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3 On the quality of the ERA-Interim ozone reanalyses

Part II Comparisons with satellite data

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Abstract

This is the second of two companion papers presenting an assessment of the quality of the ERA-Interim ozone reanalyses by comparisons with independent observations, during the period January 1989 to December 2008. Ozone profiles from SAGE, HALOE, UARS and Aura MLS, POAM II and III were used to validate the three-dimensional ERA-Interim ozone analyses. Total column ozone (TCO) from OMI and a global mean TCO reference were used to assess the quality of the TCO product. The ERA-Interim TCO is typically within ±5DU (about ±2%) from the TCO reference, while showing up to 2% lower values than OMI TCO between 50°S-50°N. Comparisons with SAGE, HALOE and MLS ozone profiles showed some degrees of consistency in the results. The ERA-Interim analyses at and above 10hPa were typically within ±10% from SAGE and HALOE, and within ±5% from MLS. Around 30hPa, positive analysis departures up to +25% and up to +35% were found before January 1996 in the cases of SAGE and of HALOE and MLS, respectively. With the active assimilation of GOME ozone profiles (January 1996 through December 2002), the level of agreement typically improved leading to residuals mostly within ±10%. Positive departures up to 20% were found in the lower stratosphere (around 70hPa), except in the tropics during the GOME ozone assimilation period when these residuals were within -5 and +10%. The comparisons at high latitudes with POAM data showed discrepancies larger than 50% at and above 10hPa, and typically within ±20% below. The analysis departures showed trends typically within ±0.5%/year. When statistically significant, these changes were normally associated to an improved agreement with time between the ERA-Interim ozone analyses and the independent data. The comparisons also showed higher quality of the ERA-Interim ozone analyses compared with the ERA-40 ones, particularly due to the assimilation of GOME ozone profiles.

1 Introduction

After completing two major reanalysis projects, ERA-15 (Gibson *et al.*, 1997), and ERA-40 (Uppala *et al.*, 2005), the European Centre for Medium-Range Weather Forecasts (ECMWF) is currently producing a new global reanalysis. This latest effort, referred to as ERA-Interim (Dee and Uppala, 2009), focusses on the period since January 1989, and extends the temporal coverage beyond the ERA-40 availability. The main reasons for producing a reanalysis over such a relatively short period were to improve the exploitation of the enormous amount of available data, particularly from satellite instruments, and to have an improved baseline for the future reanalysis production by using an up-to-date stable version of the ECMWF operational suite which included several improvements compared with the ERA-40 one. For example, in addition to improved model physics and parameterizations, the ERA-Interim data assimilation system was upgraded to a four-dimensional variational data assimilation scheme (4D-Var), as opposite to the 3D-Var scheme used in ERA-40, and it made use of a variational bias correction scheme (VarBC) for satellite radiances, that automatically detects and corrects for observation biases.

Ozone, both in the form of three-dimensional field and integrated columns, is one of the fields routinely produced by ERA-Interim. Dragani (2010) discussed the quality of the ERA-Interim ozone reanalyses by comparison with ground-based ozone measurements during the twenty year period from January 1989 to December 2008. There, comparisons of the ERA-Interim TCO analyses with ground-based Dobson measurements at four locations, representing different latitudinal situations, showed a good level of agreement. The residuals were typically within ±5% at midlatitudes in the NH and in the tropics, and within ±10% at high latitudes. The comparisons of the ozone sondes with the three-dimensional ERA-Interim (and ERA-40) ozone analyses showed a dependence on the season, latitude, as well as on the period accounted for as a consequence of the varying ozone observing system actively used. In particular, they demonstrated that the ERA-Interim ozone product benefitted from the assimilation of GOME ozone profiles (January 1996 - December 2002), particularly in the tropics. In the pre-GOME assimilation period, the residuals between the ozone sondes and their corresponding ERA-Interim ozone profiles were within ±10% in the tropics and at midlatitudes at most levels, and within ±20% at high latitudes. In the GOME and post-GOME assimilation periods, the level of agreement was within

±5% in the tropics and at high latitudes in summertime, and within ±10% at high latitudes in wintertime as well as at midlatitudes throughout the year. Dragani (2010) also showed large improvements in the fit of the ERA-Interim ozone reanalyses to in-situ data over ERA-40, especially in the tropics, where a reduction of the RMS error up to 40% in the lower stratosphere, and between 20 and 50% in the troposphere were shown.

The present paper, then, complements the study by Dragani (2010) by assessing the quality of the ERA-Interim ozone reanalyses against ozone retrievals (profiles and total columns) from a number of satellite instruments during the twenty year period from January 1989 to December 2008. Indeed, it can also be considered as a long-term validation of the independent ozone observations with ozone analyses produced with an up-to-date and invariant NWP system. For completeness, the same comparisons were also produced for the ERA-40 ozone reanalyses, and the discussion will attempt to highlight the differences between these two reanalysis projects, and the improvements achieved in ERA-Interim. In addition, deficiencies in the system that still need to be addressed by the next reanalysis project, in order to provide more accurate ozone analyses, are identified. It is believed that the results and findings of this study could be beneficial, particularly in the context of climate change studies, or to address questions regarding the recovery of the ozone hole.

Dragani (2010) discussed the main characteristics of the ozone assimilation system used in ERA-Interim, focussing in particular on the differences with that used for the ERA-40 reanalysis, in section 2. The diagnostic tools and the matching criterion used in the current study are the same of those used in the companion paper, where a full description was provided in section 3, and hence is not repeated at this stage. The results from the validation of the ECMWF ozone reanalyses against those ozone data are presented in section 2. Section 3 investigates the possibility of trends in the agreement between the ERA-Interim ozone reanalyses and the independent observations as function of vertical level and latitudinal band. A discussion with conclusions and remarks follows in section 4. Here, the lessons learnt from analyzing ERA-Interim, and from comparing it to ERA-40 will be summarized. At last, a number of recommendations and potential improvements to be applied to future reanalysis will be discussed in section 5.

2 Comparisons with satellite ozone data

We continue the discussion on the assessment of the quality of the ERA-Interim ozone analyses for the period spanning from January 1989 till December 2008 that was started in Dragani (2010). Data from several satellite instruments, as well as a global mean TCO reference created *ad-hoc* from NASA's merged satellite dataset were used in the present study. As done in the companion paper, the following discussion will also investigate the relative differences in the fit of the ERA-40 and ERA-Interim ozone analyses to the independent data, and attempt to identify the reasons for those differences. Figure 1 schematically presents the time coverage of all the independent satellite observations used in this paper to validate and assess the quality of the ozone reanalyses. Most of the data used were in the form of ozone profiles, with the exception of OMI which provided total column ozone. Details on the data version and quality are provided below.

2.1 Comparisons with a TCO reference

Figure 2 shows the time series of the monthly mean ERA-Interim and ERA-40 TCO (in Dobson Units, DU) averaged over the latitudinal band between 50°N and 50°S, compared with a mean TCO reference over the same latitudinal band. This TCO reference was obtained as a five-year running monthly mean of NASA's merged satellite ozone data sets. These consist of monthly-mean zonal and gridded average products constructed by merging individual (Nimbus 7 and Earth Probe) TOMS and (Aura) OMI total ozone as well as (Nimbus 7, NOAA-9, 11, 16, and 17) SBUV and SBUV/2 TCO and ozone profiles. An external calibration adjustment

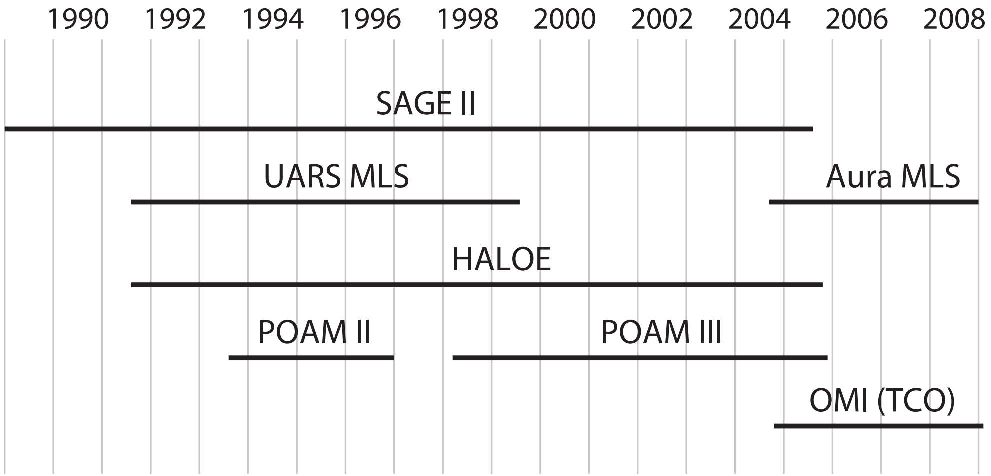

Figure 1: Time coverage of the remote sounding data used in this study. With the exception of the OMI instrument, which provided total column ozone, all the independent ozone products used in the validation were ozone profiles.

