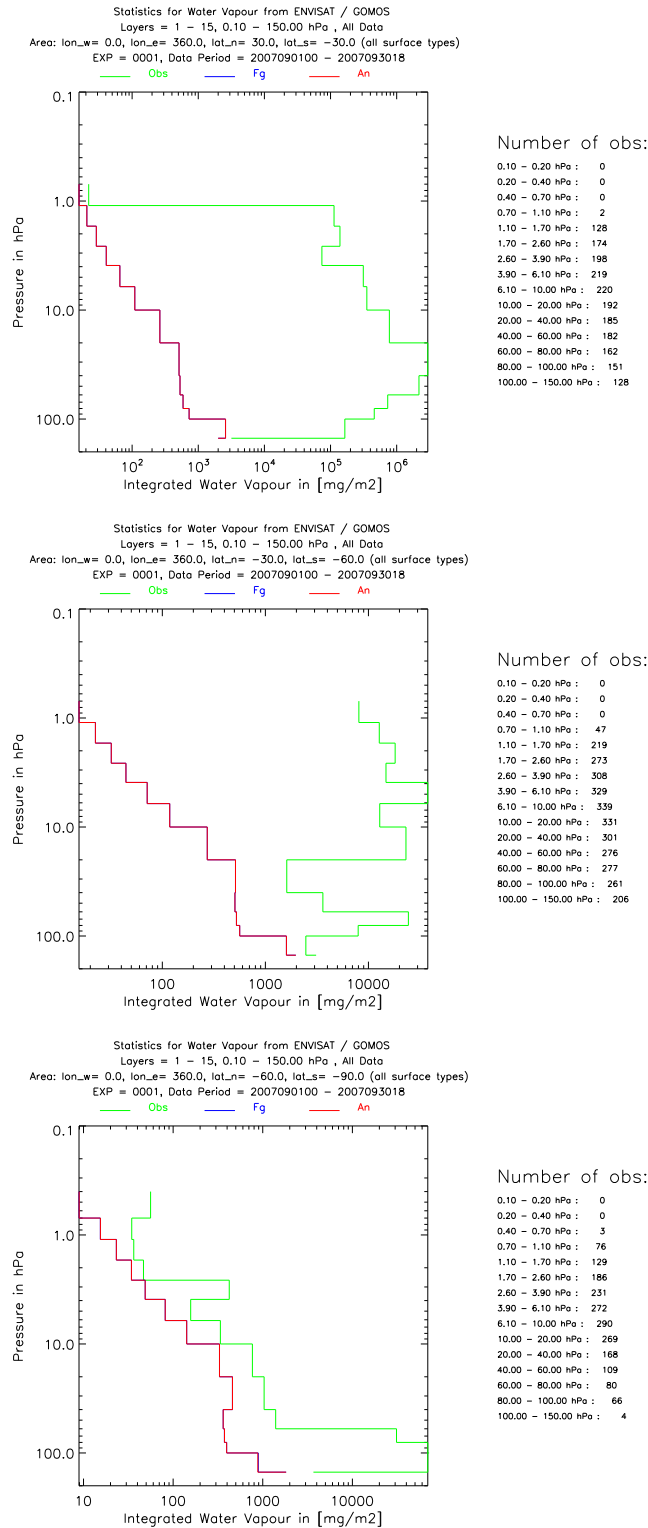


Figure 20: Comparisons between the area averaged GOMOS water vapour profiles and the area averaged ECMWF water vapour first-guess and analysis for September 2007. Top panel refers to the latitudinal band 30°N-30°S, the mid panel refers to the band ([30°-60°S]), and panels [c] refers to the latitudinal band between 60° and 90°S. Water vapour values are in mg/m².

