MONITORING AND ASSIMILATION OF ENVISAT NRT RETRIEVALS AT ECMWF

Rossana Dragani
ECMWF, Shinfield Park, Reading, RG2 9AX, UK, Email: Rossana.Dragani@ecmwf.int

ABSTRACT

NRT SCIAMACHY total ozone columns and NRT GOMOS temperature and ozone profiles are daily monitored at ECMWF as part of the ENVISAT calibration/validation activities. The monitoring of MIPAS retrievals (ozone, temperature, and water vapour profiles) was stopped on March 2004, due to instrumental problems. However, an assimilation campaign is planned to assess the impact of MIPAS ozone and water vapour profiles provided at reduced spatial resolution on the ECMWF analyses. This talk presents the general performance of ozone assimilation at ECMWF together with the results from the MIPAS assimilation campaign and from the routinely monitoring of SCIAMACHY and GOMOS data.

1. INTRODUCTION

ECMWF is contracted by ESA to provide 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 to ECMWF on ESA’s ftp servers in near-real time (NRT) in BUFR format. The Meteo data include temperature, ozone and water vapour profiles from MIPAS (MIP_NLE_2P) and GOMOS (GOM_RR_2P), as well as total column ozone (TCO) retrievals from SCIAMACHY nadir measurements (SCI_RV__2P). This paper discusses the results from the daily monitoring of NRT ENVISAT products at ECMWF over the last two to three years, and it mainly focuses on the SCIAMACHY and GOMOS data. The MIPAS assimilation campaign was, instead, delayed as the ozone and water vapour retrievals are not yet available, and therefore this topic will not be discussed in the present paper.

Because ozone is fully integrated into the ECMWF forecast model and analysis system (Dethof and Holm, 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 monitoring statistics of SCIAMACHY total column ozone and GOMOS ozone and temperature profiles showed improvements in the quality of these observations compared with those of two to three years ago, as well as a better agreement with the ECMWF ozone and temperature fields. In contrast, the quality of the GOMOS water vapour profiles and their agreement with the ECMWF water vapour analyses are still poor.

This paper is structured as follows: section 2 gives a summary of the main features of the ECMWF operational model; 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. Section 5 provides the conclusions.

2. THE ECMWF OPERATIONAL MODEL

The ECMWF model is a global spectral model with a current horizontal resolution truncation of T799, which corresponds to 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 comprises two main six 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 analyses and 0901-1500 UTC for the 12 UTC analyses. All the observation monitoring, ENVISAT data monitoring included, is done in the delayed-cut-off analyses (Dethof, 2004 and Haseler, 2004). The forecast model includes a simple ozone parameterization, which is an updated version of the Cariolle and Deque (1986) scheme. 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 univariately 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. As far as the ozone model bias is concerned, the ECMWF model
overestimates total column ozone 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 at certain times of the year in particular in the northern hemisphere during the winter (Dethof and Holm, 2004).

The ECMWF model underwent to significant changes over the last year. On 1 February 2006, the ECMWF operational model system was upgraded to model cycle CY30R1. The major changes were the increase in the horizontal and vertical resolutions (T799 L91) and the extension of the model top at 0.01 hPa. In addition, a new set of coefficients were used in the ozone chemistry scheme (Cariolle and Teyssendre, 2007). On 12 September 2006, the ECMWF model was upgraded to model cycle CY31R1 to include as a major change a variational bias correction (VarBC) scheme for radiances, alongside with a revised cloud scheme and a revised method to assimilate rain affected radiances. These changes were expected to have some little impact on the monitoring of ENVISAT products, as the new bias correction for radiances affects the temperature field and in turn ozone. On 12 December 2006, a further upgrade of the model became operational (CY31R2).

The major change that had repercussions on the monitoring of the ENVISAT ozone products was the update of the heterogeneous term in the ozone chemistry scheme (Cariolle and Teyssendre, 2007).

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 are obtained from NESDIS1. 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 observation error correlation. Besides ozone retrievals from SBUV/2, NRT SCIAMACHY ozone column produced by KNMI2 and distributed via the ESA funded project PROMOTE 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 both datasets. Temperature and water vapour retrievals are not assimilated at all in the system, although these fields are strongly constrained by the assimilation of radiances. The radiance assimilation does not include the assimilation of the ozone band in the infrared.