was applied to each satellite data set to account for and minimize any effect due to instrument changes, thus providing a continuous data set from the 70s (depending on the product) to September 2008. Data and more detailed information are available at http://acdb-ext.gsfc.nasa.gov/Data_services/merged/. The mean TCO reference used in this study made use of the gridded monthly mean TCO product available on 5° latitude by 10° longitude grid, averaged over the latitudinal band between 50°N and 50°S. It is noted that, because some of the data that NASA used to build the merged satellite dataset were also actively assimilated in ERA-Interim, the comparison does not necessary provide an independent validation. However, it is still useful to have a first indication of the quality of the reanalyzed product, but also to identify potential problems and drifts in the ERA-Interim time record due to the assimilation of other data. Figure 2 showed that in general the TCO reanalyses were in good agreement with that TCO reference with differences within ±5 Dobson Units (DU), less than 2% of the global mean value. The only exceptions were in the case of ERA-40 during 1989-1990, and in the case of ERA-Interim from April 2004 through 2007, when the reanalyses were outside the one standard deviation range around the reference mean, with differences of about 15DU from the reference. In both cases, the reduced agreement could be linked to the particular ozone data usage. In the case of ERA-40, this was due to the lack of ozone observations actively assimilated, so that the ozone analyses were completely unconstrained by observations. In the case of ERA-Interim, this was partly related to the assimilation of SCIAMACHY TCO retrieved at KNMI.

2.2 Comparisons with OMI-TOMS TCO

The Ozone Monitoring Instrument (OMI) (Levelt *et al.*, 2006a) was launched on the Aura platform in July 2004. This is a nadir sounder that is meant to continue the total column ozone measurements provided by instruments such as the Solar Backscatter Ultraviolet (SBUV) and Total Ozone Mapping Spectrometer (TOMS) (Levelt *et al.*, 2006b). In contrast with its predecessors, OMI has a higher spatial and spectral resolution. Two TCO products are available from OMI: One is retrieved using the version 8 TOMS-like algorithm (Bhartia and Wellemeyer, 2002; Balis *et al.*, 2007) referred to as OMI-TOMS product; and one is retrieved using the Differential Optical Absorption Spectroscopy (DOAS) algorithm (Veefkind *et al.*, 2006) referred to as OMI-DOAS. In ERA-Interim, the OMI-DOAS product was actively assimilated starting from 2008. In contrast, the OMI-TOMS data were used in the present paper for the independent validation. Although the two retrieval algorithms are different, e.g. in the treatment of clouds (Kroon *et al.*, 2008a), and because they used the same

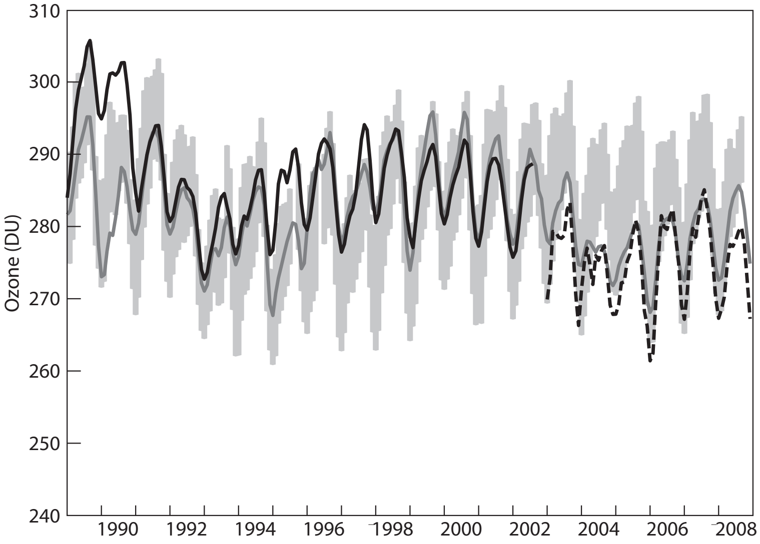

Figure 2: Time series of the monthly mean ERA-Interim TCO (grey solid line) and ERA-40 TCO (black solid line) averaged over the latitudinal band between 50N and 50S. The grey area limits the one standard deviation region around the monthly mean TCO obtained from the NASA merged satellite data set averaged over the same latitudinal band. The black dashed line covering the period from January 2003 to December 2008 refers to the mean SCIAMACHY TCO actively assimilated in ERA-Interim averaged between 50N and 50S.

radiance information it was decided not to consider the comparisons between ERA-Interim and OMI-TOMS data in 2008 as an independent validation.

Kroon *et al.* (2008b) presented a validation of the OMI TCO using remote and ground-based observations during the NASA's Aura Validation Experiment (AVE) campaigns. Their results showed that the agreement between OMI-TOMS TCO and ground based observations was generally within 1%, although the standard deviation was about 2-3%, presumably due to the combination of using a tropospheric climatology and taking measurements above clouds. Ziemke *et al.* (2006) referenced a personal communication with G. Labow regarding results from a validation study of OMI-TOMS TCO measurements against ground-based Dobson and NOAA-16 SBUV/2 data. These comparisons showed that OMI-TOMS TCO data are around 0.5% higher than the Dobson measurements and within 1% with respect to SBUV/2 for latitudes between 60° S and 60° N. In Balis *et al.* (2007), OMI-TOMS TCO retrievals were compared with Dobson and Brewer ground-based measurements for the period between August 2004 and September 2006. They found that on average the mean OMI-TOMS TCO residual with Dobson data was 0.57 ± 3.50%, and that from Brewer ground-based instruments (mainly located at midlatitudes in the NH between 30° N and 60° N) was -0.03 ± 3.50%.

Figure 3 shows the comparison between the area averaged monthly mean ERA-Interim TCO and the area averaged monthly mean OMI TCO from September 2004 to December 2008. Both the monthly mean ERA-Interim and monthly mean OMI TCO were averaged over the latitudinal band between 50N and 50S.Figure3 shows that the ERA-Interim ozone analyses have on average lower ozone values than measured by OMI, with residuals within -1.5 and +5 DU (within -0.5 and +1.8%). As mentioned above, the comparison shown here can not provide an independent validation during 2008 as the OMI-DOAS TCO was actively assimilated in ERA-Interim.

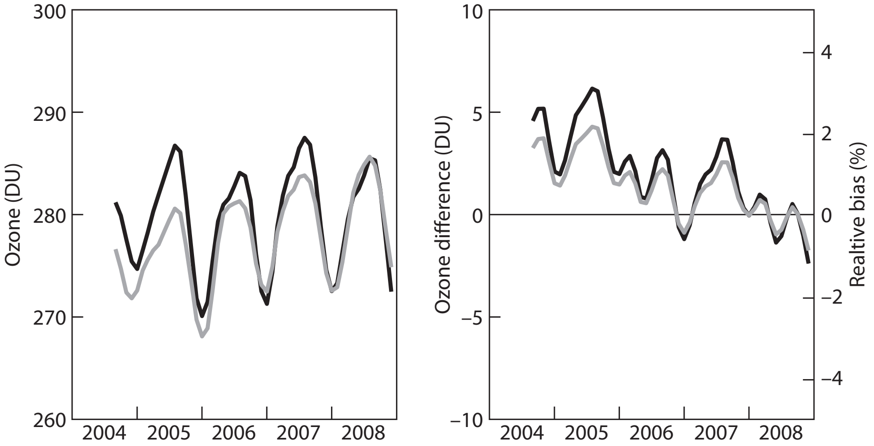

Figure 3: Time series of the area averaged monthly mean total column ozone (in DU) from Aura OMI (black) and the ECMWF ERA-Interim (grey) total column ozone reanalyses (left panel) and their absolute (black) and relative (grey) differences (right panel). Only the latitudinal range between 50N and 50S was considered in this comparison.

2.3 Comparisons with SAGE II ozone profiles

The SAGE II (Stratospheric Aerosol and Gas Experiment II) sensor was launched into a non-sun synchronous, 57 degree inclination orbit aboard the Earth Radiation Budget Satellite (ERBS) in October 1984 (Mauldin, 1985; Chu *et al.*, 1989; McCormick, 1987). The instrument provided self-calibrating, near global measurements of aerosol, ozone, water vapor and nitrogen dioxide until August 2005 covering a period of about 21 years. The instrument used the solar occultation technique to measure attenuated solar radiation through the Earth's limb in seven channels centered at wavelengths ranging from 0.385 to 1.02 micrometers. The SAGE instrument series has extensively been used to study and validate ozone long-term trends provided by global models (e.g. WMO, 2003). In the present paper, almost sixteen years of SAGE II (hereafter referred to as SAGE) version 6.2 ozone data profiles were used. Already in version 6.1 (e.g.Wang *et al.*, 2002), the agreement between SAGE ozone profiles and ozone sondes was found to be approximately 10% down to the tropopause. In particular, it was seen that SAGE tends to overestimate ozone between 15 and 20 km altitude and systematically underestimates ozone in the troposphere between 8 km and 2 km by approximately less than 5% and 30%, respectively. Above 18 km, the version 6.2 ozone product shows an agreement within 5% from correlative data (e.g. Nazaryan and McCormick, 2005). The main difference between the version 6.2 and the version 6.1 algorithms was an improvement of the water vapor product (Thomason *et al.*, 2004). For the most part, the ozone density profiles retrieved with the version 6.2 algorithm changed on the order of 0.5% from those retrieved with version 6.1 algorithm (NASA, 2003).