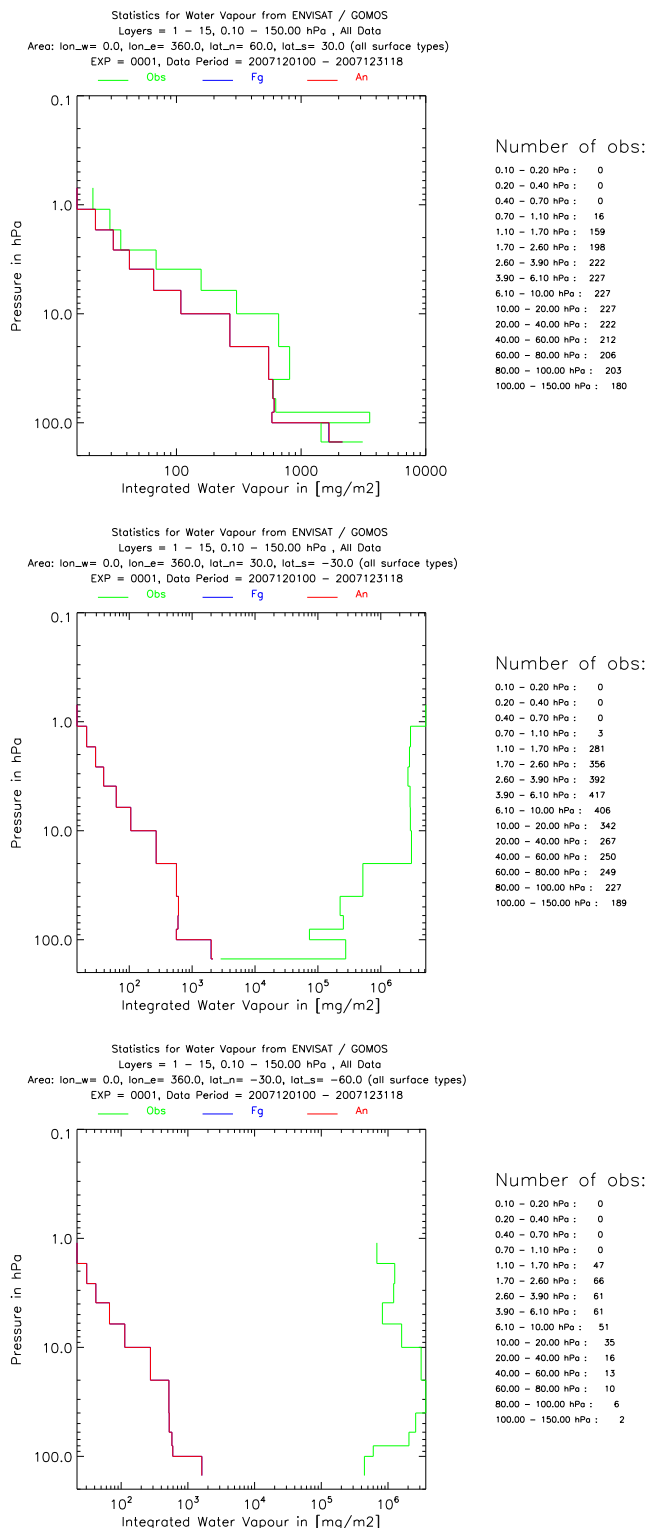


Figure 21: Like in figure 20, but the averaging period is December 2007. The top panel refers to the midlatitudes in the NH ($[30^{\circ}$ - 60° N), the mid panel refers to the tropical band ($[30^{\circ}$ N - 30° S]), and the bottom panel refers to the midlatitudes in the SH ($[30^{\circ}$ - 60° S).

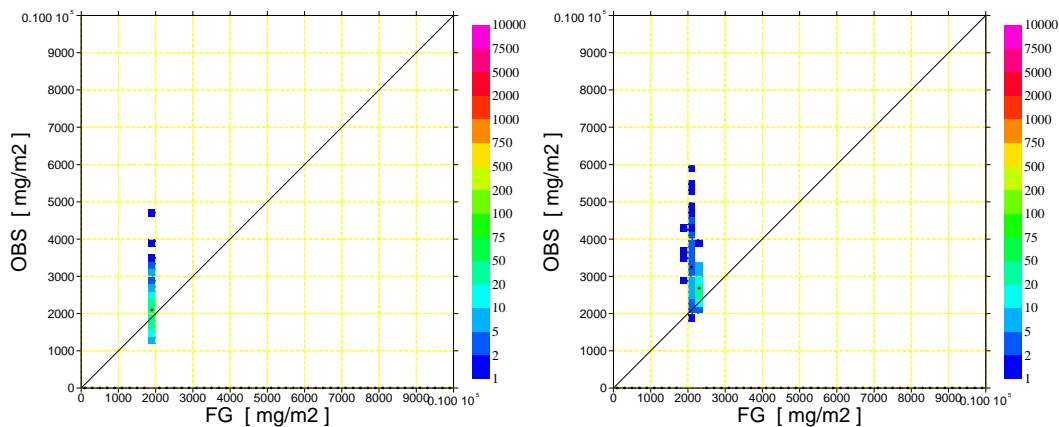


Figure 22: Scatter plots of NRT GOMOS water vapour content against the ECMWF first-guess in the integrated layer 1-100 hPa for the periods April (left), and October 2007 (right). The colours give the number of observations per bin, and the black dots the mean per bin. Values are in mg/m^2 .

5 Monitoring of MIPAS data

Owing to instrument problems, NRT Level 2 MIPAS data (MIP_NLE_2P) have not been available since 27 March 2004, so that no monitoring activity of these observations could be performed during 2007. Results from the monitoring statistics covering the period October 2003 - March 2004 were presented by [Dethof \(2004\)](#).

6 Conclusions

Under ESA contract 17585-CCN-1 (Technical support for global validation of Envisat data products) NRT GOMOS (GOM_RR_2P) products were monitored at ECMWF using the operational assimilation system. Because of instrumental problems which caused the unavailability of the NRT MIPAS (MIP_NLE_2P) product, no monitoring could be performed of these data since 27 March 2004. In addition, the monitoring of the NRT SCIAMACHY (SCI_RV_2P) product could not be performed in 2007 due to data unavailability as well. To allow the implementation of the new Level 1b algorithm (version 6.01), the dissemination of the Level 2 NRT SCIAMACHY data was stopped on 8 May 2006, and never restarted afterwards. It is understood that the KNMI TOSOMI product distributed via the ESA funded PROMOTE consortium has to be regarded as the official ESA Level 2 total column ozone retrieved from SCIAMACHY (Minute of the ESA contract progress meeting held at ECMWF on 6 December 2006).

