ESA CONTRACT REPORT

Contract Report to the European Space Agency

Validation of the reprocessed MIPAS and SCIAMACHY retrievals using ERA-Interim, and one-year assimilation of MIPAS ozone profiles at ECMWF

January 2013

Rossana Dragani

Final report for ESA contract 21519/08/I-OL CCN No. 1:

Technical support for global validation of ENVISAT data products

European Centre for Medium-Range Weather Forecasts
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Abstract

During the ENVISAT lifetime, ECMWF has been contracted to routinely monitor the ENVISAT near real time products. After the satellite loss, this activity has been readdressed to validate the reprocessed datasets against the ERA-Interim reanalyses. These datasets include ozone, temperature, and water vapour (WV) profiles retrieved from the MIPAS measurements, and ozone profiles from the limb measurements of SCIAMACHY.

The reprocessed MIPAS ozone profiles exhibit higher values than ERA-Interim at most levels, latitudes, and seasons. Above 10 hPa, the MIPAS minus ERA-Interim differences are within ±10%. In the lower stratosphere the residuals can be as large as +30% in the tropics. MIPAS minus ERA-Interim temperature differences are about -1K at all latitudes and seasons in the UTLS and in the lower stratosphere at mid and high latitudes, less than 2K (about 1%) in the tropical lower stratosphere, and within ±5K in the upper stratosphere and mesosphere. Because of a number of shortcomings, the region where the ERA-Interim and MIPAS WV datasets are reliable is a shallow layer around the tropopause, where the differences are within ±10%. Larger differences are found elsewhere.

The SCIAMACHY limb minus ERA-Interim ozone differences are within ±20% between 20 and 40 km in the extra-tropics. Larger departures are found in the tropics, particularly at 10 hPa ($>$ 100%), in contrast with the comparisons of ERA-Interim against MIPAS and previous studies.

In preparation for the forthcoming reanalysis production, a one-year assimilation study of the near real time MIPAS ozone profiles has also been performed. Comparisons with MLS and ozone sonde profiles show that the assimilation of MIPAS improves the vertical distribution of the ozone analyses in the upper troposphere and stratosphere in the extra-tropics, and in the region of the ozone maximum in the tropics.

1 Introduction

Contracted by the European Space Agency (ESA), ECMWF was involved in the monitoring and assimilation of a variety of different near real time (NRT) products from several instruments on board ENVISAT during the satellite lifetime. The outcome of these activities was documented in a number of monthly and annual reports available at `www.ecmwf.int/publications/library/do/references/list/18`. These activities were performed routinely using the ECMWF Observation Monitoring Facility which provides statistics of how different observations available in the ECMWF system compare with their model equivalent. The set of monitored products, limited to the three atmospheric instruments on board ENVISAT, included temperature, ozone and water vapour profiles retrieved from MIPAS and GOMOS, as well as total column ozone retrievals from SCIAMACHY nadir measurements. These were normally referred to as the Meteo products.

With the sudden lost of ENVISAT on 8 April 2012 and the unavailability of NRT time products, the ECMWF work was readdressed to focus on the newly available reprocessed datasets from the ENVISAT atmospheric sensors. These reprocessed products from the ENVISAT atmospheric instruments are compared with their collocated model equivalent from the ECMWF ERA-Interim (Dee et al., 2011) archive. ERA-Interim is the latest ECMWF global atmospheric reanalysis and covers the period from January 1979 to present. As the name suggests it represents an interim production made in preparation of a new atmospheric reanalysis to replace ERA-40 that will extend back to the early part of the twentieth century. A reasons for using the reanalysis dataset instead of the weather analyses from the operational forecasting system is that, unlike the latter, reanalyses are obtained with a single, fixed version of the data assimilation system and forecast model. This means that a reanalysis is not affected by changes in the model.

The ERA-Interim reanalyses are produced with a recent version of the ECMWF high resolution model that was used operationally from December 2006 to June 2007. It uses a horizontal resolution truncation of T255, which corresponds to about 79 km grid spacing, and 60 vertical levels with the model top at 0.1 hPa. The model relies on a four-dimensional variational (4D-Var) scheme (Rabier et al., 2000) to assimilate observations available within a 12-hour time window. An important aspect in ERA-Interim is the inclusion of a completely automated scheme for correcting biases in satellite radiance observations (Dee, 2005; Auligné et al., 2007). Bias corrections for individual sensor channels are expressed in terms of a small set of predictors, which can depend on the atmospheric state at the observed location or on the state of the instrument itself. A set of bias parameters determine the linear combination of predictors used for correcting each radiance observation. These parameters are continuously adjusted by the variational analysis to minimise inconsistencies among the available sources of information, including all observations and their background equivalent. It is noted that an ozone bias correction scheme was only introduced in the ECMWF high resolution system in September 2009 (Dragani, 2009), and therefore not yet available at the time the ERA-Interim reanalysis production started.

The ENVISAT reprocessed datasets available for the present study include ten years of ozone, temperature and water vapour profiles retrieved from MIPAS (version 6), and ozone profiles from the SCIAMACHY limb measurements (version 5.02). The GOMOS reprocessed dataset was not considered here as it was only made publicly available on 19 December 2012. Total column ozone (TCO) retrieved from the nadir measurements of SCIAMACHY was not considered either as the NRT TOSOMI TCO retrieved at KNMI from the same level 1b measurements were actively assimilated in ERA-Interim, and therefore the two datasets cannot be regarded as independent.

This report is structured as follows: Section 2 presents a brief summary of the quality of the ERA-Interim analyses restricted to the model fields that were used for the validation of the ENVISAT reprocessed data. The diagnostic tools and the matching criterion used in the present study are described in section 3. The results from the comparisons between the ERA-Interim analyses and MIPAS and SCIAMACHY reprocessed data are presented in sections 4 and 5, respectively. Section 6 presents an assessment of one-year assimilation of MIPAS ozone profiles in a lower resolution version of the ECMWF operational system. This is based on NRT retrieved data and represents an extension of the work presented in Dragani (2012). Conclusions and remarks follow in section 7.

2 The ERA-Interim reanalyses

A thorough discussion and assessment of the ERA-Interim reanalysis project can be found in Dee et al. (2011), which also include a detailed discussion on the changes in the used observing system. Here, a brief review of the quality of the model fields used in the validation of the ENVISAT reprocessed datasets is provided.

2.1 Ozone

Dragani (2010, 2011) presented an assessment of the quality of the ERA-Interim ozone based on twenty year comparison with in-situ and remotely sensed independent ozone data.

The ERA-Interim TCO was typically found within ±5DU (about ±3%) from a TCO reference generated from the NASA merged satellite TCO as a monthly mean for five consecutive years. Comparisons with OMI TCO showed up to 2% lower total ozone values in the ERA-Interim dataset between 50°S-50°N. The vertical distribution of the ozone concentrations compares well with the sonde and satellite ozone measurements in the tropics with the ozone maximum normally localised at the observed levels. However, the ozone maximum values are often underestimated. Modelling of stratospheric ozone transport and depletion at high latitudes, particularly during winter times, still show problems in the ERA-Interim production. The reanalyses tend to place the ozone maximum too high, with deeper depletion in the middle stratosphere just below the peak. This is mainly due to the limited amount of ozone observations available at this time of the year and latitudes. Improvements are expected in the next reanalysis production as ozone sensitive radiances from Infrared sounders are expected to be assimilated. Dragani and McNally (2012, 2013) showed the value of these observations particularly in improving the quality of the ozone analyses in the UTLS region and at high latitudes in the winter hemisphere. In general, the vertical distribution of the ozone analyses benefits from the assimilation of any height resolved ozone retrievals, as demonstrated by their improved quality during the years ERS-2 GOME ozone profiles were assimilated (1996-2002, Dragani, 2011).

Overall, comparisons with SAGE, HALOE and (UARS and Aura) MLS data show consistent results both in the tropics and extra-tropics, with mean residuals typically within ±5% around 5hPa and within ±10% in the region of the ozone mixing ratio maximum at 10hPa. Mean residuals of about +10% (but up to +20% at times) and within ±20% are found both in the tropics and extra-tropics for all instruments near 30hPa and in the lower stratosphere around 65hPa, respectively.

Although, a lot of effort was devoted in improving the homogeneity of the ERA-Interim production compared with that of ERA-40, the ERA-Interim ozone analyses still show limited consistency in time as a consequence of the biases between the ozone observations from different instruments. Although an adaptive ozone bias correction is currently used in the ECMWF weather forecasting system, this was not yet available at the time the ERA-Interim production started. This aspect will be improved in the forthcoming reanalysis production.

2.2 Temperature

Temperature (and water vapour) analyses are mostly constrained through the assimilation of radiances observations and a number of in-situ observations. The observation operator used for simulating satellite radiance observations in ERA-Interim is based on RTTOV version 7, which incorporates the fast transmittance model described by Matricardi et al. (2004). This represents a largely improved version of the RTTOV radiative transfer model. Matricardi et al. (2004) showed, for example, that the differences between fast-model and line-by-line calculations of transmittances are greatly reduced at all pressure levels when using RTTOV-7. Improvements in the treatment of surface emissivity allowed a better exploitation of many surface and near-surface peaking channels over land. The adaptive bias correction applied to all radiance observations greatly improved the consistency in time and homogeneity of the ERA-Interim temperature and water vapour analyses. This is particularly the case in the troposphere and lower stratosphere. Systematic discrepancies between analyses produced with observations from different satellite instruments still remain in the middle and upper stratosphere, and mesosphere. This is a consequence of the limited availability of observations that can be used as a reference to correct for the upper stratospheric biases (Kobayashi et al., 2009). A further improvement, particularly in the ERA-Interim stratospheric temperature analyses, occured in 2006 when the assimilation of GPS radio occultation data started.

Overall, the tropospheric and lower stratospheric temperature analyses are expected to be affected by small biases, typically less than 1K. Larger biases should instead be expected in the upper stratosphere and mesosphere.

2.3 Water Vapour

As in the case of temperature, also the water vapour analyses are mainly constrained by the assimilation of humidity sensitive radiances. Compared with the previous reanalysis production, ERA-40, the ERA-Interim humidity analyses are based on a completely revised humidity analysis scheme that was developed by Hólm (2003). The new scheme involves a nonlinear transformation of the humidity control variable to have nearly Gaussian humidity background errors. Humidity observations are not accurate enough to produce sensible analysis increments in the stratosphere. As a consequence, humidity increments are not allowed in the stratosphere realised by prescribing very small humidity background errors above the diagnosed tropopause. An account of the modifications to the formulation of the humidity analysis and its impact on the assimilation of humidity-sensitive observations, from conventional as well as satellite instruments, is presented by Andersson et al. (2005). That study showed through comparison with in-situ data that the model's performance with respect to boundary layer humidity, which provides the largest contribution to the total column water vapour, is often within the absolute accuracy of most current humidity observing systems (around 5% in relative humidity).

3 Matching criterion and diagnostic tools

The comparisons with all the ENVISAT observations made use of the same matching criteria. The 3D ERA-Interim analysis closest in time to the independent measurements was interpolated to the observation location. Based on this criterion and given the availability of four analyses per day (at 00, 06, 12, and 18 UTC), a temporal mismatch of up to 3 hours between observation time and analysis valid time should be expected. Then, the ERA-Interim analysis profiles and the observations were interpolated on a common vertical grid (with pressure levels at [0.18, 0.25, 0.5, 0.72, 1, 1.3, 1.6, 2, 2.5, 3, 5, 7, 10, 13, 15, 20, 30, 41, 52, 70, 100, 150, 200, 300, 385]hPa).

The results are presented in terms of mean absolute and relative residuals (RRs) computed between the independent observation ($\mathbf{X^{Obs}}$) and its reanalysis equivalent ($\mathbf{X^{EI}}$) over the whole period of data availability. The mean (indicated by $\overline{()}$) RRs were calculated as follows:

$$\mathbf{RR} = 100 \times \overline{\frac{\mathbf{X^{Obs}} - \mathbf{X^{EI}}}{\mathbf{X^{Obs}}}} \tag{1}$$

4 Validation of MIPAS profiles

MIPAS was a Fourier transform spectrometer for the detection of limb emission spectra in the middle and upper atmosphere. Because it observed a wide spectral interval throughout the mid infrared (from 4.15 μm to 14.6 μm) at high spectral resolution, MIPAS could detect and spectrally resolve a large number of emission features of atmospheric minor constituents, thus playing a major role in atmospheric chemistry. MIPAS was one of the first ENVISAT instruments to be fully operational after the launch, providing very high quality observations, and NRT MIPAS ozone profiles (MIP_NLE_2P) were actively assimilated at ECMWF from October 2003 until the end of March 2004 (Dethof, 2004) when due to instrumental problems the instrument had to be switched off. Operations could only be resumed in January 2005 when the original high spectral resolution was reduced from 0.025 cm^{-1} to 0.0625 cm^{-1}. The reduction in the spectral resolution led to a proportional reduction in the measurement time from 4.5 seconds to 1.8 seconds, that was exploited to increase the number of measured spectra in each scan in order to have a finer vertical limb grid in the upper troposphere and lower stratosphere (UTLS), and an altitude range coverage from 6 to 70 km. The reduction in the measurement time coming from the use of a lower spectral resolution also resulted in a reduced horizontal spacing between two contiguous limb scan measurements. Originally, operations were also restricted to operate MIPAS with a reduced duty cycle (<50%, then relaxed to 60%). Based upon the instrument reliability, ESA decided to restart the MIPAS operations at 100% duty cycle in December 2007. However, because of completely independent issues, the production of the Level 2 data was further delayed, and fully resumed only at the beginning of 2011. After a number of assimilation experiments confirmed the value of these observations, ECMWF restarted the operational assimilation of MIPAS ozone profiles on 8 December 2011. Preliminary results from that study were already discussed in Dragani (2012), while results from an extension of it are presented in section 6 of this report. Here, the focus is on the validation of the reprocessed ozone, temperature and water vapour profiles retrieved from the MIPAS instrument (version 6) against their collocated ERA-Interim reanalyses.