Figures 4 and 5 show the time series of the mean SAGE (grey areas representing the observation uncertainty range around the observation mean) and ERA-Interim (black lines) ozone reanalyses at four stratospheric pressure levels, and over three latitudinal bands (the northern hemisphere extra-tropics for latitudes northern than 30°N, the southern hemisphere extra-tropics for latitudes southern than 30°S, and the tropics between 30°N and 30°S. The pressure levels selected here are two levels above the ozone peak (5 and 10hPa), one in the region of the ozone maximum (about 30 hPa), and finally one level in the lower stratopshere below the maximum (about 70hPa). The grey curve in each panel refers to the mean relative residual computed as in equation 1 ofDragani (2010).

The comparisons in figure 4 show a general good agreement between SAGE and ERA-Interim at 5 and 10 hPa at all latitudinal bands, with differences generally within the observation standard deviation. The relative bias is generally within ±10% at all latitudinal bands and on both levels. The seasonal variability of the ozone field also seems well captured. Though the comparisons, especially at 5hPa in the NH, show an annual cycle in the residuals with maxima occurring in winter and minima occurring during the summer time.

At 30hPa (panels **a** to **c** in figure 5), the level of agreement is poorer than previously discussed. Here, ERA-Interim generally exhibits lower ozone values than measured by SAGE, particularly in the tropics (panel **b**), with relative differences of about 25-30% before January 1996, and apart from a few exception within ±10% afterwards. Part of these differences can certainly be explained by the fact that the ECMWF ozone system tends to underestimate the tropical ozone amount in the region of the ozone maximum (Dethof and Hólm, 2004), and partly related to the SAGE overestimated ozone values at these altitudes (Wang *et al.*, 2002). Despite the poorer agreement, the general seasonal variability of the ozone distribution observed by SAGE was reasonably captured in the reanalyses. From January 1996, the level of agreement between SAGE and ERA-Interim improves, particularly in the tropics. This coincided with the start of the assimilation of GOME ozone profiles.

Below the ozone peak (panels **d** to **f** in figure 5), the fit of the ERA-Interim ozone analyses to SAGE is good in the northern hemisphere extra-tropics (panel **f** in figure 5), with residuals being mainly within the observation standard deviation and relative differences being mainly within -10 and +20%. There are similarities in the seasonal variability. A sometimes poorer level of agreement was seen in the tropics and in the southern hemisphere extra-tropics, depending on the year. Overall, the relative differences between SAGE and ERA-Interim were generally positive and up to +40% in the SH extra-tropics and within -20 and +60% in the tropical band.

During the period GOME ozone profiles were actively assimilated (January 1996 to December 2002), the ERA-Interim fit to the SAGE data improved also in the lower stratosphere below the ozone maximum, particularly noticeable in the SH where the percentage departures were normally within -10 and +20%. It is also worthwhile noticing the good comparison during 2003 and the beginning of 2004 (most levels and latitudinal bands) that can instead be associated with the assimilation of the Michelson Interferometer of the Passive Atmospheric Sounding (MIPAS) ozone profiles. Dethof (2003) showed that the assimilation of MIPAS ozone profiles into the ECMWF system can substantially improve the quality of the ozone analyses.

Figure 6 shows the time series of the difference between the RMS of the SAGE ozone profiles minus the co-located ERA-Interim ozone profiles and that of SAGE minus the corresponding ERA-40 ozone profiles as function of pressure, and for three latitudinal bands (from top to bottom: the NH extra-tropics, the tropics, and the SH extra-tropics). The regions where the ERA-Interim ozone analyses fit the SAGE observations better than the corresponding ERA-40 are given by negative values and represented in the plot by the shaded areas. Contours over white areas show the regions where the ERA-40 ozone analyses fit the SAGE data better than the corresponding ERA-Interim ones. Because the ERA-40 production covered the period until August 2002, the plot does not span the whole period of the SAGE data availability. At all latitudinal bands, the ERA-Interim analyses compare better with SAGE then their ERA-40 equivalent in most of the lower stratosphere and upper troposphere (UTLS), typically below the ozone maximum peak (at pressure levels larger than 40hPa), but not at levels above, at least until December 1995. From January 1996 when the assimilation of GOME ozone profiles was activated, the representation of the ozone vertical distribution seemed improved in the ERA-Interim reanalysis, and in the region of the ozone peak even better than that provided by the ERA-40 reanalysis when compared to SAGE. Some problems still remained in the upper stratosphere, particularly in the SH extra-tropics.

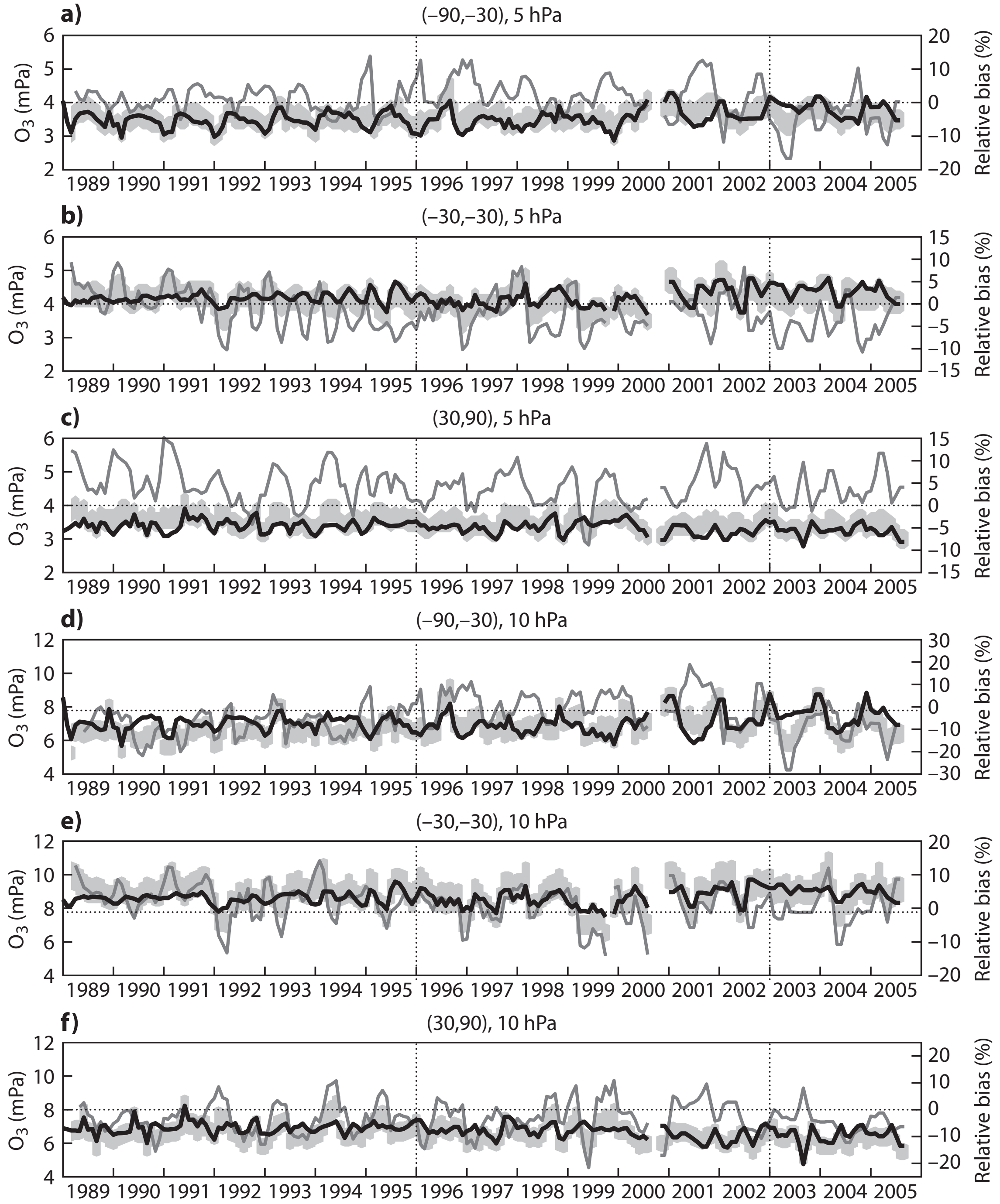

Figure 4: Comparisons between SAGE II ozone retrievals and the co-located ERA-Interim ozone reanalyses. The black lines show the time series of the area averaged monthly mean ERA-Interim ozone reanalyses (in mPa). The grey shading refers to the observation one standard deviation around the mean SAGE II time series. Only the SAGE II sun set events were considered. Panels a) to c) show the comparisons at 5hPa; panels d) to f) refer to the comparisons at 10hPa. Panels a) and d) refer to the comparisons in the SH extra-tropics ([30,90]S); panels b) and e) refer to the comparisons in the tropics ([30N,30S]); finally, panels c) and f) show the comparisons in the NH extra-tropics ([30,90]N). The ozone data are in mPa. The grey solid lines show the mean relative bias (SAGE II - ERA-Interim) limited within the right vertical axis range. The two vertical dashed lines delimit the period (Jan 1996 - Dec 2002) during which the GOME ozone profiles were actively assimilated in the ERA-Interim reanalyses.