The NRT GOMOS products (GOM_RR_2P) were available during the whole 2007, with only a few short periods of unavailability. The longest of these periods was at the beginning of 2007. Changes in the settings of the local air density and of the local temperature (both set equal to zero) in the new Level 2 processor (IFP 5.0) for GOMOS data switched on 8 August 2006 forced the ozone and temperature retrievals to be set to “MISSING” in the BUFR files, and so unusable for monitoring. This problem was solved and the dissemination of the NRT GOMOS products restarted on 17 January 2007.

Upon the data availability, an indication of the timeliness of the ENVISAT products during the period 2006-2007 was provided. Overall, about 91% of the data from SCIAMACHY were delivered by ESA on time for the delayed-cut-off analyses (data based on the period from 1 January to 8 May 2006). The timeliness of the TOSOMI products as downloaded by KNMI was lower than that for ESA (89% in 2006, and just over 83% in 2007). As far as GOMOS products are concerned, about 96% of the data were received in time for the delayed-cut-off analyses during 2006, and just below 95% during 2007. Because the information required to calculate

these statistics is only stored for a period of about two years, no record was available for MIPAS data, as their dissemination was stopped in March 2004.

The quality of the GOMOS temperature profiles was stable during 2007, and consistent with that reported by Dragani (2006). On average, the GOMOS temperature departures are less than -1% (-2 K) in most of the stratosphere and slightly larger (up to -3%, about -6K) in the mesosphere between 0.2 and 0.4hPa. With the dissemination started on 17 January, the temperature profiles in the GOMOS BUFR files were retrieved as the "Tangent Point Temperature from External Model" stored in the GAD, namely the ECMWF 24-hour temperature forecasts in the lower part of the profile (up to 1hPa) and of the MSIS90 climatology in the upper part of the profile with a smooth transition around the pressure level of 1hPa. The results from the monitoring statistics seemed to highlight some problems on the actual nature of the temperature data. In particular, the mean departure between the temperature profile in the GOMOS files and the ECMWF temperature analyses seemed to exceed the expected mean departure between the ECMWF 24-hour temperature forecasts and the ECMWF temperature analyses themselves. While the latter is typically within $\pm 0.3^\circ$ in the stratosphere, the former exhibits values within -2 and $+1^\circ$ at the same altitude range. This should be further investigated, especially if the temperature profiles are used to infer information in the retrieval process of other variables.

On 17 January 2007, for the first time since the beginning of the dissemination of the NRT GOMOS data, information on water vapour became available in the GOM_RR_2P BUFR files and was continuously provided for the whole 2007. However, the quality of the water vapour data was generally poor, even after the bright, twilight and straylight observations were filtered out. The monitoring statistics for 2007 showed the GOMOS water vapour values were from one to four orders of magnitude larger than those given by the model at all stratospheric levels and latitudinal bands. The largest differences were found in the upper stratosphere, where not only did the GOMOS observations exhibit values of four order of magnitudes larger than their model equivalent on average, they also were larger than the mean GOMOS tropospheric observation. A slightly higher level of agreement was found at midlatitudes in the NH during December 2007. Here the GOMOS WV observations still exhibited higher values than their model equivalent, but the departures were considerably smaller than those seen in the other latitudinal bands. In addition, the water vapour content decreases with height as one would expect.

As far as the NRT GOMOS ozone profiles are concerned, the global mean annual mean first-guess and analysis departures are within -5 and +10% in most of the stratosphere (for pressure values smaller than 40hPa), but larger departures were found on average in the lower stratosphere (for pressure values larger than 40hPa), and in the mesosphere. The standard deviations of the departures were found larger than 50% in most vertical layers. When averaging over latitudinal bands, the level of agreement just discussed is usually confirmed. The agreement between the GOMOS ozone observations and their model equivalent is better than the GOMOS ozone one standard deviation limit at all vertical levels and latitudinal bands. The largest differences are found in the lower stratosphere, typically for pressure values larger than 40 hPa, and in the upper mesosphere where the first-guess and analysis departures can be larger than 20%. Also the first-guess and analysis departure standard deviations are very large with values larger than 50% in places indicative of noise in the ozone retrievals. Despite that, it should be acknowledged that the GOMOS ozone product has continuously improved during the years. Comparisons of the monthly scatter plots for July from 2004 to 2007 showed a reduction in the scatter of the GOMOS ozone observations as well as a much improved level of agreement with their model equivalent since the start of the dissemination.

7 Acknowledgements

Information to calculate the statistics discussed in section 2 was provided by Susan Madry (ECMWF). The OMI data were obtained from <ftp://toms.gsfc.nasa.gov/pub/omi/data/ozone/Y2007/>.

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