4.1 The reprocessed ozone profiles

Figure 1 shows the seasonal mean differences between MIPAS and co-located ERA-Interim ozone analyses during the ENVISAT lifetime (2002-2012). Absolute differences are plotted to the left; relative differences computed according to equation 1 are presented on the right panels. Each row refers to a particular season across the ten year lifetime of ENVISAT: (from the top to bottom) December-January-February (DJF), March-April-May (MAM), June-July-August (JJA), and September-October-November (SON). The vertical stripes in figure 1 are due to the combined plotting of several years together. On average, MIPAS ozone profiles exhibit higher ozone values than their ERA-Interim ozone equivalent at most levels, latitudes, and four seasons. These results confirm the outcome of the VALID study (van Gijsel, 2011) that showed MIPAS ozone profiles could exhibit up to 8% higher ozone concentrations than collocated lidar measurements. In the comparisons with ERA-Interim, the largest differences are found in the tropics in the region of the ozone mixing ratio maximum between 10 and 20 hPa, where MIPAS ozone values are on average 1 ppmm (about 10%) higher than their ERA-Interim equivalent. Dragani (2010, 2011) showed that, although the vertical distribution of the tropical ERA-Interim ozone analyses well compared with independent data, the values at the peak are often underestimated. The plots also show that on average at pressure levels smaller than 15 hPa the MIPAS minus ERA-Interim differences are within ±10%. In the lower stratosphere these differences are positive and normally larger, particularly in the tropics where they can reach +30%.

Figure 2 shows the standard deviation of the seasonal mean differences plotted in figure 1 (left panels). In general, these standard deviations are largest at high latitudes in the winter stratosphere where the ERA-Interim ozone analyses are least constrained due to lack of ozone observations. During spring/autumn time, the largest standard deviation values are limited to a shallow layer in the region of the ozone mixing ratio maximum between 10 and 20 hPa where they can be as large as 1.5 ppmm (10%).

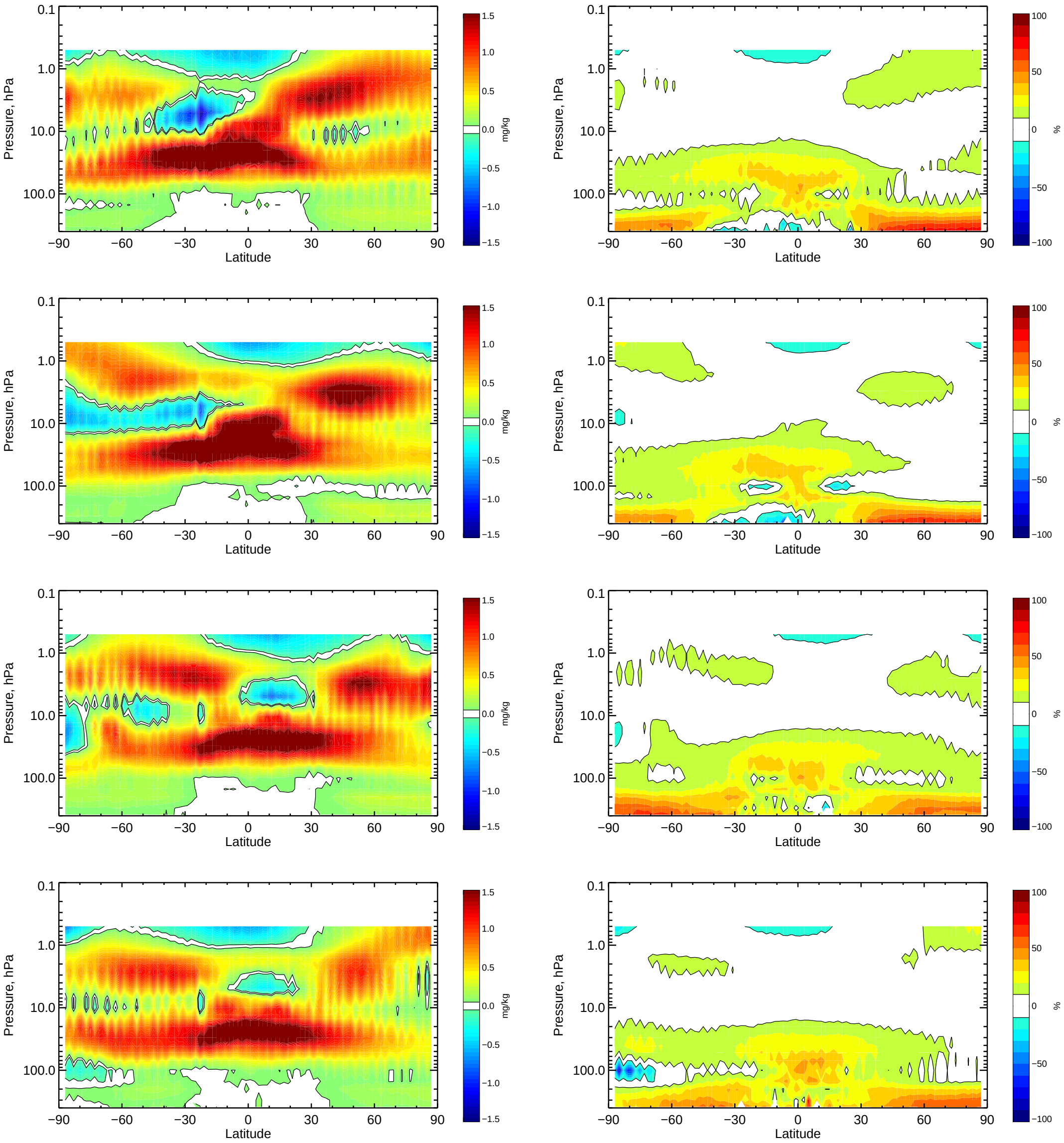

Figure 1: Seasonal mean difference between MIPAS and co-located ERA-Interim ozone analyses during the ENVISAT lifetime (2002-2012). Absolute differences are plotted to the left; relative differences computed with respect to the MIPAS observations are presented on the right panels. Each row refers to a particular season: (from the top to bottom) DJF, MAM, JJA, SON. Data are in mass mixing ratio (left) and % (right), respectively.

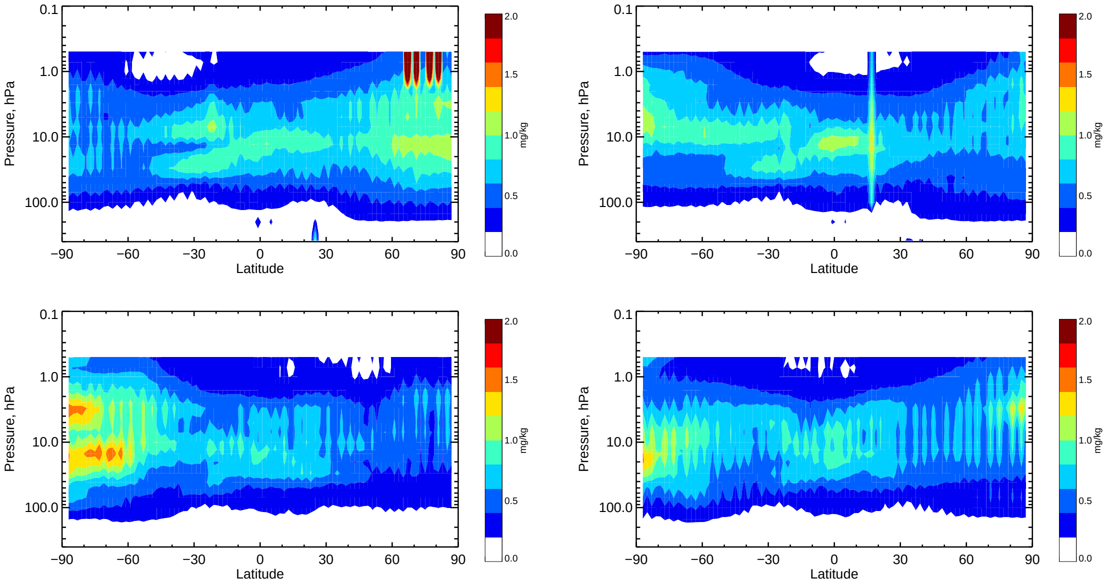

Figure 2: Standard deviation of the seasonal mean difference between MIPAS and co-located ERA-Interim ozone analyses during the ENVISAT lifetime (2002-2012). Each panel refers to a particular season: DJF and MAM on the top row (left and right panels, respectively), JJA and SON on the bottom row (left and right panels, respectively). Data are in mass mixing ratio.

Figure 3 shows the pressure-time mean differences between MIPAS ozone profiles and their ERA-Iterim equivalent averaged over three latitudinal bands (the tropics and extra-tropics). In the northern hemisphere, the MIPAS minus ERA-Interim mean residuals appear small (less than 1 ppmm) at all vertical levels and during the whole lifetime of ENVISAT. In the tropics, the mean residuals are positive, i.e. MIPAS shows higher ozone values than ERA-Interim. This is particularly the case in the tropical region between 10 and 30 hPa where the ozone mixing ratio peaks during the years 2005-2007, where the residuals are as large as 3 ppmm. This reduced level of agreement between observations and reanalyses is likely due to the changes in the ozone observing system assimilated in ERA-Interim. The ozone reanalyses benefitted from the assimilation of GOME ozone profiles until December 2002, then from the assimilation of MIPAS ozone profiles between 2003 and March 2004 (the comparisons for this period cannot be regarded as independent), and since 2008 from the assimilation of MLS ozone profiles. The assimilation of all these vertically-resolved ozone products led to improvements in the vertical distribution of ozone. In the southern hemisphere extra-tropics, MIPAS shows slightly smaller ozone concentrations than ERA-Interim in the region above the ozone maximum during the winter months, and higher concentrations at the maximum region or just below it during the summer/fall months.

Figure 4 presents the latitude-time mean differences between MIPAS ozone profiles and their ERA-Iterim equivalent at four pressure levels in the stratosphere. These four stratospheric pressure levels were selected as follows: one level at 10 hPa, near the typical ozone volume mixing ratio maximum; one level above and one level below the ozone maximum, at 5 and 30 hPa, respectively; and, finally, one level in the lower stratosphere at 65 hPa. These levels correspond to the four pressure levels overplotted in figure 3. Figure 4 confirms the large differences in the tropics, particularly between 2005 and 2007, as well as negative ozone differences at mid and high latitudes in the SH during the winter months at 10 hPa. This is a consequence of the lack of any ozone observation at high latitudes in the winter hemisphere. The level of agreement between MIPAS and ERA-Interim improves after the assimilation of MLS ozone profiles started in reanalysis.

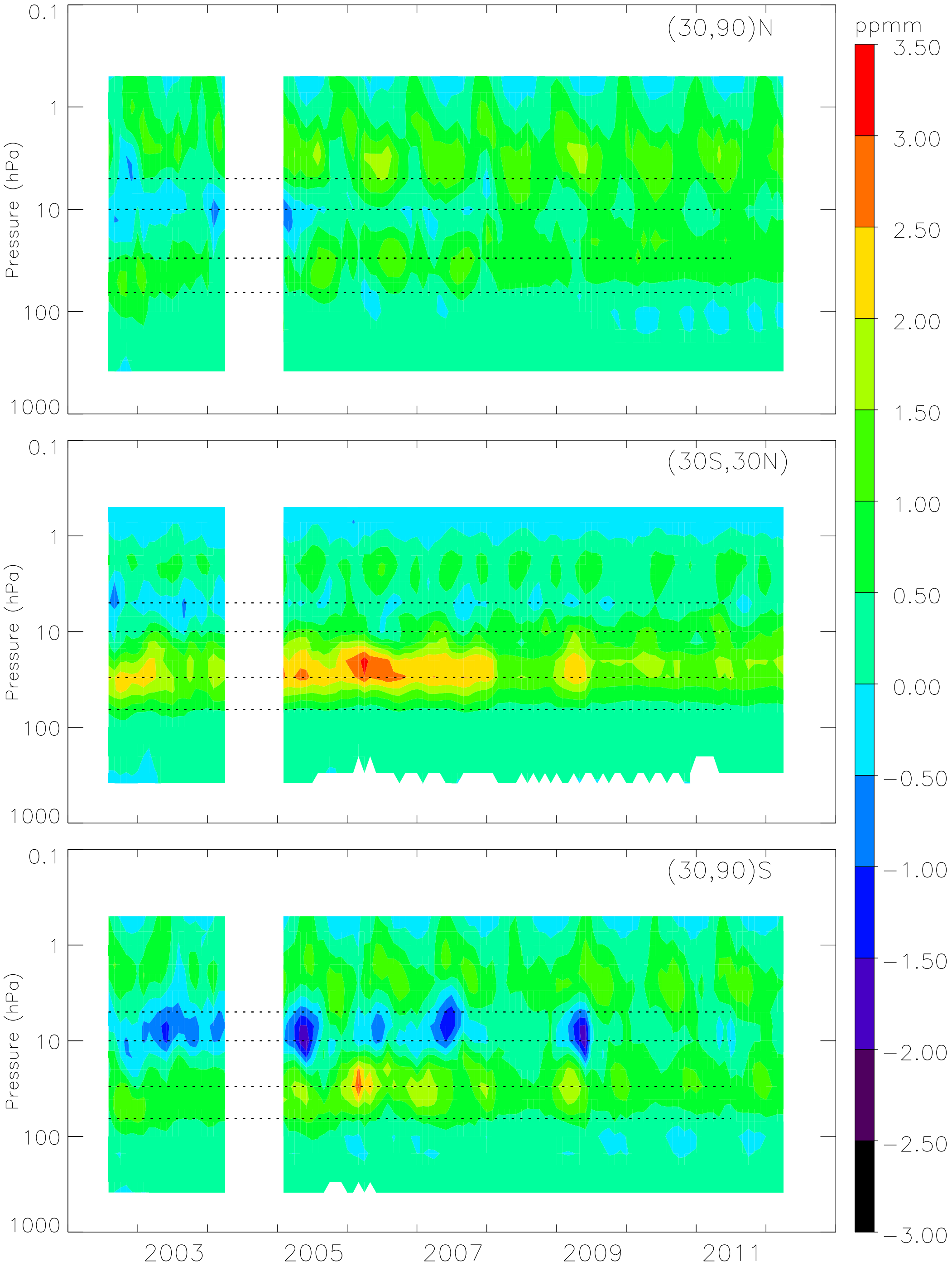

Figure 3: Pressure-time cross-sections of the zonal mean difference between MIPAS ozone profiles and co-located ERA-Interim ozone analyses averaged over three latitudinal bands. The four dotted lines indicate the 5, 10, 30 and 65 hPa levels. Data are in mass mixing ratio.