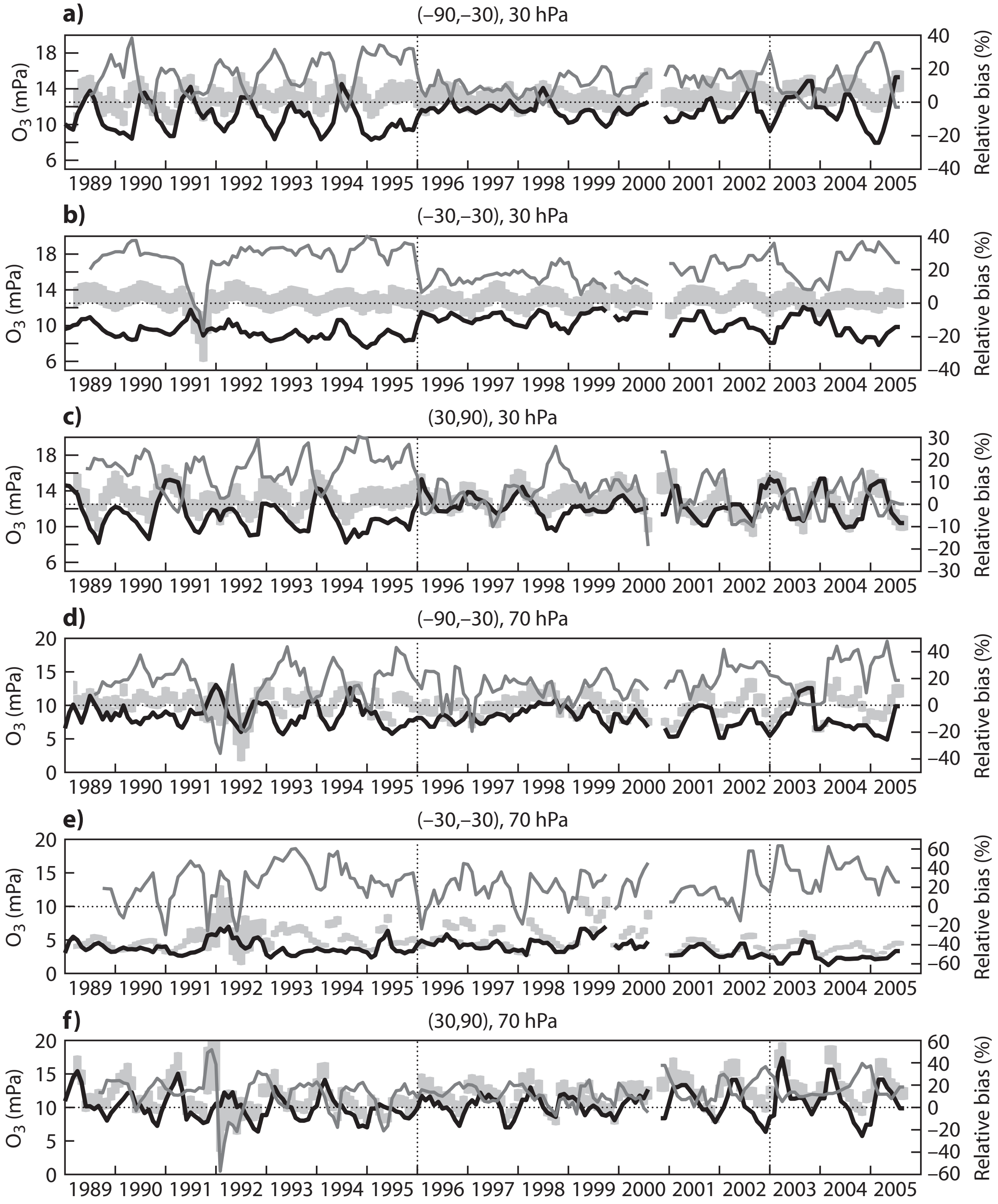

Figure 5: As in figure 4, but at 30 hPa (panels a) to c)) and 70hPa (panels d) to f)).

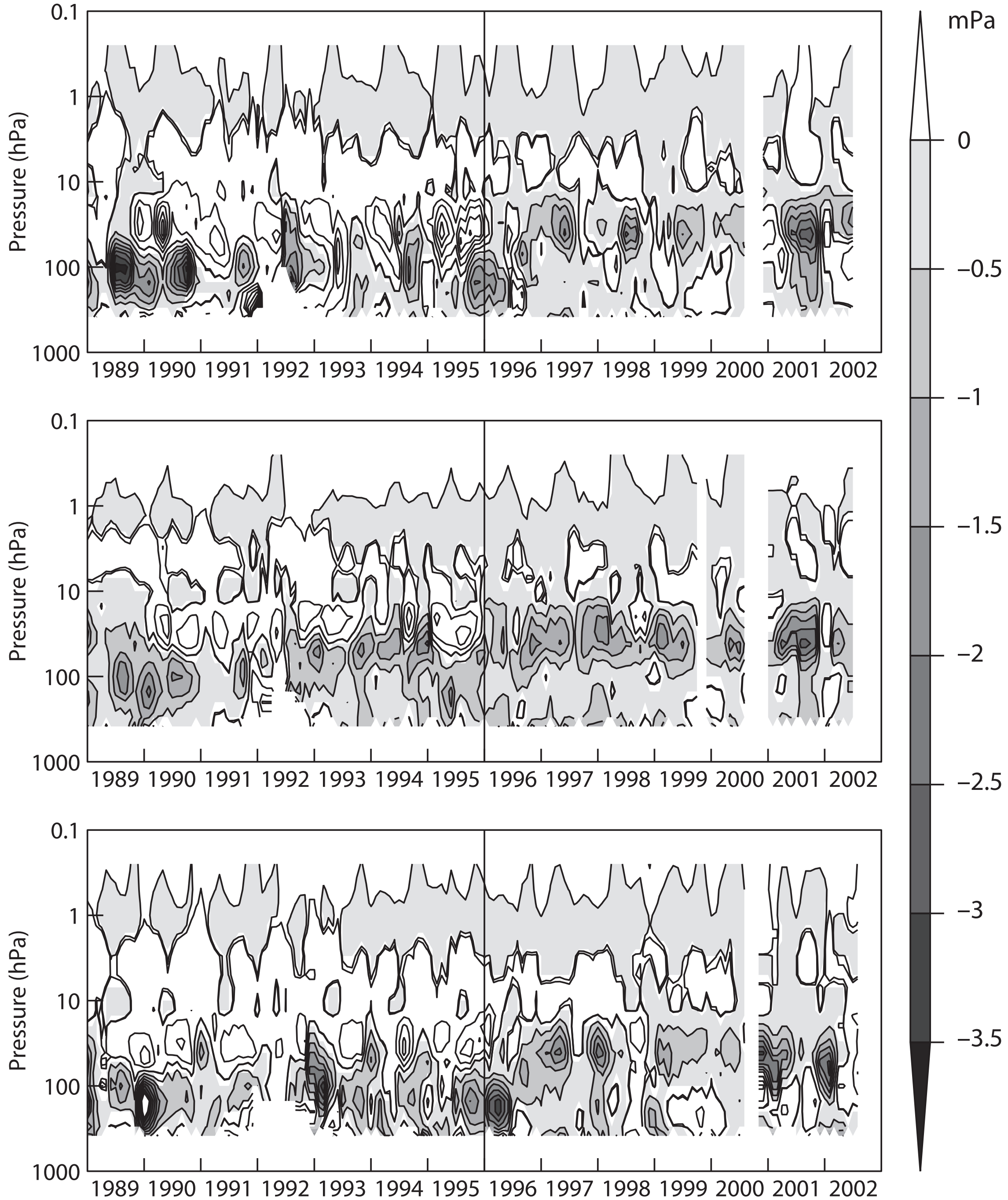

Figure 6: Time series of the difference between the RMS of (SAGE-ERA-Interim) and that of (SAGE-ERA-40) as function of pressure. The top panel shows the comparisons averaged over the NH extra-tropics ([30,90]N); the middle panel shows the comparisons averaged over the tropics ([30N,30S]); the bottom panel shows the comparisons averaged over the SH extra-tropics ([30,90]S). Negative values (shaded areas) mean a better fit of ERA-Interim ozone analyses to SAGE observations than those from ERA-40. Positive values (contour over white areas) mean a better fit of ERA-40 ozone analyses to SAGE observations than those from ERA-Interim. Data are in mPa, and increments are 0.5mPa. The vertical solid line delimits the period (Jan 1996 - Dec 2002) during which the GOME ozone profiles were actively assimilated in the ERA-Interim reanalysis.