1See http://orbit-net.nesdis.noaa.gov/crad/sit/ozone/ for more details.

3. MONITORING AND ASSIMILATION OF SCIAMACHY NRT TOTAL COLUMN O₃

SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY) (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 the 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 are produced operationally by ESA and also by KNMI. The current operational ESA algorithm is based on the older GOME data processor. The KNMI total column ozone is retrieved with a scheme based on the OMI Differential Optical Absorption Spectroscopy (DOAS) algorithm, the so-called TOOSMI algorithm. This is a modified version of the DOAS (Differential Optical Absorption Spectroscopy) method, initially developed to retrieve total column ozone fields from OMI (Ozone Monitoring Instrument) (Veekind and de Haan, 2002).

The ESA NRT SCIAMACHY ozone retrievals have been monitored passively at ECMWF in the operational suite since February 2003, and carried on until 8 May 2006, when the dissemination of the Level 2 products was stopped, to allow the implementation of a revised Level 1b scheme (version 6.01), but never restarted afterwards. It is now understood that the TOOSMI product will be regarded as the official ESA Level 2 total column ozone retrieval from SCIAMACHY (Minute of the ENVISAT progress meeting held at ECMWF on 6 December 2006).

The TCO retrieved at KNMI were passively monitored from March 2004 to 27 September 2004. As the assimilation of NRT TOOSMI SCIAMACHY data was seen to improve the ECMWF total column ozone analyses, as well as the ozone vertical distribution (Dethof, 2004), KNMI NRT ozone retrievals have been actively assimilated in the ECMWF operational system since 28 September 2004, when the model was updated to cycle CY28R3. Hence, from 28 September 2004 onwards the comparison of ESA total column ozone against the ECMWF ozone field does not give an independent validation anymore as it rather compares ESA with KNMI SCIAMACHY retrievals.

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°×1°.

Figure 1 shows the time series of global mean first guess (blue line) and analysis (red line) departures for ESA SCIAMACHY (top panel), and KNMI TOSOMI (bottom panel) averaged over 6-hourly analysis cycles for the period January- April 2006. The dissemination of SCIAMACHY NRT data for 2006 started only on 3 January, as a consequence of a wrong handling of the seasonal index 3 during the last months of 2005 that was solved with the implementation of the Instrument Processing Facility (IPF) 6.00. During the period from 1 to 10 February, the monitoring could not be performed because of technical problems that arose after the cycle CY30R1 was switched on.

During the last three days of March, the first guess and analysis departures suddenly increased to -12 and -8 DU respectively. This jump was identified as the consequence of the use of a wrong climatology (Angelika Dehn, SERCO, private communication). A similar episode also occurred at the end of March 2005. The quality of the SCIAMACHY data recovered at the beginning of April when both the first guess and analysis departures went back to the values found before the end of March 2006. On 6 April, a series of anomalies occurred on-board of ENVISAT leading to the interruption of the payload, including SCIAMACHY. The recovery from these anomalies required the payload to be switched on and off a few times during the following two weeks. After these anomalies, the quality of SCIAMACHY data started to degrade. This degradation is certainly related to the level 2 retrieval scheme, as the monitoring statistics for the KNMI retrievals are not affected and still remain at the same levels registered before the anomalies.

Figure 2 shows the monthly mean geo distribution of the first-guess departures for March 2006, from the ESA SCIAMACHY (top panel) and the KNMI TOSOMI (bottom panel) monitoring statistics. Figure 2 shows large departures at the end of the orbits that might point to a problem with the ozone retrieval at high solar zenith angle. The geographical plot of the first-guess bias also reveals relatively large positive biases north of 40°N especially over Canada, and Europe, as well as large negative biases over the Norwegian and Barents Seas.