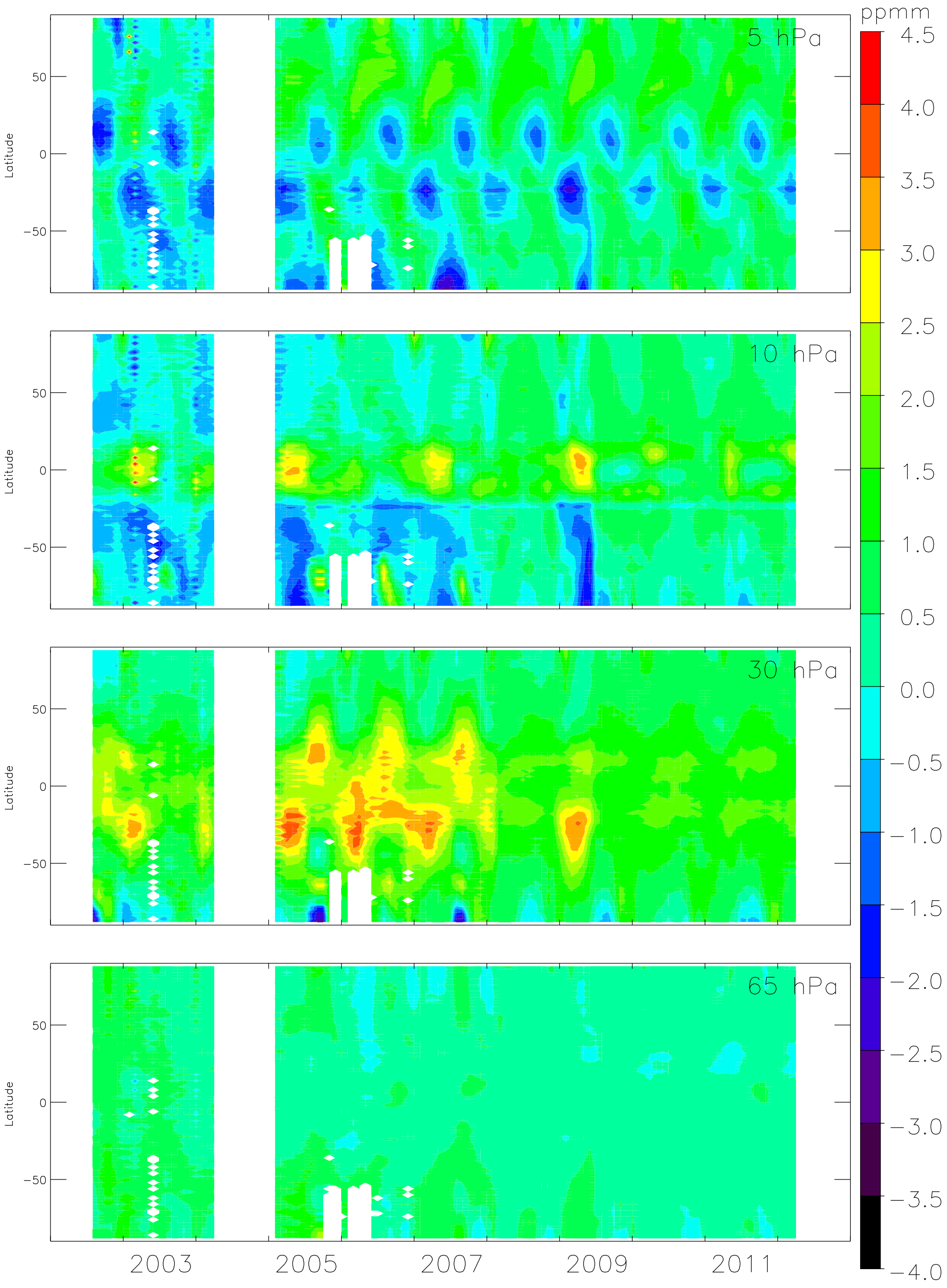

Figure 4: Latitude-time cross-sections of the zonal mean difference between MIPAS ozone profiles and co-located ERA-Interim ozone analyses at four pressure levels in the stratosphere: (from top to bottom) 5, 10, 30, 65 hPa. Data are in mass mixing ratio.

4.2 The reprocessed temperature profiles

The seasonal mean differences between MIPAS and co-located ERA-Interim temperature analyses (left panels) and their standard deviations (right panels) during the ENVISAT lifetime (2002-2012) are plotted in figure 5. On average, MIPAS temperature profiles are colder than their ERA-Interim temperature equivalent at all latitudes and seasons in the UTLS region and normally in the lower stratosphere at mid and high latitudes, where the differences are up to about 1K. In the tropical lower stratosphere MIPAS exhibits higher temperature than ERA-Interim, with differences of less than 2K (about 1%). At all latitudes and seasons in the upper stratosphere, the temperature differences are normally positive (the MIPAS temperatures are higher than the ERA-Interim temperatures) with differences of 4-5K. Above the stratopause, this behaviour is reverted with MIPAS being up to 5K colder than ERA-Interim. The standard deviation of the seasonal mean differences (left panels of figure 5) are generally about 2K at most levels and latitudes, as well as seasons.

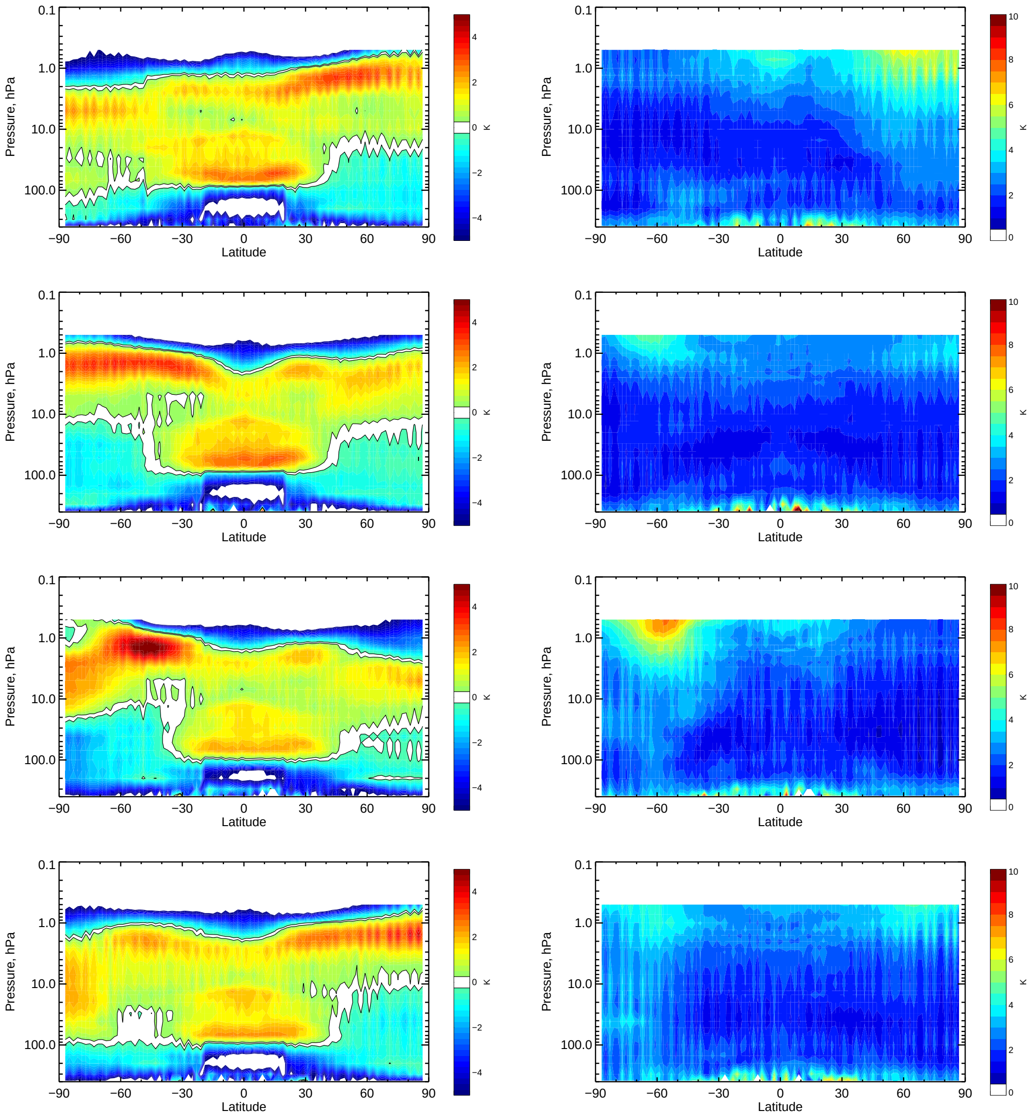

Figure 5: Seasonal mean difference between MIPAS and co-located ERA-Interim temperature analyses (left panels) and the standard deviations of the differences during the ENVISAT lifetime (2002-2012). Each row refers to a particular season: (from the top to bottom) DJF, MAM, JJA, SON. Data are in K.

Figures 6 and 7 show the pressure-time and latitude-time cross-sections of the zonal mean difference between MIPAS temperature profiles and co-located ERA-Interim analyses. The time series plots confirm the results of figure 5. The MIPAS temperatures are normally warmer than their ERA-Interim equivalent in the tropics, with differences up to 2 K. In the extra-tropics, the MIPAS temperatures are typically colder than ERA-Interim in the lower stratosphere and warmer in the middle and upper stratosphere, where the largest residuals can be as large as 5K in wintertime just below the stratopause. Arguably the quality of the ERA-Interim temperature analyses is lower at these level than in the troposphere and lower stratosphere, because the amount of available observations to constrain the analyses decrease substantially, as the number of observations to be used to anchor the bias correction. In the upper troposphere, the MIPAS minus ERA-Interim temperature residuals are also large and up to -5K in places. This is most likely due to large bias in the MIPAS data. Although MIPAS observations can extend down to 6 km altitude, they are optimized for the study of the stratosphere (Carli et al., 2012).

In the lower stratosphere from 30 down to 65 hPa, the MIPAS temperature appears to be about 1K colder than the ERA-Interim stratospheric temperature during winter at high latitudes (bottom two panels in figure 7). Figure 7 also shows a clear jump in the time homogeneity of the MIPAS temperature dataset between the first two years and the following years from 2005 to 2012. This is particularly evident in the middle stratosphere at 5 and 10 hPa.

Overall, the mean residuals between the MIPAS temperature and the ERA-Interim temperature analyses are within ±1% in the stratosphere.

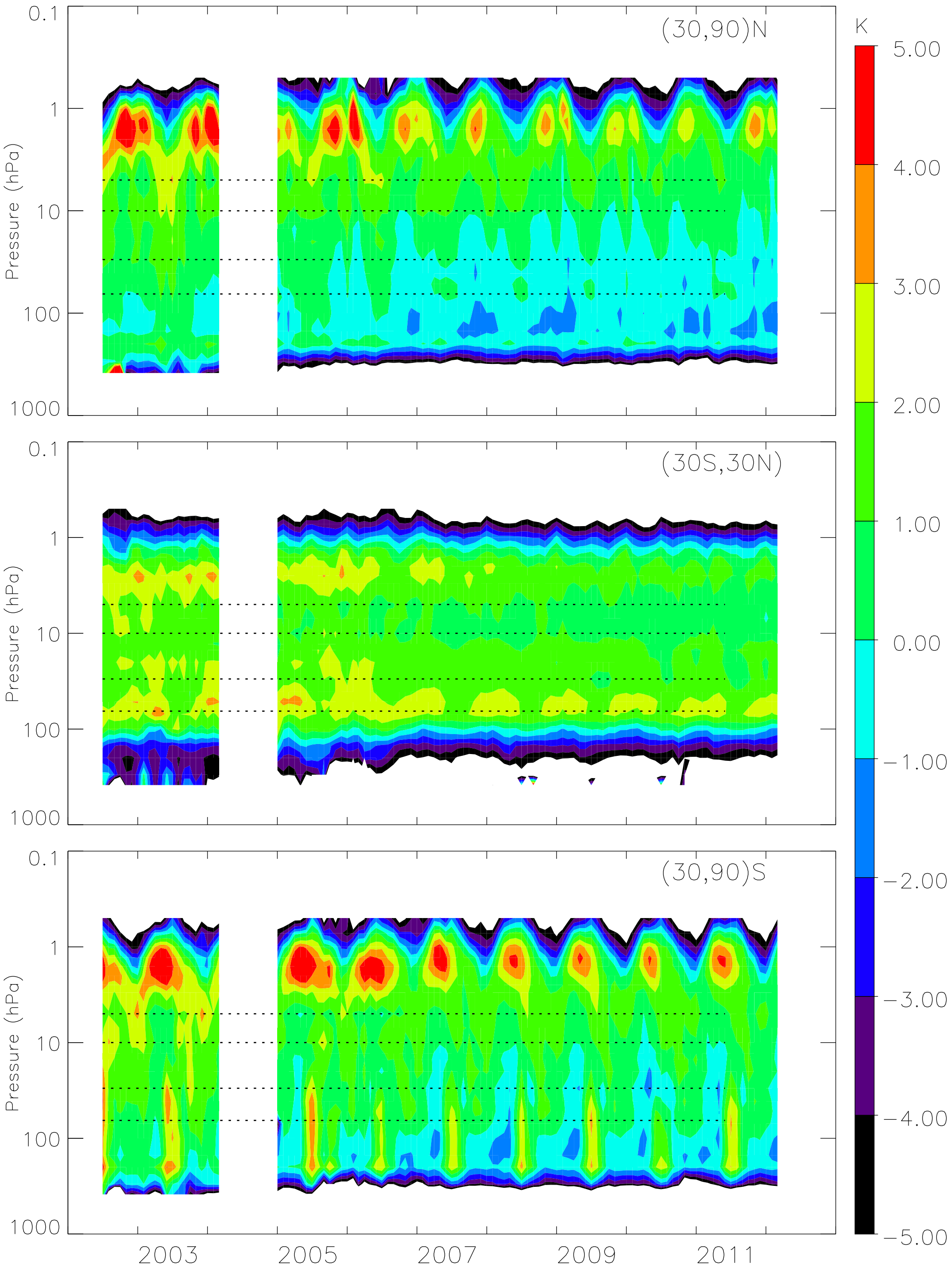

Figure 6: Pressure-time cross-sections of the zonal mean difference between MIPAS temperature profiles and co-located ERA-Interim temperature analyses averaged over three latitudinal bands. Data are in K.