2.4 Comparisons with HALOE ozone profiles

The HALogen Occultation Experiment (HALOE) sensor was launched onboard the NASA's Upper Atmosphere Research Satellite (UARS) spacecraft (Reber *et al.*, 1993) on 1991, with the objective to improve understanding of stratospheric ozone, especially ozone depletion due to chlorine chemistry. The instrument measured concentrations of several chemical species, including ozone. The latitudinal coverage was from 80°S to 80°N over the course of one year and included extensive observations of the Antarctic region during spring. The altitude range of the measurements extends from about 15 km to 60-130 km, depending on the species.

Several validation studies of the HALOE ozone profiles were published over the years and for the various versions of HALOE retrievals. Comparisons of version 18 (V18) HALOE ozone observations with ozone sondes showed an agreement of about 10% on average down to 10 hPa in the tropical and subtropical regions, as well as down to 200 hPa in the extratropics (Bhatt *et al.*, 1999). Low mean bias (within ±7%) was found between V18 HALOE and in-situ measurements from instruments aboard the NASA ER-2 aircraft (Lingenfelser *et al.*, 1999) during four different campaigns (AASE II, SPADE, ASHOE/MAESA, and STRAT) at ER-2 cruise altitudes between 50 and 70hPa. Here, we have used the level 3AT ozone profiles retrieved with the version 19 (V19) algorithm, which had a further correction scheme for cirrus clouds compared with the version 18 data used. However, little differences were found in the HALOE ozone retrieved with V18 and version 19 (V19) (Bhatt *et al.*, 1999). HALOE v19 retrievals were compared with the SAGE v6.0 data in Morris *et al.* (2002) and with the SAGE v6.1 data in Randall *et al.* (2003), respectively. Both studies found small systematic differences between 20 and 30 km, SAGE exhibiting higher values than HALOE. Randall *et al.* (2003) also found residuals within ±5% from 12 to 50 km, with increasing positive differences above 40 km up to ±11%. An agreement typically within ±5% was also found with version 2.2 Aura MLS ozone profiles, even though larger residuals normally up to 10% were seen at lower stratospheric levels (Froidevaux *et al.*, 2008).

Figures 7 and 8 show the comparisons between the V19 HALOE ozone retrievals and the co-located ERA-Interim ozone analyses at different pressure levels and averaged over the tropics and extra-tropics during the period of HALOE data availability. Similarly to the comparisons with SAGE, a good level of agreement was found between observations and co-located analyses at 4 and 10 hPa, with residuals generally within the observation standard deviation at all latitudes and over the entire period. At both vertical levels, the relative residuals show seasonal variations with values typically within ±5% in the tropics and within ±10% in the extra-tropics.

At 31 hPa, the HALOE observations usually exhibited higher ozone values than their ERA-Interim equivalent at all latitudes.The ozone seasonal variability in the reanalyses showed some differences with that observed by HALOE, both in terms of amplitude of the signal and occurrence, in particular in some cases the ozone minima and maxima seem to occur later in time than observed by HALOE. It should be noticed that on a annual basis the HALOE and ERA-Interim level of agreement was generally better during winter-spring than during summer-fall. Overall, some improvements were seen towards the end of the 90s, particularly from 1996 in the NH extra-tropics and from 1997 in the tropics and in the SH extra-tropics. The relative differences were typically up to +35% during the first period, then up to 10% in the NH from 1996 and up to 20% in the tropics and SH after 1997.

Also in the lower stratosphere (around 68 hPa) the HALOE observations showed higher valuer than their model equivalent, with relative differences generally up to +20%. The level of agreement is usually good in the tropics and in the NH extra-tropics, particularly after January 1996. The ozone seasonal variability is well represented in the NH, and in the tropics, but in the SH extra-tropics there are problems in capturing the amplitude of minima and maxima, particularly before 1997.

The comparisons of both ERA-Interim and ERA-40 with HALOE data in figure 9 show a sustantially improved fit of the ERA-Iterim analyses to the observations after January 1996, at all latitudes in the lower stratosphere.

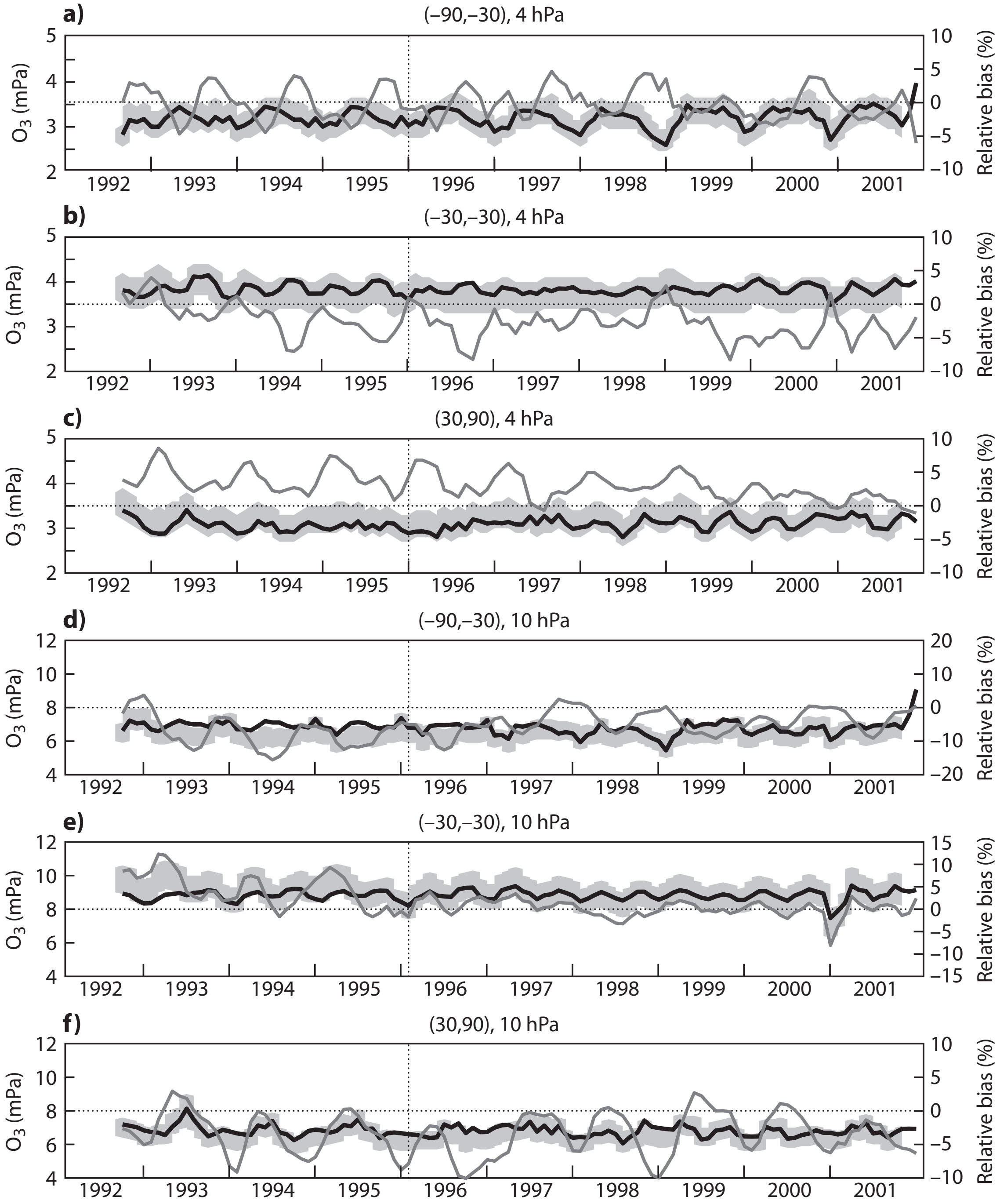

Figure 7: As in figure 4, but for HALOE at 4hPa (panels a) to c)) and 10hPa (panels d) to f)).