Figure 3 shows the scatter plots of the first-guess departures for KNMI TOSOMI (l.h.s panels) and ESA SCIAMACHY (r.h.s panels), for March 2005 (top), March 2006 (middle), and March 2007 (bottom). Note that the ESA SCIAMACHY TCO was not available in 2007. The KNMI TOSOMI showed in both 2005 and 2006 a higher level of agreement with the ECMWF ozone field than the ESA SCIAMACHY, in particular at mid and high latitudes in the Northern hemisphere. To be noted that the comparison is slightly in favour of the KNMI data, as they are actively assimilated. Improvements can be seen for both retrievals in the level of agreement with the ECMWF ozone first-guess in 2006, compared with the same period in 2005. In March 2007, the level of agreement of the TOSOMI product with the model ozone seems to further improve compared with previous years, with a mean first-guess departure of -0.56 DU in March 2007, as opposite to the -10.54 DU and -7.28 DU of March 2005 and 2006 respectively. The changes introduced in the ECMWF operational model (and discussed in section 2) are partly responsible for these improvements. However, the
substantial increase in the density of the data with almost zero bias with respect to the model ozone in 2007 has to be related to improvements in the KNMI product, as the changes implemented in the ECMWF operational suite after March 2006 had little impact on the global mean ozone.

With the exception of a few sporadic episodes, where the departures are larger than 10 DU, generally the agreement between observation and model is very high. A striking feature noticeable in the time series is the jump in the first-guess departures which occurred each time the KNMI data delivery was temporarily stopped. This is a consequence of the fact that this product is actively assimilated, and thereby the system needs a short period of adjustment when the dissemination restarts.

In general, both ESA and KNMI SCIAMACHY ozone data depict well the seasonal cycle of total ozone column, such as high ozone values in the northern hemisphere during the late northern winter and early northern spring, and low ozone in the tropics. Figure 5 shows the time series of the zonal mean total column ozone values computed from ESA SCIAMACHY (top panel), KNMI TOSOMI (middle panel), and OMI (Ozone Monitoring Instrument) data (bottom panel) for the period from 1 January to 8 May 2006.

The high level of agreement between the TOSOMI product and the ECMWF ozone field during 2007 is also confirmed by the time series of most recent data. Figure 4 shows the global time series of the observations, first-guess and analyses (top panel) and first-guess and analysis departures (bottom panel) for the six-month period between October 2006 and March 2007 for the KNMI TOSOMI total column ozone.

Figure 4: The time series of the observations, first-guess, and analyses (top), and first guess and analysis departures for KNMI TOSOMI for the period from October 2006 to March 2007. Values are in DU.

Figure 5: The time series of the zonal mean ESA SCIAMACHY (top panel), KNMI TOSOMI (middle panel) observations, and OMI TCO (bottom panel) for the period from 1 January to 8 May 2006. Values are in DU.

Figure 5 indicates a good agreement between the NRT SCIAMACHY ozone retrievals and OMI observations.
over most of the globe, and shows the ability of the SCIAMACHY retrievals to well represent the global distribution of the total column ozone. However, compared with OMI, the SCIAMACHY total ozone values are, in general, underestimated in the tropics (about 20 to 30 DU lower than OMI), and at midlatitudes in the SH (25 to 50 DU lower than OMI).

Overall, the quality of the NRT ESA SCIAMACHY data improved during the first months of 2006, compared with that on 2005. However, the quality of the KNMI product seems to be more stable, and the KNMI retrieval scheme appears to be more reliable (e.g. during the anomalies occurred on board ENVISAT in April 2006). There are still some problems at the orbit ends in both hemispheres (although it seems that the differences between the two datasets are not as large as during 2005), and in the Northern hemisphere between 40°N and 70°N, in particular over Canada and the Norwegian and Barents seas.

4. MONITORING OF GOMOS DATA

GOMOS (Global Ozone Monitoring by Occultation of Stars) makes use of the occultation measurement principle by tracking stars as they set behind the atmosphere. GOMOS has an UV-visible and a near-infrared spectrometer, covering the wavelength region 250-950 nm. It allows the retrieval of atmospheric trace gas profiles in the altitude range 100-15 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 O₃, NO₂, NO₃, OCIO, H₂O and temperature.

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. Information on water vapour has not been available in BUFR format until 18 January 2007.

GOMOS data quality is strongly dependent on the illumination of the limb through which the star is observed (Meijer et al., 2004). According to GOMOS quality disclaimer, data in dark limb conditions have good quality for scientific applications, whereas data in bright, twilight or straylight limb conditions have degraded quality and should be filtered out. A filter to convert into BUFR format only the data retrieved from dark limb measurements was recently implemented in the converter from PDS to BUFR (PDS2BUFR), and it will shortly become operational.