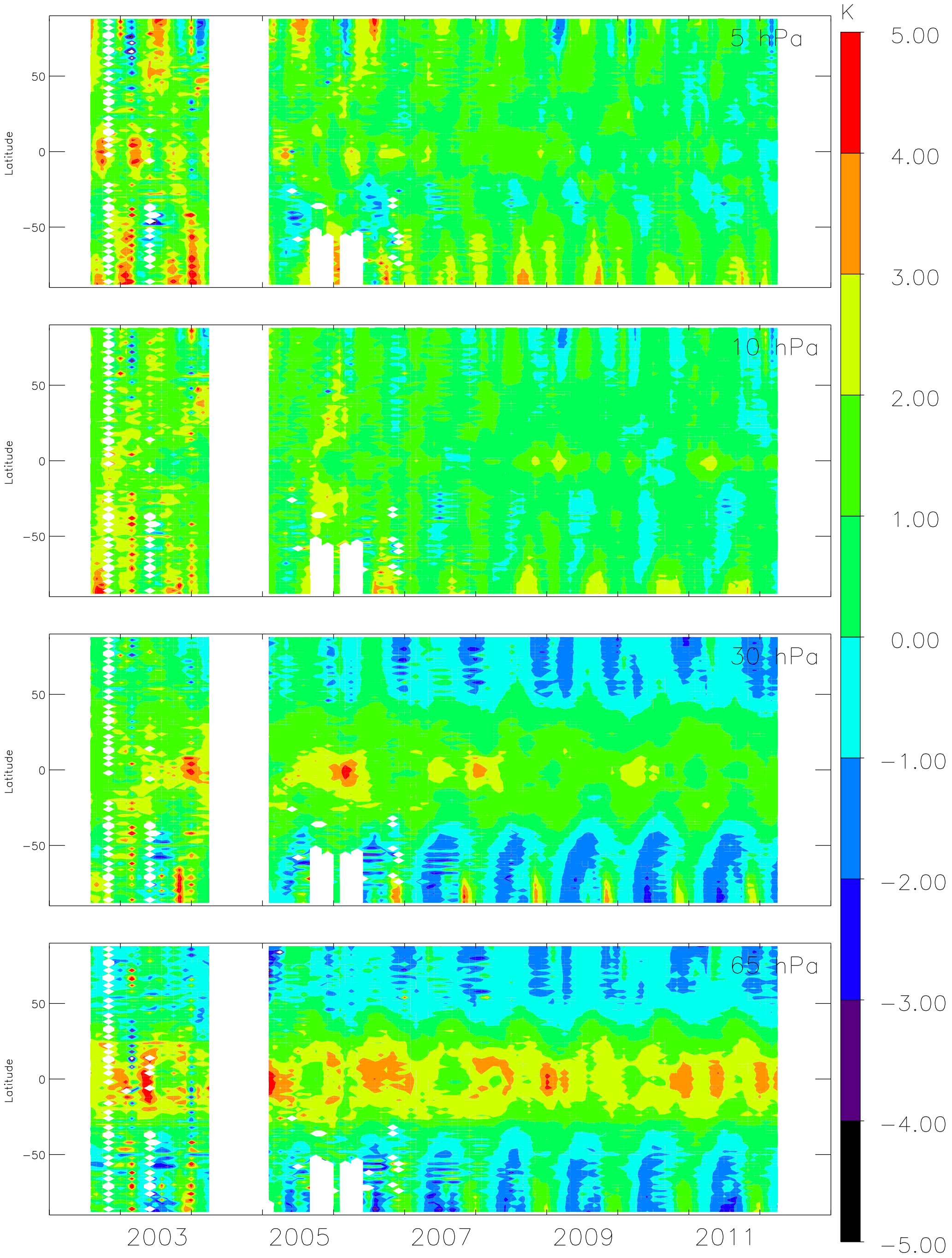

Figure 7: Latitude-time cross-sections of the zonal mean difference between MIPAS temperature profiles and co-located ERA-Interim analyses at four pressure levels in the stratosphere: (from top to bottom) 5, 10, 30, 65 hPa. Data are in mass K.

4.3 The reprocessed water vapour profiles

The comparison between the MIPAS water vapour and their ERA-Interim equivalent can only provide an indication of the quality of the dataset. That is because while MIPAS observations are optimized for the study of the stratosphere, and they normally show large biases in the upper troposphere, the ERA-Interim water vapour analyses may be better constrained in the troposphere than in the stratosphere. As anticipated above, the humidity scheme used in ERA-Interim does not allow the observation to generate any increment in the stratosphere by having very small humidity background errors. Therefore, the vertical range over which both MIPAS and the ERA-Interim water vapour datasets can be compared is limited to a layer across the tropopause.

Around the tropopause, the residuals between MIPAS and ERA-Interim water vapour are normally within ±10% (figure 8). In the upper troposphere between 300 and 150 hPa, the water vapour residuals are negative and tipically between 30 to 50%. In this region, the standard deviation of the departures are also very large, larger than 100% in places (right panels of figure 8).

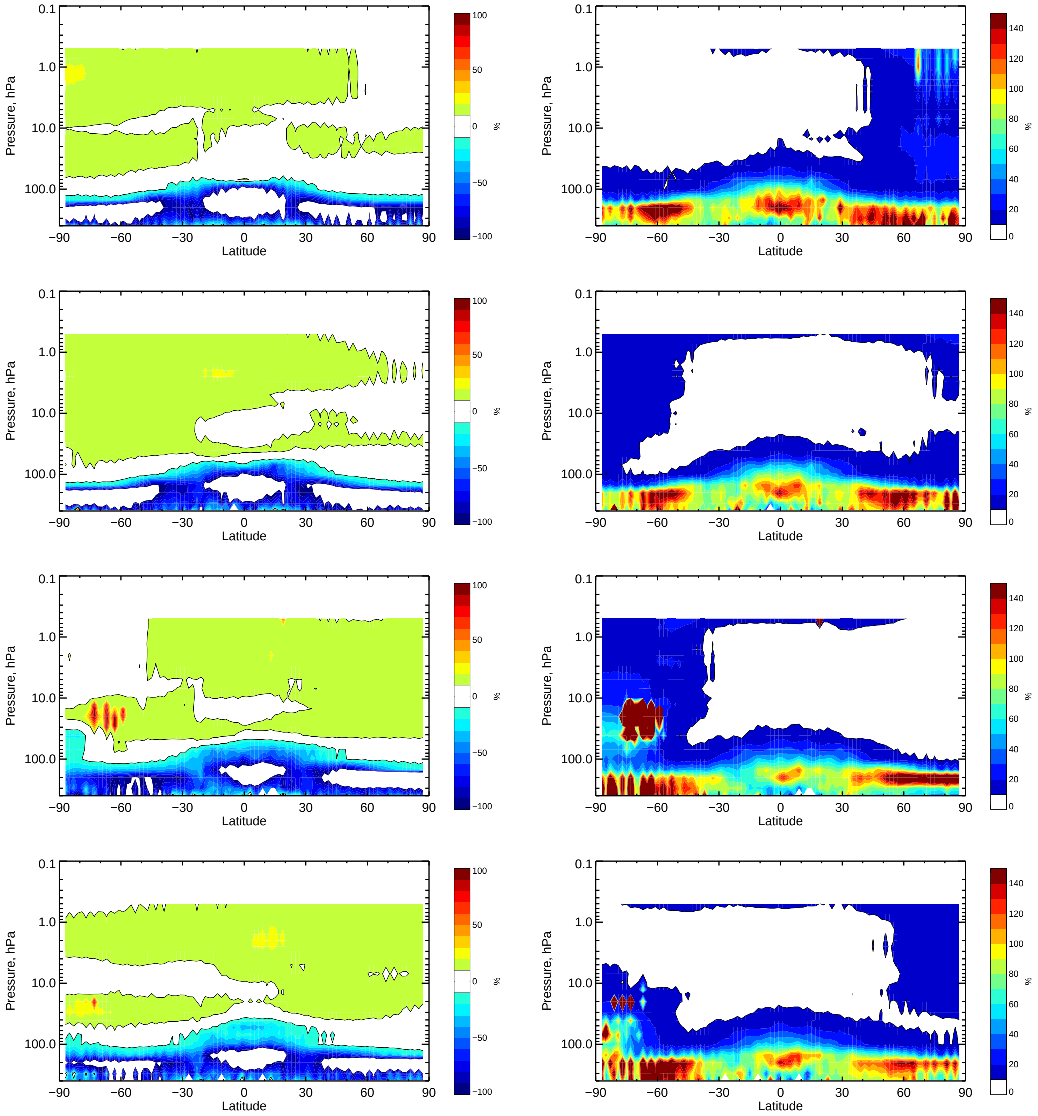

Figure 8: Like in figure 5, but for the water vapour normalised to the ERA-Interim analyses. Data are in %.

Figure 9 show large differences in the upper stratosphere, particularly in winter time. The latitude-time cross-sections of the water vapour residuals at four levels in the UTLS region (65, 85, 100, 115 hPa) are presented in figure 10. Though, the quality of the ERA-Interim water vapour analyses is questionable at some of these levels, a discontinuity after the instrumental problem of 2004 can be seen in the water vapour dataset, particularly in the lower stratosphere (top two panels in figure 10).

Overall, the region of the atmosphere where the comparison between the MIPAS water vapour profiles and their ERA-Interim equivalent can provide a fair indication of the data quality is limited to a layer around the tropopause. In that region, the level of agreement between observations and analyses is within 10%. Elsewhere, the differences are much larger than 10%.

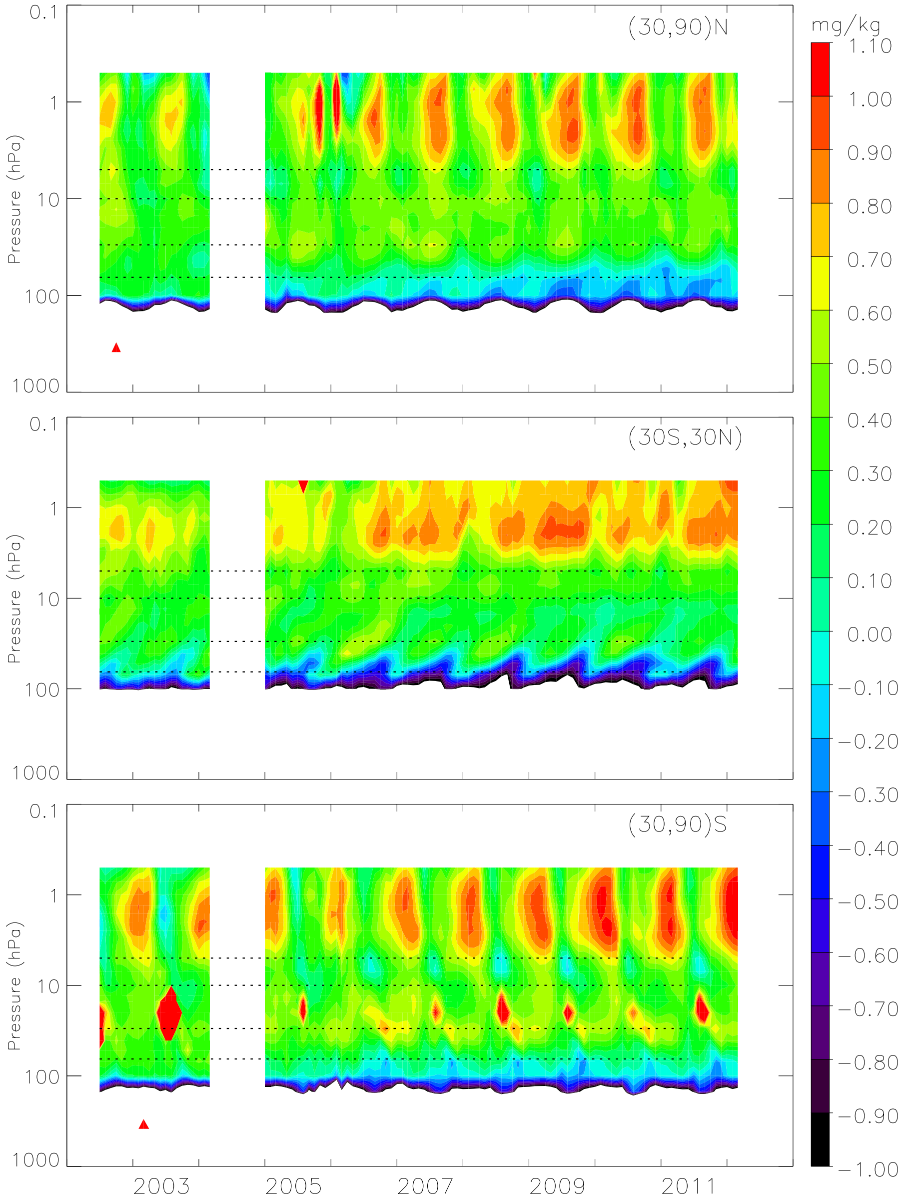

Figure 9: Pressure-time cross-sections of the zonal mean difference between MIPAS water vapour profiles and co-located ERA-Interim analyses averaged over three latitudinal bands. Data are in mg/kg.