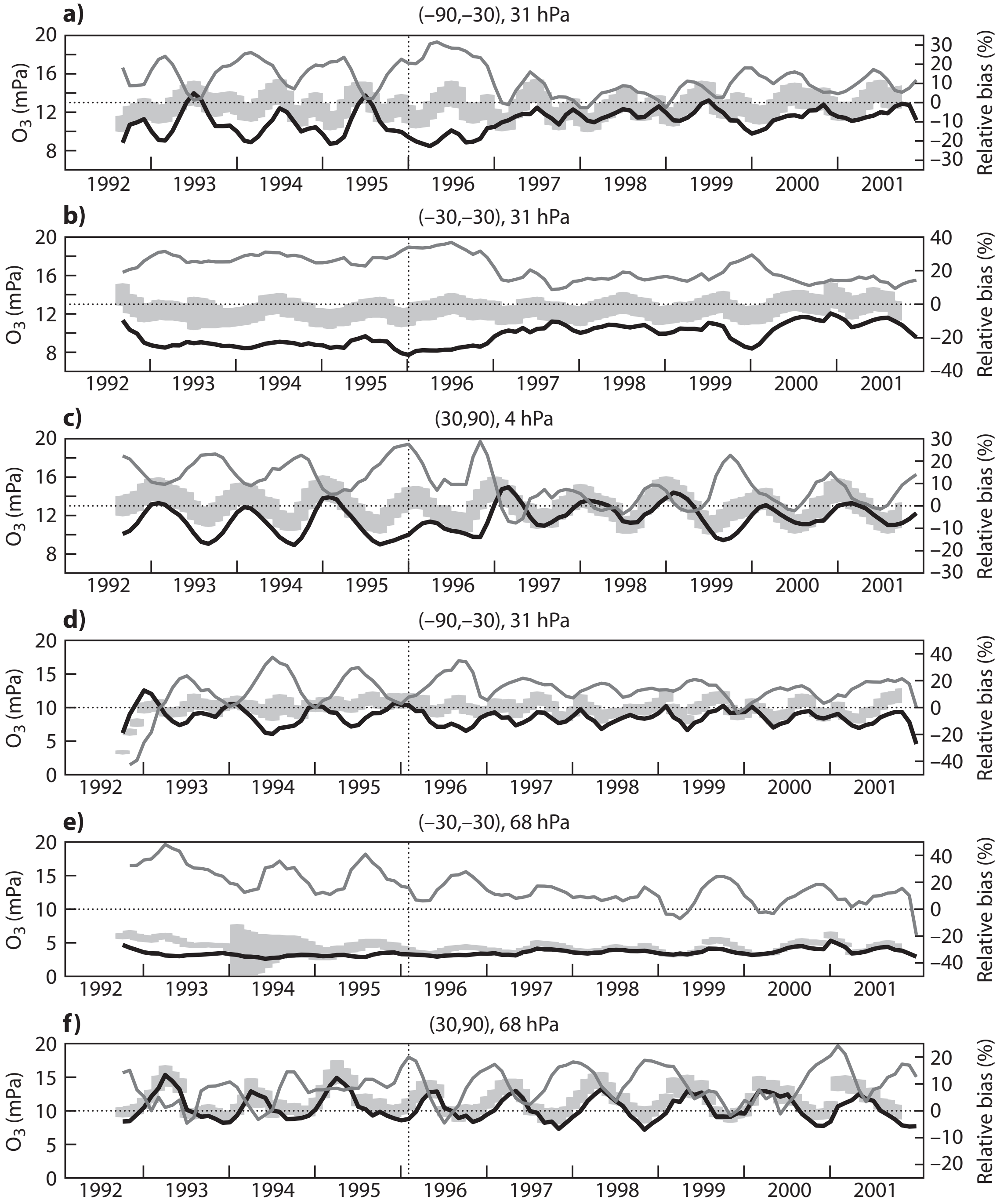

Figure 8: As in figure 7, but at 31hPa (panels a) to c)) and 68hPa (panels d) to f)).

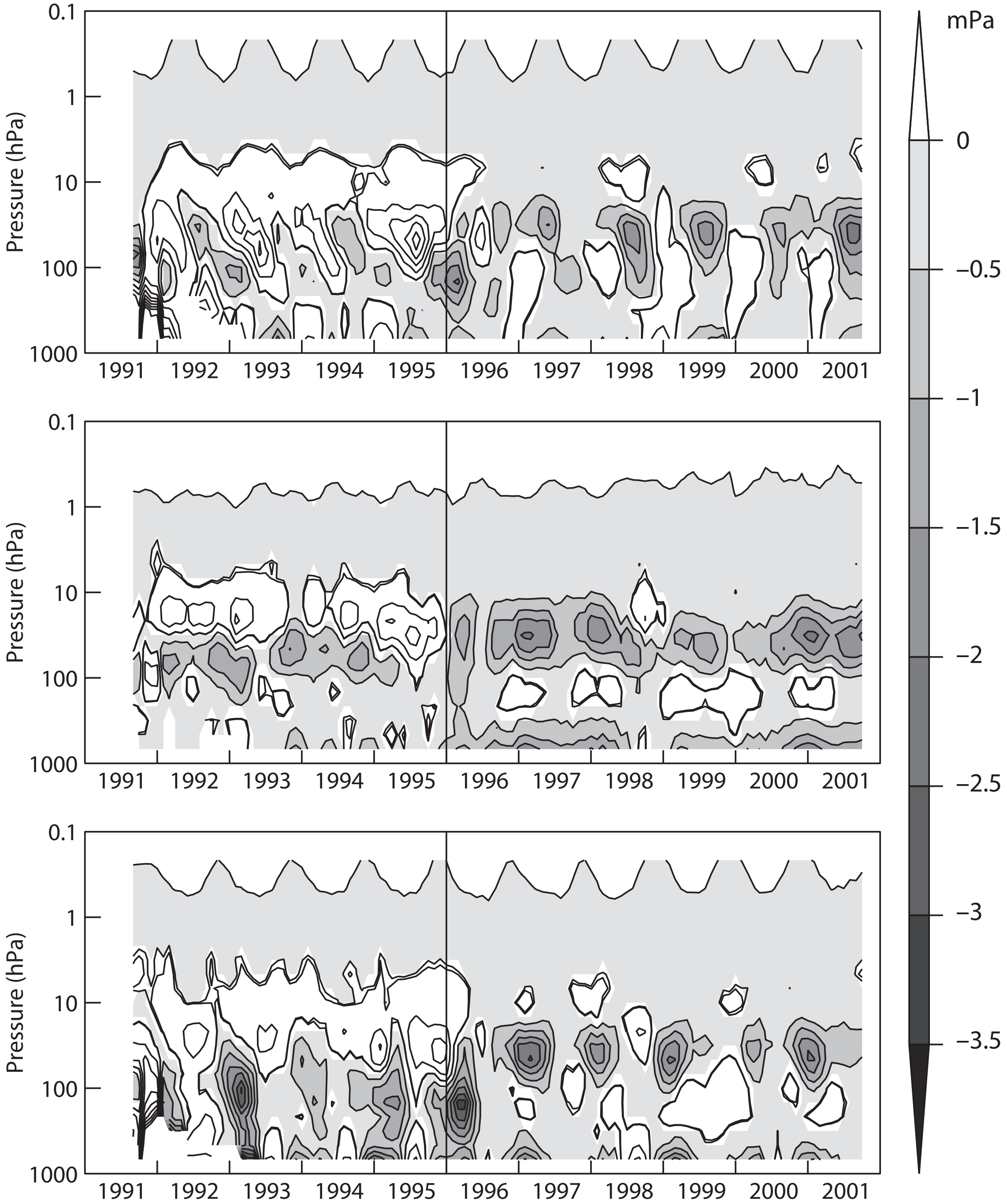

Figure 9: As in figure 6, but for the comparisons with HALOE.

2.5 Comparisons with UARS and Aura MLS ozone profiles

The Microwave Limb Sounder (MLS) measures naturally-occurring microwave thermal emission from the limb of the Earth's atmosphere to remotely sense vertical profiles of selected atmospheric gases, temperature and pressure. The first MLS experiment in space flew on UARS. The primary UARS MLS data products were vertical stratospheric profiles of ozone (O_3) at 183 and 205 GHz, chlorine monoxide, water vapor, and temperature. In this study we used the MLS level 3AT ozone profile data (version 5). These are daily time-ordered data, arranged at time intervals of about 65 seconds, or about 495 km intervals along the instrument's line of sight (LOS) tangent track. Only the retrievals from the 205 GHz measurements were considered as they are more accurate than those at 183 GHz (Froidevaux *et al.*, 1996). Cunnold *et al.* (1996) discussed the quality of the UARS ozone retrievals compared with SAGE-II data. They showed that UARS MLS values were typically larger than SAGE II values by approximately 5% in the region between 1 and 32hPa. Below 32hPa, differences up to 50% were found between MLS and CLAES measurements in the tropics. Comparisons against ozone sondes showed that MLS values were approximately 20% too small in the tropical lower stratosphere around 46hPa particularly during the first 6 months (October 1991 to April 1992) of the UARS mission. In July 2004, the UARS follow on mission, Aura, was launched (Schoeberl *et al.*, 2006). The Aura orbit is Sun-synchronous at 705 km altitude with a 98° inclination and ascending node equator-crossing time roughly at 1345 local time. This satellite carried in space the second MLS experiment. In this study, the Version 2.2 (v2.2) Aura MLS ozone profiles were considered (Livesey *et al.*, 2008). Froidevaux *et al.* (2008) compared the v2.2 Aura MLS ozone retrievals with matching ozone data from ground-based and satellite observations, and found that the differences are generally a few percent compared with remotely sounded data at stratospheric levels and within 5% when compared with ground-based microwave measurements in the mesosphere. For simplicity, the plots are produced for both instruments together, but the reader is advised that differences may exist between the two datasets. It is also worthwhile to remind the reader that the v2.2 MLS ozone profiles were actively assimilated in the ERA-Interim reanalyses during 2008, and therefore the comparisons shown below do not represent an independent validation of the quality of the ozone reanalyses during that year.