In the following subsections, the results from the monitoring statistics of NRT ozone, temperature and water vapour retrieved from GOMOS measurements are presented.

4.1. Monitoring of GOMOS ozone:

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

Figure 6 shows the mean GOMOS ozone profiles and mean GOMOS departures for March 2007 averaged over the globe. The agreement between GOMOS NRT ozone values and ECMWF ozone profiles is much improved over the years, in particular in the Stratosphere. In contrast, it is still poor in the mesosphere and upper troposphere. The largest differences are found in the mesosphere, with the first-guess and analysis departures being usually larger than 20%. Also the first-guess and analysis departure standard deviations are very large, greater than 50% at most vertical levels.

Figure 6: Profiles of time and globally averaged GOMOS and ECMWF ozone values (left) and GOMOS departures (right). Averaging period is March 2007. Ozone values are in DU and departures are in %.

When compared with past years, some improvements can be detected. Figure 7 shows the scatter plots of the observations against first guess (lhs) and of the first guess departures against latitudes (rhs) for March 2006 (top panels) and March 2007 (bottom panels) for the layer between 20 and 40 hPa.

Figure 7: Scatter plots of the observations against first guess (lhs) and of the first guess departures against latitudes (rhs) for March 2006 (top panels) and March 2007 (bottom panels) for the layer 20-40 hPa.
Figure 7 shows that the quality of the data has improved over the last year. In March 2006 (top panels) the observation exhibited unrealistically low values (0 DU), as well as unrealistically high observations. These extreme values led to a large scatter of the first guess departures around zero at all latitudes. In March 2007, the overall performance of the GOMOS ozone retrievals seems to be improved. The 0 DU values are no longer detected, and the density of outliers is very much reduced. Similar level of improvement can be seen at most vertical levels in the Stratosphere. The statistics are expected to improve further once the new PDS2BUFR converter will become operational.

4.2. Monitoring of GOMOS temperature:

This section discusses the results from the monitoring of the NRT GOMOS Level 2 temperature profiles.

Figure 8 shows the mean GOMOS temperature profiles (lhs) and mean GOMOS departures (rhs) for March 2007 averaged over the globe.

Overall, figure 8 show that GOMOS NRT temperature profiles agree well with the ECMWF temperatures. The ECMWF temperature analyses are, in general, warmer than the GOMOS observations at all latitudinal bands, and at all levels, with a few exceptions in the mesosphere at high latitudes in the northern hemisphere. In the global mean, GOMOS temperature departures are less than -1% (about -2 K) in the stratosphere. Larger departures (up to 2%, about 4-5 K differences) are found in the mesosphere. The first-guess and analysis departure standard deviations are about 1% up to 1 hPa, and slightly larger (up to 3%) in the mesosphere.

Although the level of agreement of the temperature retrievals with the ECMWF model was already good, quite significant improvements were found in the monitoring statistics in 2007 compared with that of 2006. Figure 9 shows the comparisons of the temperature departures for March 2006 (lhs) with those obtained in March 2007 (rhs) for three latitudinal bands: (a) [60N-90N] (top panels); (b) [30N-30S] (middle panels); (c) [60S-90S] (bottom panels). Figure 9 shows that the agreement between the observations and the model improved in the lower stratosphere at high latitudes in both hemisphere during March 2007, compared with the same period in 2006. By contrast, the level of agreement between model and observations for 2007 is comparable to that for 2006 in the mesosphere. Some improvements are also found in the standard deviations of the departures, which are slightly reduced in the 2007 monitoring statistics. Negligible differences were seen in the tropics between the 2006 and 2007 statistics.

The scatter plots (not shown) of the observation versus model temperature and of the temperature departures confirm the level of agreement discussed above.

4.3. Monitoring of GOMOS water vapour:

The GOMOS water vapour became available in BUFR format only in January 2007. The monitoring statistics so far show a poor level of agreement between
observations and the ECMWF water vapour, at all levels and latitudinal bands.