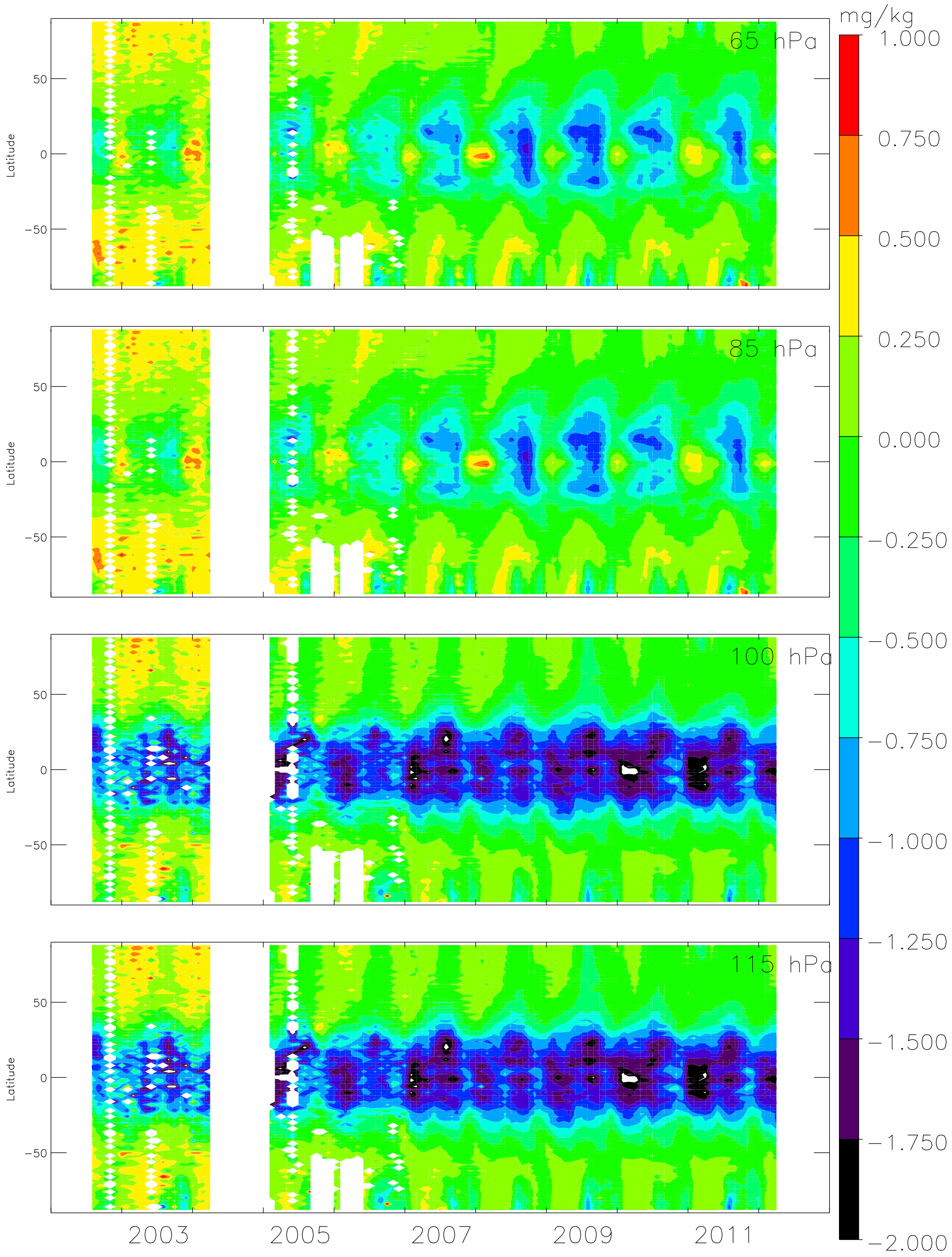

Figure 10: Latitude-time cross-sections of the zonal mean difference between MIPAS water vapour profiles and co-located ERA-Interim analyses at four pressure levels in the stratosphere: (from top to bottom) 5, 10, 30, 65 hPa. Data are in mass mg/kg.

5 The SCIAMACHY reprocessed dataset

SCIAMACHY (SCanning Imaging Absorption SpectroMeter for Atmospheric CHartographY, Burrows et al., 1988) was one of the atmospheric instruments on the ENVISAT satellite. The main scientific objective of SCIAMACHY was to measure 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) in order to derive global distributions of a number of atmospheric chemical species. SCIAMACHY measurements were performed in three viewing modes: nadir, limb and occultation. Depending on the measurement mode, global coverage could be achieved within 3 to 6 days, e.g. nadir measurements provided global coverage in about 6 days. Nadir UV/visible measurements provide global column distributions of O_3, NO_2, BrO, SO_2, OClO and H_2O, as well as cloud and aerosol parameters. Nadir infrared measurements are used to generate column distributions of CO. Limb observations provide vertical stratospheric profiles of O_3, NO_2 and BrO for UV/visible wavelength range.

Total column ozone from the nadir measurements were actively assimilated in the ERA-Interim production, and therefore their comparison with ERA-Interim cannot be regarded as an indipendent validation.

In this report, the focus is instead on the ozone profiles retrieved from the limb observations. These data were not available in NRT and therefore their quality could never be characterised against the ECMWF ozone analyses. The dataset was reprocessed for the whole ENVISAT lifetime with version 5.02 of the IPF algorithm. The off-line limb processor uses SCIAMACHY limb spectra within the 15 to 40 km tangent height range and a 3.3 km vertical resolution. Above about 40 km the sensitivity to O_3 becomes too small due to the small optical depths of these species. Below about 15 km, the sensitivity is strongly reduced because the atmosphere becomes optically thick in limb viewing mode. The lowest tangent height used for the retrieval is determined by the highest cloud free measurement from the Limb cloud product. This means that the retrieval starts at the first cloud free measurement. If no clouds are detected, it uses the the standard minimum height. Because of the limited sensitivity to ozone in limb mode below 15 km and above 40 km, the retrieval errors are considerably higher in these regions.

The height-resolved ozone product is provided in both mixing ratio and number density formats. The present study made use of the former as the ERA-Interim reanalyses are also available as mixing ratio.

Figures 11 and 12 show the pressure-time cross-sections of the zonal mean difference between SCIAMACHY limb ozone profiles and co-located ERA-Interim ozone analyses averaged over the tropics and the extra-tropics in absolute and relative values, respectively. According to the data disclaimer, the usable vertical range of SCIAMACHY limb ozone profiles is that within the two horizontal solid lines. In this region of the atmosphere the level of agreement between SCIAMACHY limb retrievals and the ERA-Interim ozone analyses are normally within ±20% in the extra-tropics. Here, the residuals are normally negative (positive) in the upper (lower) stratosphere indicating higher (lower) ozone values in the reanalyses than in SCIAMACHY. Outside this vertical range, the extra-tropical residuals show larger positive (negative) values below (above) the usable vertical range. In the tropics, large residuals are found in the region of the ozone maximum mixing ratio at 10hPa. Such differences are often larger than 100%. Such large negative residuals (up to -9 ppmm) are in clear contrast with the comparisons with MIPAS ozone profiles that showed instead positive residuals at 10 hPa up to about +3ppmm.

The reason for such a discrepancy is not at all clear. An initial validation of the version 5.01 ozone profiles found ozone biases in the tropics as large as 23% when compared with in-situ data. However, these differences were localised around 18 km, roughly 75hPa rather than at 10hPa. Here, two hypotheses are made that could have produced this result. Neither of them, however, can explain the reason why these large differences can be mostly found around 10 hPa in the tropics. One hypothesis is that these differences could partly be due to the SCIAMACHY data being used as volume mixing ratio instead of number density profile information.

The problem is that the calculation of the volume mixing ratio profile information needs additional information about the real pressure and temperature distributions, and these are not fully provided in the product, but are taken from the McLinden climatology, as for the *a priori*. It is possible that the use of climatological, rather than flow-dependent information in the converversion from number density profiles into their corresponding mixing ratio profiles could have led to large biases, and affected in particular the region of the ozone volume mixing ratio maximum at 10hPa. Additionally, it seems that the profile retrievals are computed without prior correction for tangent height errors in the Level 1b-2 processing step. This could also have introduced errors in the vertical coordinate that is used when deriving the observation equivalent from ERA-Interim. It is unclear if such errors could have a dependence on the vertical region of the atmosphere, and therefore be larger at some levels than at others. On the model side, the tropical ERA-Interim ozone analyses although show a good ozone vertical distribution with well vertically localised ozone maximum, the actual values are often not very well captured. Comparisons with a number of different independent ozone observations showed that the tropical ERA-Interim ozone analyses at 10 hPa are normally within ±10% from the measurements (Dragani, 2011), and therefore much smaller than what is indicated by the comparisons with SCIAMACHY.

Figure 13 refers to the latitude-time cross-sections of the zonal mean difference between MIPAS ozone profiles and co-located ERA-Interim analyses at four pressure levels in the stratosphere. With the exception of 65 hPa, all the other levels should be within the SCIAMACHY usable vertical range. These plots confirm the large negative differences around 10 hPa discussed above. At 30 hPa (third panel from the top) the SCIAMACHY minus ERA-Interim differences are normally positive in the tropics and slightly negative in the extra-tropics. At this level, it is clear that the level of agreement between the observations and reanalyses varied during the ten year lifetime of ENVISAT, with a better agreement during 2003 to spring 2004, and then again from 2008 onwards. This is a consequence of changes in the ozone observing system used in ERA-Interim. The ozone reanalyses benefitted from the assimilation of MIPAS ozone profiles in 2003 till March 2004 when the instrument had to be switched off, and since 2008 from the assimilation of MLS ozone profiles. The assimilation of these two limb instruments helped improve the distribution of the ozone analyses, particularly in the tropics between 10 and 30 hPa. Because the relative differences are very large at 10 hPa, the level of agreement hardly shows any difference during the ten years under assessment as a consequence of the changes in the ozone observing system assimilated in ERA-Interim.

In the upper stratosphere (5hPa), the level of agreement between reanalyses and observations is good with very small biases. In the lower stratosphere (65hPa), the agreement is also reasonably good at midlatitudes, while in the tropics these biases are larger than 50%. It should be noted that this level is just outside the usable range in the tropics that starts from about 56hPa. At 65hPa, large biases are also seen at high latitudes in the SH during winter. Although not to the extent showed in this comparison, the problem at these latitudes and time of the year is partly due to inaccuracy in the ozone analyses that have less constraints than in other periods of the year, and partly due to the observations that according to the data disclaimer should not be used at large solar zenith angles.

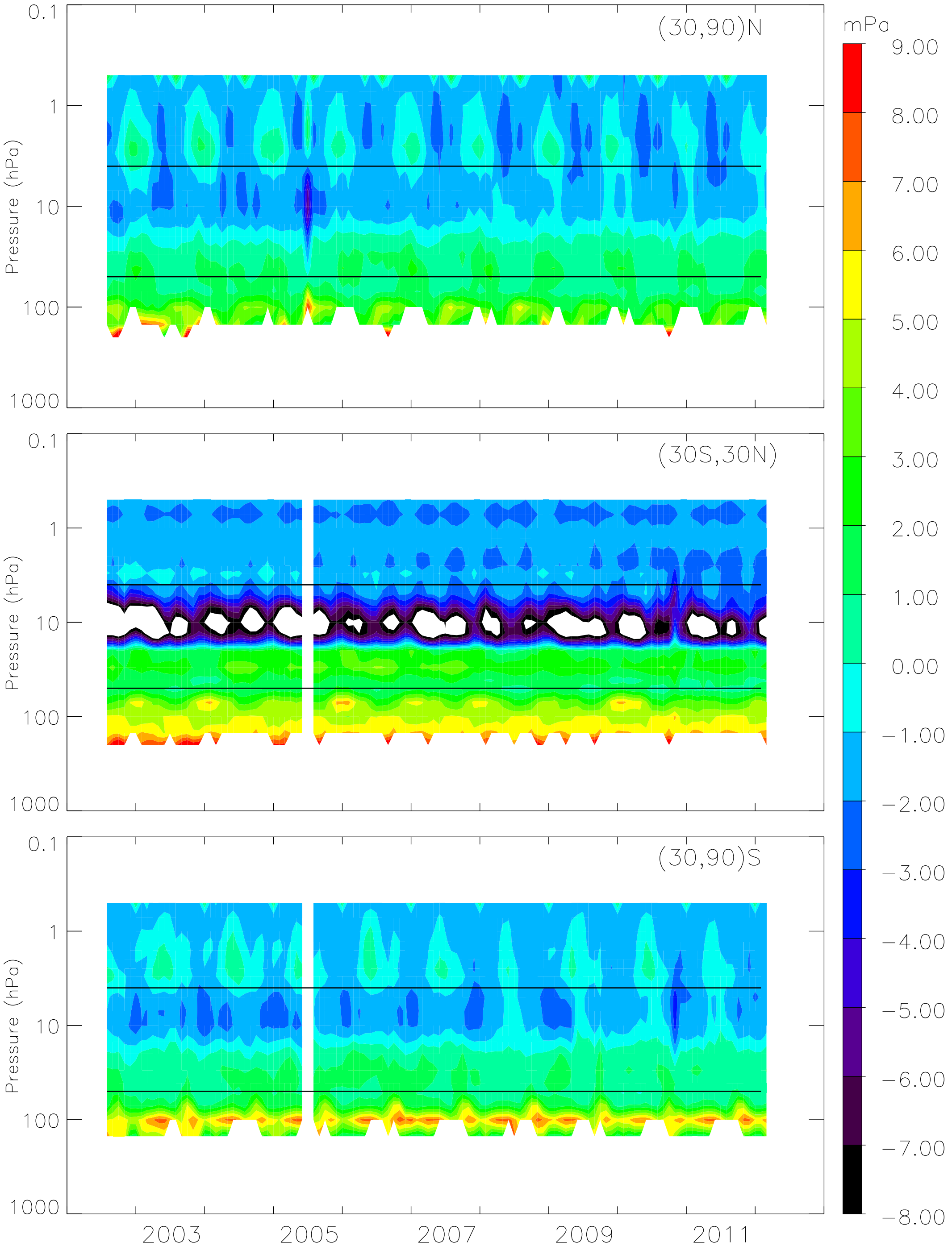

Figure 11: Pressure-time cross-sections of the zonal mean difference between SCIAMACHY limb ozone profiles and co-located ERA-Interim ozone analyses averaged over three latitudinal bands. The two solid lines indicate the vertical range where the SCIAMACHY ozone retrievals could be used according to the data disclaimer. Data are in mass mixing ratio.