The ERA-Interim and MLS comparisons are shown in figures 10 and 11 at four vertical levels and averaged over three latitudinal bands. At 4 and 10hPa (figure 10), the ERA-Interim and the MLS data are generally in good agreement, with residuals generally being within ±5%, and occasionally larger with values within ±10% (e.g. in the SH extra-tropics at 4hPa). The ozone seasonal variability is typically well represented in the ERA-Interim and in good agreement with that shown in the MLS observations, but as noted in the comparisons with SAGE the residuals show an annual cycle, especially at 4hPa in the NH, with maximum values typically in winter and minimum values during the summer time.

The level of agreement between the MLS ozone parofiles and ERA-Interim reanalyses is degraded in the lower stratosphere. At 31hPa, the mean residuals are usually positive (observations showing larger ozone values than the reanalyses) and up to +35% before January 1996, and up to 20% afterwards, confirming that the ERA-Interim reanalyses likely benefitted from the assimilation of GOME ozone profiles, as discussed above. The ozone seasonal variability shown by the data is captured at the right time, but the amplitude is not always the same. The comparisons with Aura MLS show a good agreement particularly in the NH extra-tropics, but they also confirm problems in the tropics, where the ozone amount given by the ERA-Interim is too low. This is a known shortcoming of the model and it was already discussed by Dethof and Hólm (2004). At 68hPa (panels **d** to **f** in figure 11), the MLS ozone data still exhibit higher values than the ERA-Interim reanalyses, with differences of about +30% against the UARS sensor and up to about 20% against Aura MLS. At this level, the ozone variability is well-represented by the model in the NH extra-tropics, but problems are highlighted in the SH extra-tropics during the UARS period. However, Cunnold *et al.* (1996) found large residuals between MLS and correlative measurements below 32hPa that could partly explain these results. In the tropics, during the

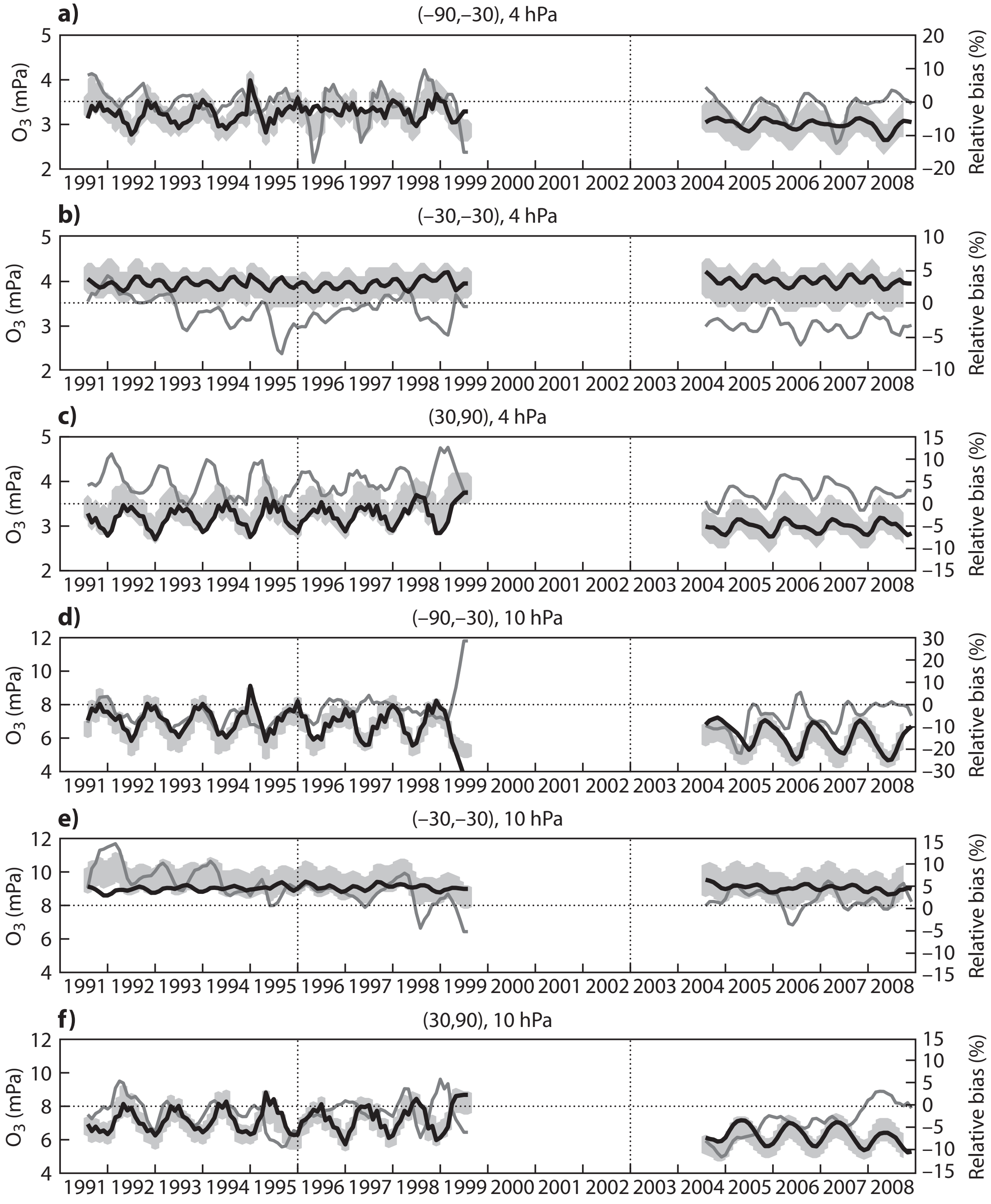

Figure 10: As in figure 4, but for MLS data at 4hPa (panels a) to c)) and 10hPa (panels d) to f)). The first period until 1999 refers to the comparisons with UARS MLS ozone profiles; the second period from 2004 to 2008 refers to the comparisons with Aura MLS. The vertical dashed line marks the beginning of the period (Jan 1996 - Dec 2002) during which the GOME ozone profiles were actively assimilated in the ERA-Interim reanalyses.

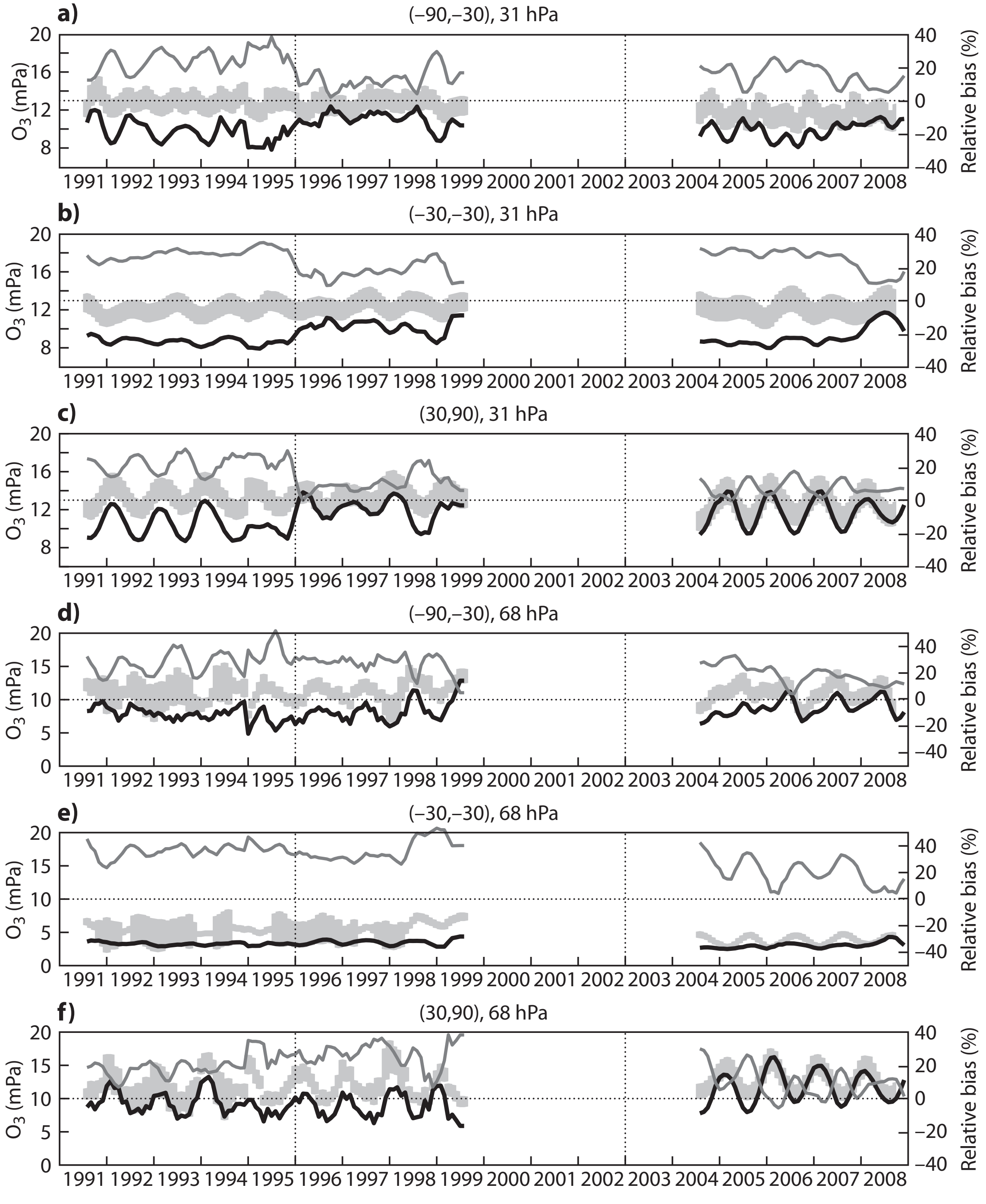

Figure 11: As in figure 10, but at 31hPa (panels a) to c)) and 68hPa (panels d) to f)).