Figure 10 shows, as an example, the time series of the observations, first guess and analyses (top panel) and of the water vapour departures (bottom panel) for February and March 2007 for the layer between 60 and 80 hPa. Currently, unrealistically high water vapour data are found in the BUFR files. These spurious data lead to excessively high mean observation values that make the comparison with the model water vapour meaningfulness sometimes.

![Figure 10: Time series of the observation, first-guess and analysis, and WV departures at 60-80 hPa.](image)

Despite the currently poor agreement, the comparisons between GOMOS water vapour profiles and the ECMWF first guess and analyses are expected to significantly improve from the operational use of the new PDS2BUFR converter.

5. CONCLUSIONS

Contracted by ESA, ECMWF provides technical support for global validation of ENVISAT NRT data products retrieved from SCIAMACHY, GOMOS and MIPAS, using its operational assimilation system. This paper discussed the results from the daily monitoring of NRT (ESA and KNMI) SCIAMACHY total column ozone and GOMOS ozone, temperature, and water vapour retrievals at ECMWF over the last two to three years. For what concerning the monitoring and assimilation of MIPAS profiles, this was stopped in March 2004 due to instrumental problems. The NRT-like assimilation campaign that will assess the contribution of MIPAS ozone and water vapour profiles retrieved at a reduced spatial resolution was, instead, delayed as the ozone and water vapour retrievals are not yet available.

The monitoring of the ESA NRT SCIAMACHY product could be performed only until 8 May 2006, when the dissemination was stopped to allow the implementation of the new Level 1b algorithm (version 6.01), but never restarted afterwards. It is now understood that the KNMI TOSOMI product has to be regarded as the official ESA Level 2 total column ozone retrieved from SCIAMACHY. The monitoring of NRT SCIAMACHY observations showed that its data quality improved compared with that of 2005; the product is more stable and the agreement with ECMWF ozone model is also significantly better than that in 2005. In the global mean, the ESA SCIAMACHY first-guess departures decreased from values around -15 DU at the beginning of January 2006 to values around -8 DU in March. Despite the improvement in the data quality there are still issues to be addressed. The Level 2 retrieval scheme seems to be not very reliable, or at least less reliable than the KNMI algorithm. For example, after a series of anomalies started on 6 April on board of ENVISAT, the quality of these data was seen to gradually deteriorate, and almost double within two weeks. This was suggested to be related with the Level 2 retrieval algorithm, as the KNMI TOSOMI monitoring statistics did not show this degradation. There are still some problems of large positive departures at the northern end of the orbits between January and March, and at the southern ends during April and May, that might indicate problems with the retrieval scheme at high SZA.

The monitoring of the NRT GOMOS products showed that:

- The GOMOS temperature profiles are in good agreement with the ECMWF temperatures. In the global mean, GOMOS temperature departures are less than -1% (-2 K) in the stratosphere and slightly larger (up to -3%, about -5K) in the mesosphere. Improvements were seen at high latitudes in the lower stratosphere where almost zero temperature departures were found. The standard deviations of the first guess and analyses departures were also reduced.

- The quality of the GOMOS NRT ozone profiles generally improved in 2007 compared with that in 2006. The unrealistically low (0 DU) values seen in 2006 were no longer found in the 2007 monitoring statistics at most levels in the Stratosphere. The scatter of the data was also seen to be reduced, leading to a smaller scatter of the ozone departures at all latitudinal bands.

- The dissemination of NRT GOMOS water vapour profiles started in January 2007. The quality of these data and their agreement with the ECMWF water vapour are currently poor. Exceedingly high data were found in the BUFR files, that compromised the level of their agreement with the model water vapour field.

One of the reasons for the poor agreement between the GOMOS retrievals and the ECMWF model fields is that at the moment the monitoring statistics make use of all the observations available in the BUFR files, regardless their quality, as determined by the star illumination
conditions. A filter to retain only the highest quality GOMOS observations was recently implemented in the converter from PDS to BUFR format, and it is now under final tests at ESA. The level of agreement between the GOMOS NRT data and the ECMWF first guess and analyses is expected to improve as soon as this new converter from PDS to BUFR will become operational.

ACKNOWLEDGEMENTS
The OMI data were obtained from http://toms.gsfc.nasa.gov/index.html.

REFERENCES