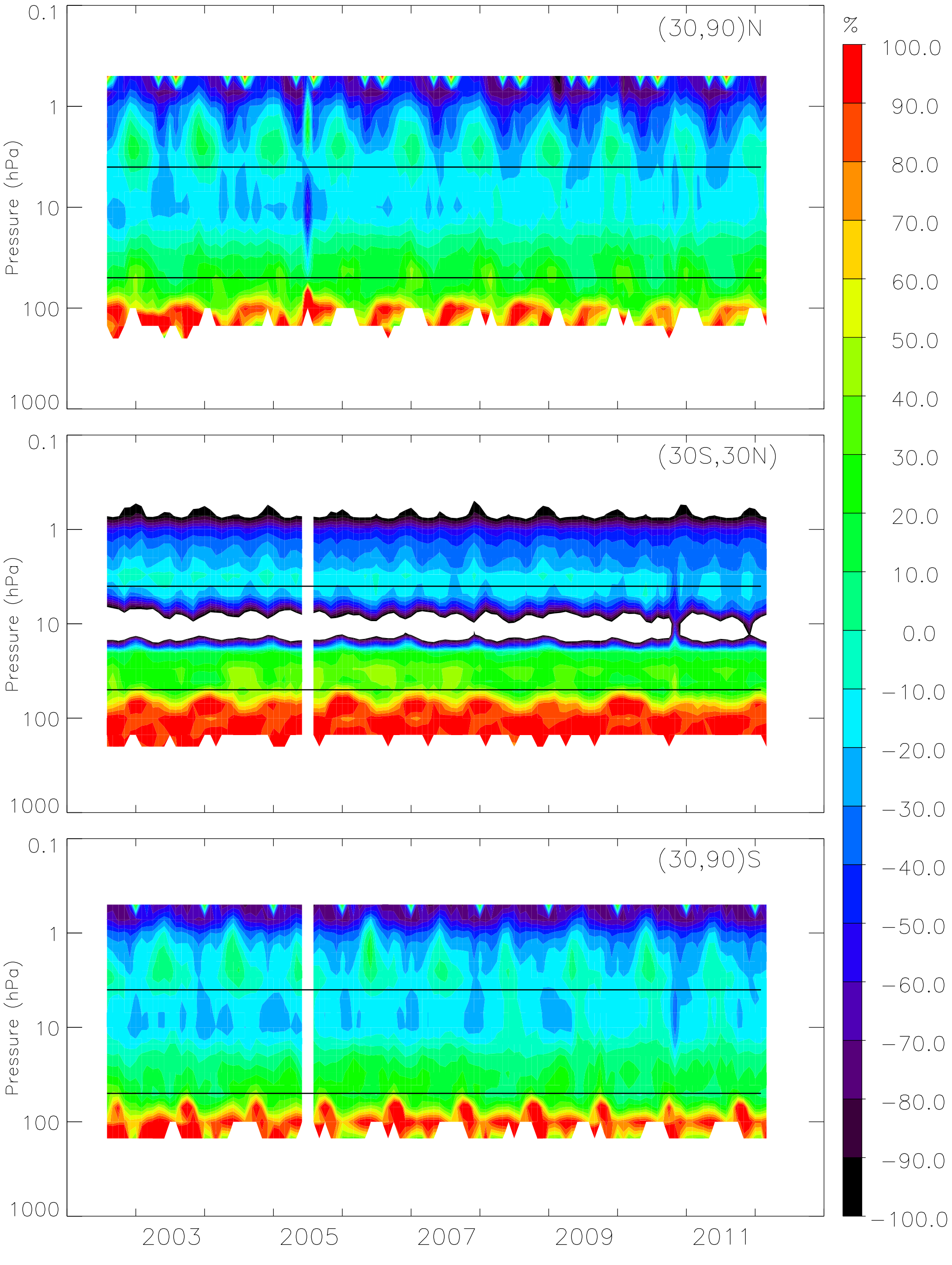

Figure 12: Like in figure 11, but data are in percentage.

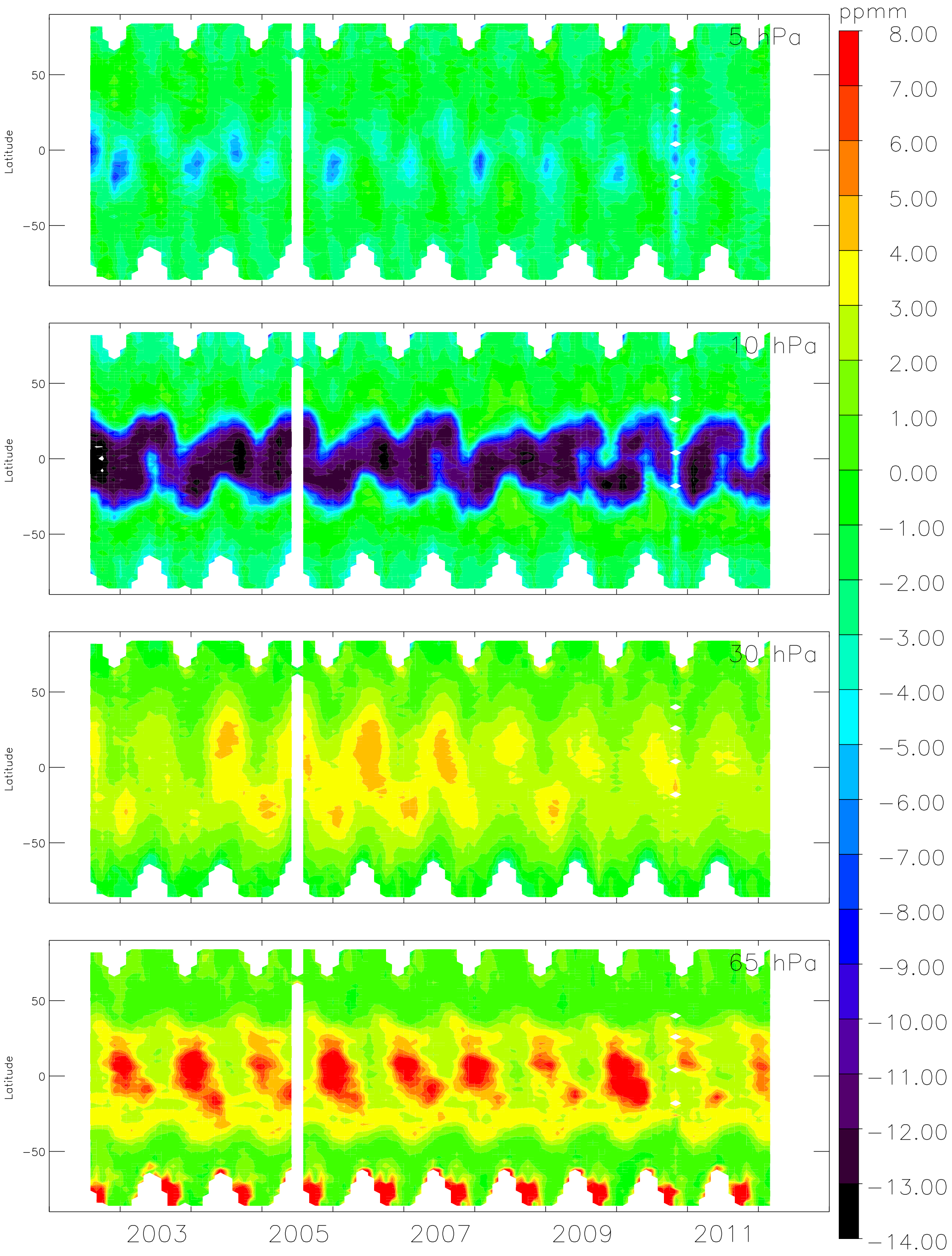

Figure 13: Latitude-time cross-sections of the zonal mean difference between MIPAS ozone profiles and co-located ERA-Interim analyses at four pressure levels in the stratosphere: (from top to bottom) 5, 10, 30, 65 hPa. Data are in mass mixing ratio (ppmm).

6 One year assimilation of NRT MIPAS ozone profiles

Dragani (2012) reported on preliminary results from an assimilation study of NRT MIPAS ozone profiles in the ECMWF weather forecasting system. The results from that study clearly showed that till the end of the ENVISAT mission MIPAS provided high quality observations that could substantially improve the distribution of the stratospheric ozone analyses. For that study, two sets of experiments were performed. In the first set, MIPAS ozone profiles were assimilated in the ECMWF data assimilation system run at two different resolutions (T255 and T799) to assess the impact of the model resolution and indirectly the representivity error that comes from not accounting for the observation horizontal smoothing. The results showed that although the model resolution is an important factor - the higher the model resolution the worse the agreement of the ozone analyses with independent observations - the improvements to the vertical distribution of the ozone analyses produced by the MIPAS assimilation were by far more important and substantial. The second set of experiments was performed 1) to assess the potential synergy of MIPAS ozone profiles with ozone-sensitive radiances in the IR spectral range (that started operationally with cycle CY37R3 on 15 Novemebr 2011), and 2) to identify the set-up for the ozone bias correction. The results showed a very good synergy between the IR ozone channels, MIPAS and the UV ozone products. The analysis of both sets of experiments neither showed negative impact on the fit to other observations and their bias corrections, nor a degradation on the ECMWF forecasts scores. Based on these results, the assimilation of the NRT MIPAS ozone profiles was restarted on 8 December 2011.

We now report on the final test that was performed using a one-year long record of NRT MIPAS ozone profiles to assess the long term and seasonal impact of these observations. This is an important step towards a potential assimilation of the MIPAS reprocessed ozone profiles in the forthcoming reanalysis production that will replace the current ERA-Interim reanalyses. The results presented below were run at a T511 horizontal truncation and on the standard 91 vertical levels during the period from March 2011 to February 2012. The results are presented in terms of seasonal averages for the periods March-April-May (MAM), June-July-August (JJA), September-October-November (SON) 2011, and December 2011-January-February 2012 (DJF).

To assess the impact of assimilating MIPAS ozone profiles in the ECMWF system we have compared the ozone analyses obtained from two experiments - a control that had the same set-up and assimilated the same observations as the operational weather forecasting system, but used a lower horizontal resolution, and an experiment that also assimilated MIPAS ozone profiles - against MLS and sonde ozone profiles. These ozone profiles are not assimilated in the two experiments and so the comparisons provide an independent validation of the quality of the analyses.

Figure 14 shows the mean differences between MLS and the analyses from the control (left) and MIPAS experiment (right), respectively. Each panel refers to a different season as discussed above. At all latitudes and seasons, the assimilation of MIPAS ozone profiles improves the agreement between the corresponding analyses and the MLS ozone profiles. Furthermore, small reductions in the standard deviations of the MLS minus collocated analyses can also be seen when MIPAS observations are actively used (figure 15).

Table 1 provides a summary table of the minimum, maximum and global mean values of the MLS minus analysis differences and their standard deviations plotted in figures 14 and 15, respectively.

Comparisons with ozone sondes retrieved from the World Ozone and UV Data Centre (WOUDC) archive are presented in figures 16 to 20. The root mean square (RMS) fit to the ozone sondes are averaged over five latitudinal bands, the tropics, the NH and SH midlatitudes, and the NH and SH high latitudes and for the four seasons as above. When the MIPAS ozone profiles are assimilated, the ozone analyses show an improved agreement with ozone sondes in the troposphere and at most stratospheric levels although in some cases the number of available profiles is likely to be too low to make the results statistically significant. Particularly noticeable is the improved fit at mid and high latitudes in the both hemispheres (figures 16 to 19) at most levels in the stratosphere and upper troposphere. In the tropics (figure 20), the assimilation of MIPAS ozone profiles helps improving the characterisation of the ozone analyses in the region of the ozone maximum.

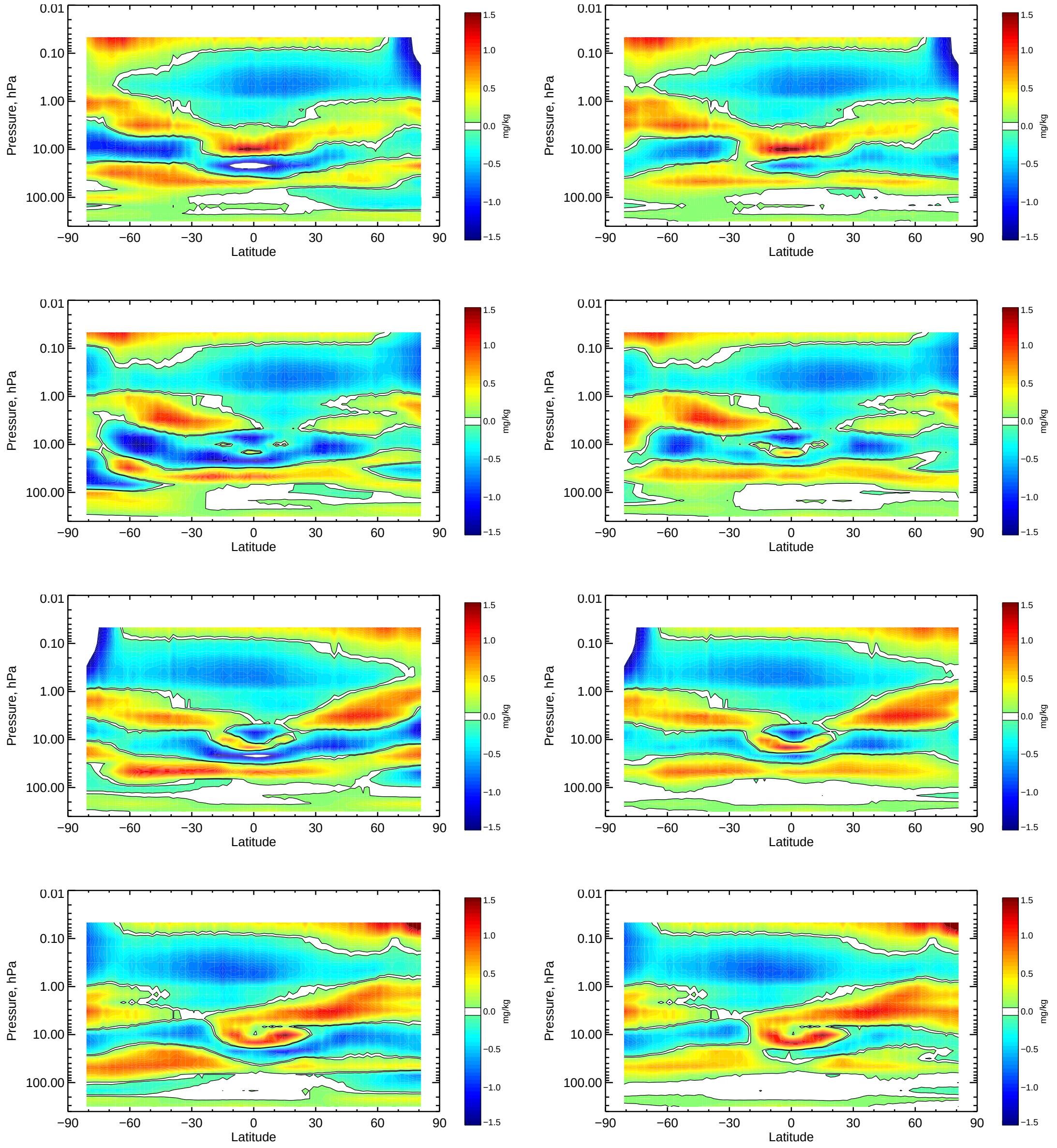

Figure 14: Seasonal mean difference between the (v2.2) MLS ozone profiles and the co-located ozone analyses computed for CTRL (left panels) and Exp/Mipas (right panels) averaged over (from top to bottom) March-April-May (MAM), June-July-August (JJA), September-October-November (SON) 2011, and December 2011-January-February 2012 (DJF). Data are in mass mixing ratio.

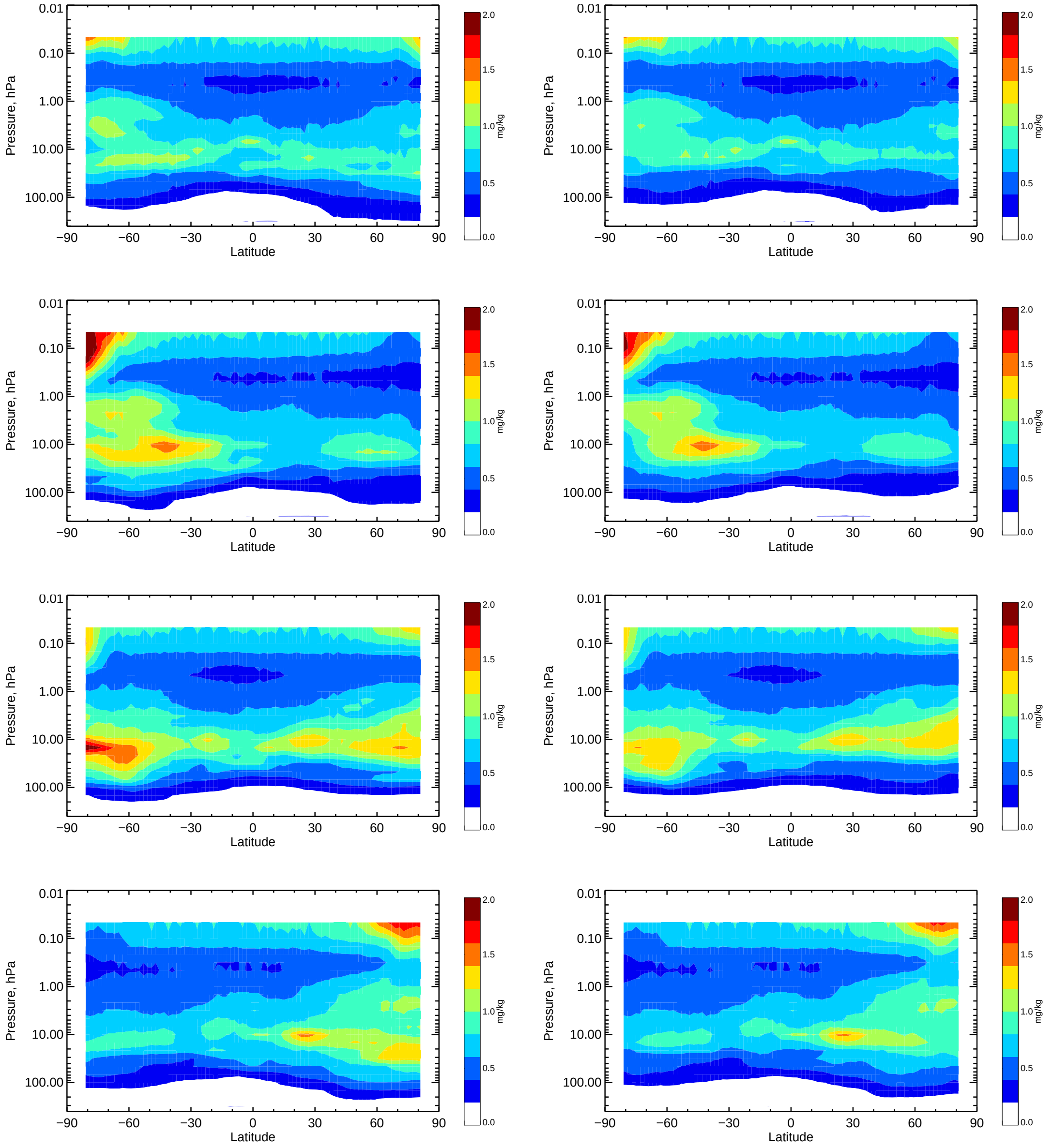

Figure 15: Like in figure 14, but for the standard deviation of the MLS minus ozone analysis differences.

	Residuals			Standard deviation		
Experiment	**Min**	**Mean**	**Max**	**Min**	**Mean**	**Max**
CTRL	-2.268	-0.016	1.770	0.054	0.584	1.519
Exp/MIPAS	-2.077	0.007	1.855	0.053	0.555	1.422
CTRL	-1.534	-0.077	1.289	0.048	0.616	2.392
Exp/MIPAS	-1.268	-0.019	1.292	0.047	0.584	1.897
CTRL	-2.433	-0.030	1.264	0.058	0.658	1.987
Exp/MIPAS	-2.394	$-1.5\ 10^{-4}$	1.529	0.061	0.629	1.422
CTRL	-1.105	0.003	2.017	0.056	0.606	1.779
Exp/MIPAS	-0.918	0.032	2.024	0.056	0.575	1.719

Table 1: Summary of the minimum, maximum, and global mean values of the MLS minus analysis residuals and their standard deviations computed for the two experiments (CTRL and Exp/MIPAS) and the four periods displayed in figures 14 and 15.

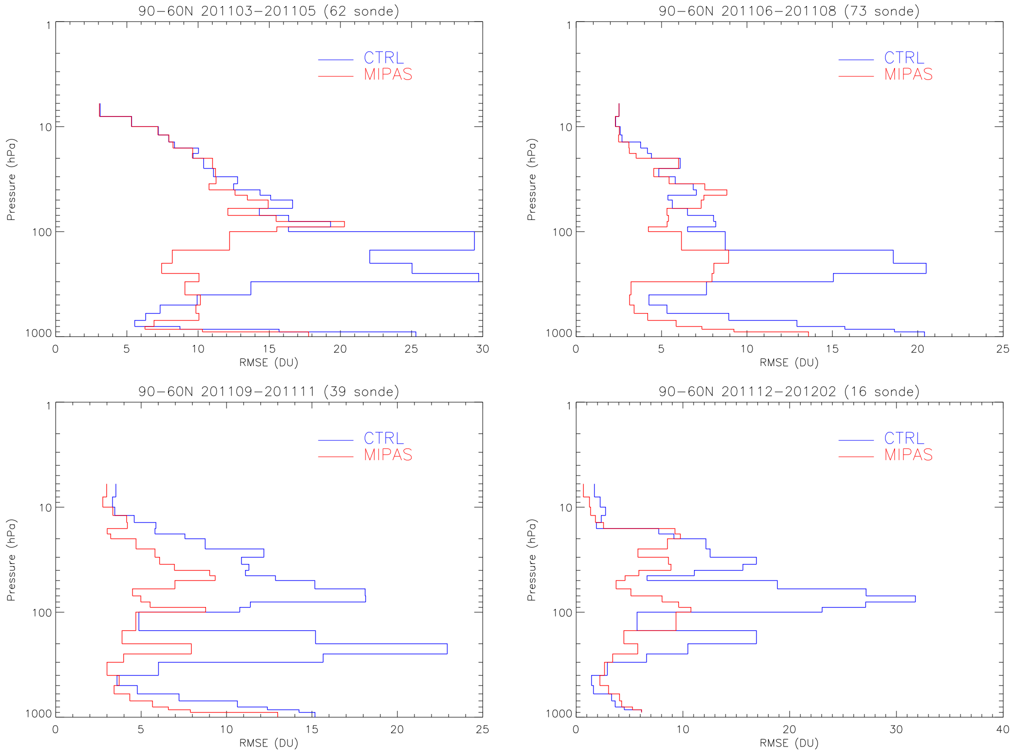

Figure 16: RMS fit of the MIPAS (red lines), and CTRL (blue lines) mean ozone analyses to ozone sondes averaged over the high latitudes in the northern hemisphere. The comparisons were computed for the four seasons, as follows: March-May 2011 (top left), June-August 2011 (top right), September-November 2011 (bottom left) and December 2011- February 2012 (bottom right). The number of ascents included in the average can be found in the title of each panel. Data are in DU.

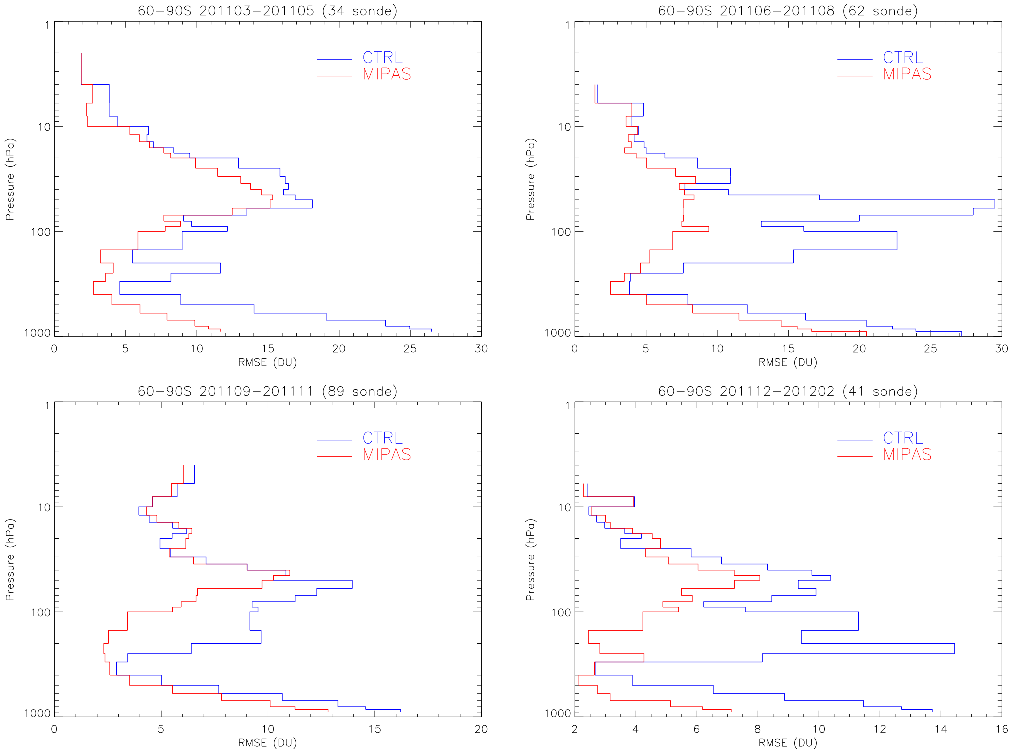

Figure 17: Like in figure 16, but for the high latitudes in the southern hemisphere.

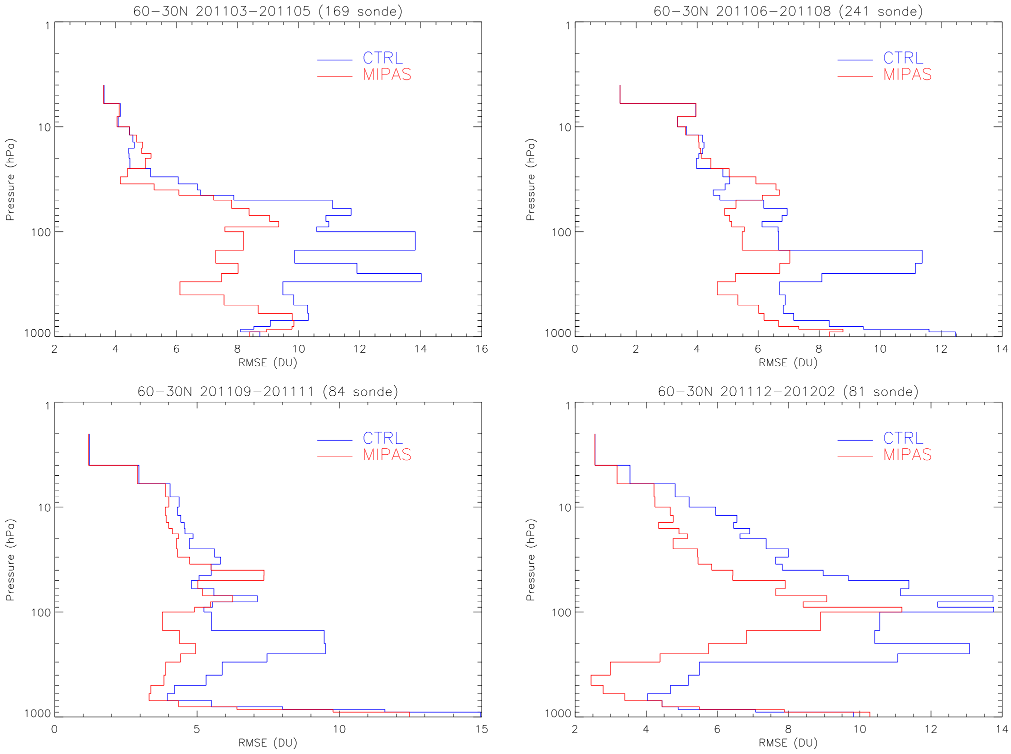

Figure 18: Like in figure 16, but for the midlatitudes in the northern hemisphere.

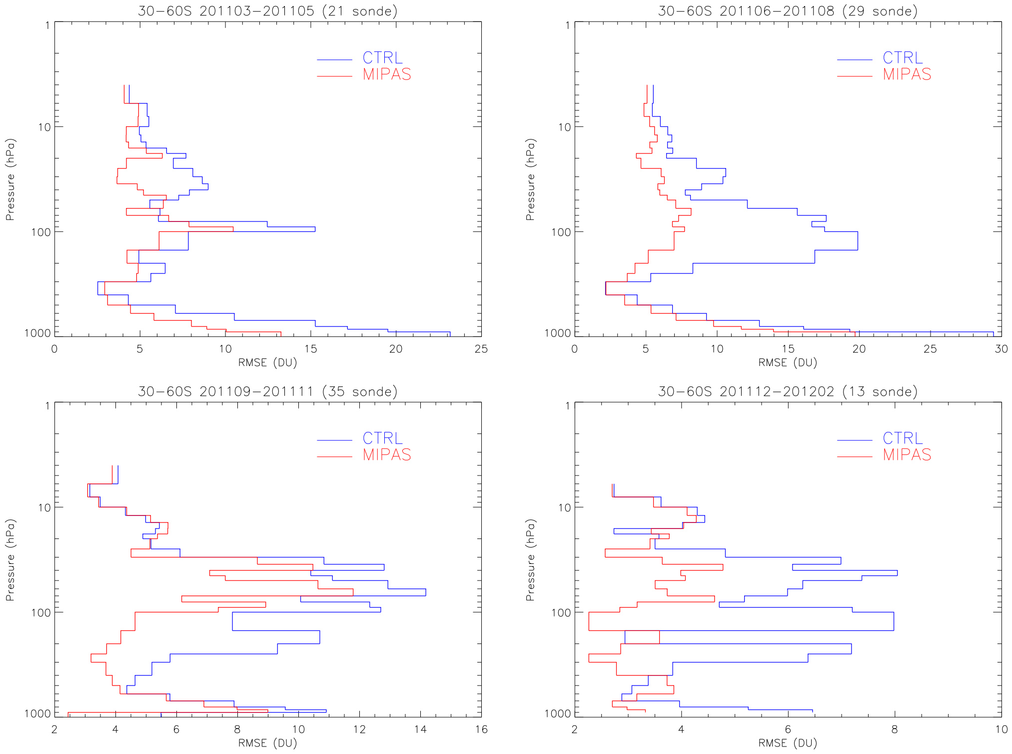

Figure 19: Like in figure 16, but for the midlatitudes in the southern hemisphere.

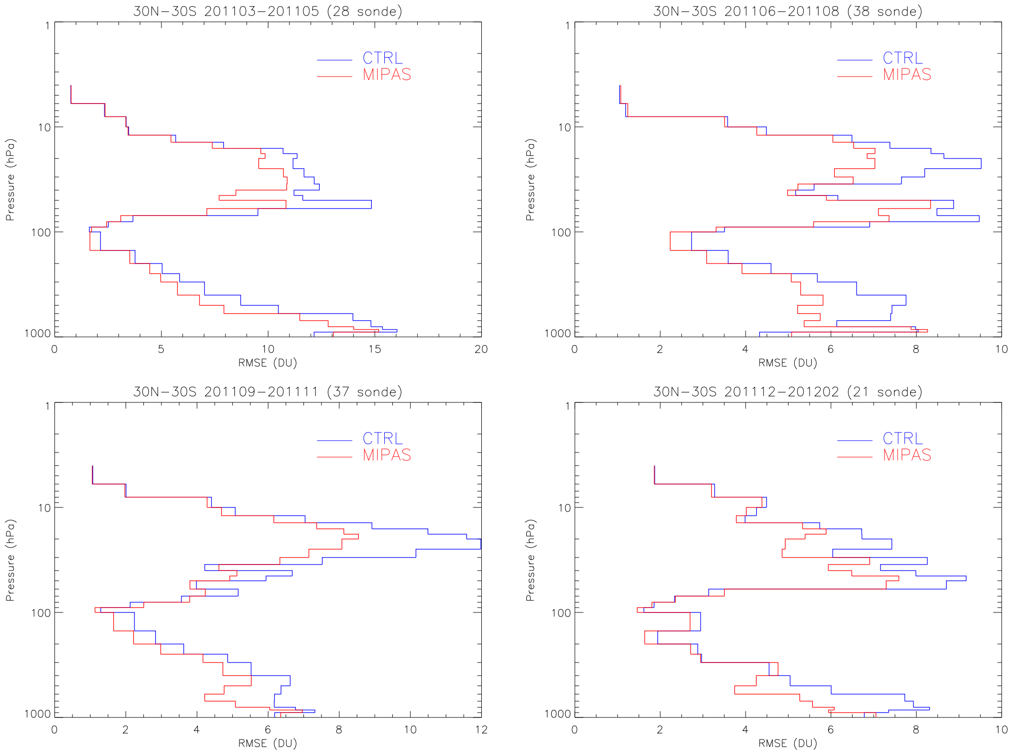

Figure 20: Like in figure 16, but for the tropics.

7 Conclusions

Under the ESA contract 21519/08/I-OL (Technical support for global validation of Envisat data products), ECMWF routinely monitored NRT products retrieved from the three atmospheric instruments on board ENVISAT within its operational assimilation system. These products consisted of ozone, temperature, and water vapour profiles from MIPAS and GOMOS, as well as total column ozone retrieved from the SCIAMACHY nadir measurements. With the sudden lost of the ENVISAT satellite on 8 April 2012, the ECMWF activity was readdressed to validate the newly available reprocessed datasets from these instruments against the latest ECMWF reanalysis production, ERA-Interim. The validation activity focussed on the ozone, temperature, and water vapour profiles reprocessed from the almost ten-year measurements of the MIPAS instrument, and ozone profiles retrieved from the limb measurements of SCIAMACHY. The reprocessed total column ozone retrievals from the SCIAMACHY nadir observations were not assessed against the ERA-Interim reanalyses as the NRT version of those retrievals were assimilated in the ERA-Interim production, and so a comparison could not provide an independent validation. The quality of the GOMOS reprocessed dataset could not be assessed as it was publicly released in its final form only in the second half of December 2012.

The reprocessed MIPAS ozone profiles exhibit higher ozone values than their ERA-Interim ozone equivalent at most levels, latitudes, and seasons. These results are in line with the outcome of the VALID study that showed MIPAS ozone profiles have up to 8% higher ozone concentrations than collocated lidar measurements. In the comparisons with ERA-Interim, the largest differences are found in the tropics in the region of the ozone mixing ratio maximum between 10 and 20 hPa, where MIPAS ozone values are on average 1 ppmm higher than their ERA-Interim equivalent. At pressure levels smaller than 15 hPa, the MIPAS minus ERA-Interim differences are typically within ±10%. In the lower stratosphere these differences are positive and normally larger, particularly in the tropics where they can reach values as large as +30%.

MIPAS temperature profiles are colder than their ERA-Interim temperature equivalent at all latitudes and seasons in the UTLS region and often in the lower stratosphere at mid and high latitudes, where the differences are up to about 1K. In the tropical lower stratosphere MIPAS exhibits higher temperature values than ERA-Interim, with differences of up to about 2K (about 1%). At all latitudes and seasons in the upper stratosphere, the temperature differences are normally positive (the MIPAS temperatures are higher than the ERA-Interim temperatures) with differences of 4-5K. Above the stratopause, this behaviour is inverted with MIPAS being up to 5K colder than ERA-Interim. Arguably the quality of the ERA-Interim temperature analyses is lower at these levels than in the troposphere and lower stratosphere, because the amount of available observations to constrain the analyses decrease substantially, as does the number of observations used to anchor the bias correction. In the upper troposphere, the MIPAS minus ERA-Interim temperature residuals are also large and up to -5K in places. This is most likely due to large bias in the MIPAS data. Although MIPAS observations extend down to 6 km altitude, they are optimized for the study of the stratosphere. The standard deviation of the seasonal mean differences are generally about 2K at most levels and latitudes, as well as seasons.

The comparison between the MIPAS water vapour and their ERA-Interim equivalent can only provide an indication of the quality of this dataset. That is because while MIPAS observations are optimized for the study of the stratosphere, and they normally show large biases in the upper troposphere, the ERA-Interim water vapour analyses may be better constrained in the troposphere than in the stratosphere. The humidity scheme used in ERA-Interim does not allow the observations to generate increments in the stratosphere. This is achieved by imposing very small humidity background errors in the stratosphere. Therefore, the vertical range over which both MIPAS and the ERA-Interim water vapour datasets are reliable and thus comparable is limited to a layer across the tropopause. In this layer, the residuals between MIPAS and ERA-Interim water vapour are normally within ±10%. In the upper troposphere between 300 and 150 hPa, the water vapour residuals are negative and tipically about 30 to 50%. In this region, the standard deviation of the departures are also very large, larger than 100% in places. Althogh the quality of the ERA-Interim water vapour analyses is questionable in the mid and upper stratosphere, the comparisons at these levels show a discontinuity after the MIPAS instrumental problem of 2004, which would suggest an impact of the spectral and integration time changes to the MIPAS settings on this variable.

Comparisons between the SCIAMACHY limb ozone profiles and collocated ERA-Interim ozone analyses in the range where the observations should be used (typically between 20 and 40 km according to the data disclaimer) show residuals within ±20% in the extra-tropics. Here, the residuals are normally negative (positive) in the upper (lower) stratosphere indicating higher (lower) ozone values in the reanalyses than in SCIAMACHY. In the tropics, large residuals are found in the region of the ozone maximum mixing ratio at 10hPa. Such differences are often larger than 100%. These large negative differences (up to -9 ppmm) are in clear contrast with the comparisons between MIPAS ozone profiles and the collocated ERA-Interim ozone analyses that showed instead positive residuals at 10 hPa up to about +3ppmm, as well as with comparisons with a number of other datasets (MLS, SAGE, HALOE, sondes) presented by Dragani (2010, 2011). An initial validation of the version 5.01 ozone profiles found ozone biases in the tropics as large as 23% when compared with in-situ data. However, these differences where localised around 18 km, roughly 75hPa rather than at 10hPa. Therefore, the reason for such a discrepancy is not clear. Two hypotheses were made that could have led to this result. One hypothesis is that these differences could partly be due to the SCIAMACHY data being used as volume mixing ratio instead of number density profile information. The convertion of the number density profile into volume mixing ratio profile requires additional information about the pressure and temperature distributions, and these are not fully provided in the product, but are taken from the McLinden climatology. Furthermore, it seems that the SCIAMACHY limb retrievals are computed without prior correction for tangent height errors in the Level 1b-2 processing step. This could also have introduced errors in the vertical coordinate that is used when deriving the observation equivalent from the ERA-Interim ozone analyses.

In addition to the ten-year validation of the reprocessed datasets, a one-year assimilation study of the near real time ozone profiles retrieved from MIPAS was also performed. The study is important to quantify the long term impact of assimilating these observations in the ECMWF system that could be used as an initial assessment in preparation for the forthcoming reanalysis production that will replace the current ERA-Interim reanalysis. The period under consideration was March 2011 to February 2012. Two experiments were run using a lower horizontal resolution version of the ECMWF weather forecasting system. A control experiment was run as a baseline and made use of all data used in the ECMWF high resolution system; a perturbed experiment also assimilated the MIPAS ozone profiles. The impact of MIPAS was assessed by comparing the ozone analyses from these two experiments against independent, unassimilated ozone data from ozone sondes and the MLS instrument. The assimilation of MIPAS ozone profiles was seen to improve the level of agreement of the ozone analyses with the independent datasets. At mid and high latitudes in both hemispheres, improvements were found at most levels in the upper troposphere and stratosphere. In the tropics, they were limited to the region of the ozone maximum. It is known that, although the tropical vertical distribution of the ozone analyses show well localised features (e.g. the ozone maximum peaks at the right vertical levels), the actual values can be slightly underestimated. Based on these results, it is concluded that the MIPAS ozone profiles provide valuable information to constrain the vertical distribution of the ozone analyses both in the stratosphere and in the upper troposphere and therefore the assimilation of the corresponding reprocessed dataset should be considered in the forthcoming ECMWF reanalysis production.

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