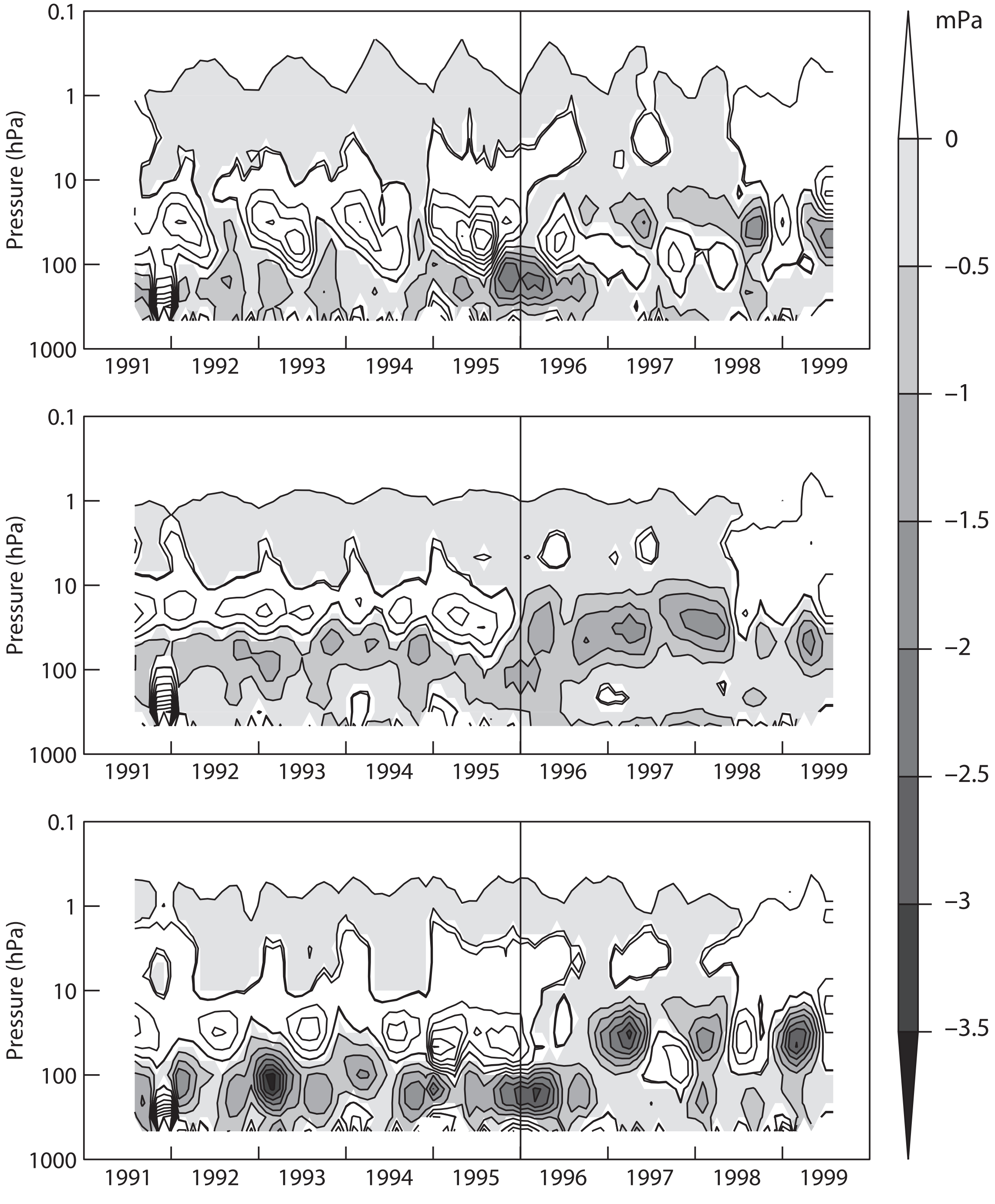

Figure 12: As in figure 6, but for the comparisons with UARS MLS.

Aura period, the ERA-Interim reanalyses show much less variability than the MLS data. There is no indication that the assimilation of GOME ozone profiles was particularly beneficial at this level.

The difference between the RMS error of UARS MLS and the corresponding ERA-40 and ERA-Interim analyses (figure 12) clearly highlights a better constrained ERA-Interim ozone in the UTLS before January 1996 than that from ERA-40, but also problems in the region of the ozone maximum, where the ERA-40 reanalyses seem to be in better agreement with MLS. The assimilation of GOME ozone profiles, started in January 1996, appears to be beneficial and improve the reanalyses particularly in the tropics.

2.6 Comparisons with POAM II and III ozone profiles

The Polar Ozone and Aerosol Measurement (POAM) II and III (hereafter simply referred to as POAM) sensors (Lucke *et al.*, 1999) were launched onboard of the third and fourth Satellite Pour l'Observation de la Terre (SPOT-3 and -4), respectively. They were both near-polar, sun-synchronous solar occultation instruments sampling in nine wavelength channels between 0.353 and 1.02 μm. The set of available products included high vertical resolution profiles of ozone. POAM made year-round measurements at high latitude in both hemispheres, with nominal latitude ranges between about 55° and 70° in the NH, and between about 65° and 88° in the SH. Here, we used the version 6 POAM II and the version 4 POAM III ozone profiles. Deniel *et al.* (1997) compared NH measurements from the POAM II instrument against electro-chemical cell (ECC) ozone sondes and found that the residuals were about 2-3% near the lowest and highest altitudes of profile overlap (17 and 30 km) and up to 7.6% from 21 to 24 km. Rusch *et al.* (1997) compared the POAM II ozone data against MLS, SAGE II and HALOE measurements and found residuals typically within 5-7% in the stratosphere between 6 and 50hPa, and up to 20% in the UTLS. Very small biases were found in the comparison of POAM III measurements with both SAGE II and HALOE, being typically of ±5% (or less) between 30 and 60 km (Randall *et al.*, 2003), and between -7 and +10% with targeted aircraft and balloon observations between 14 and 30 km during the SAGE III Ozone Loss and Validation Experiment (SOLVE) campaign (Lumpe *et al.*, 2002). For simplicity, the plots are produced for both instruments together as it was done for MLS, but the reader is equivally advised that differences may exist between the two datasets.

Because of the instrument coverage, the comparisons could only be made at high latitudes. Here, the ozone reanalyses are normally less constrained, particularly in winter and spring when the stratospheric ozone transport and depletion inside the polar vortex are difficult to model accurately. This reflects in a poorer level of agreement of the ERA-Interim ozone analyses with this set of independent data as shown in figures13 and 14. In contrast to the comparisons shown so far, the level of agreement with POAM is worse at 5 and 10 hPa than in the lower stratosphere. In the middle stratosphere the ERA-Interim ozone analyses seem unable to reproduce the ozone seasonal variability as shown by the data, besides their values are generally much larger than those measured, with relative differences up to 50% in the NH and larger than 100% in the SH (because of these large differences the relative biases were omitted in panels **a** and **c** of figure 13). The level of agreement between POAM and MLS, SAGE and HALOE correlative measurements, discussed in the literature, does not seem to reflect in the differences found in the comparisons of each single dataset with the ERA-Interim ozone analyses. However, the different latitudinal coverage used in the comparisons presented here could partly explain these differences.

In the NH, the occurrence of the ozone minima and maxima also seems to be lagged compared with that in the POAM data. In the lower stratosphere, a higher level of agreement was found. At 28 and 66hPa, the ozone seasonal changes appear to be better represented in the reanalyses and in better agreement with the POAM data, both in terms of amplitude and temporal occurrence. Differences are still noticeable, but they are now typically within ±20%. Additionally, there are features in the data that were captured by the reanalyses albeit with different amplitude, such as the relative minima occurred during 2003, 2004 and 2005 at 28 hPa in the SH

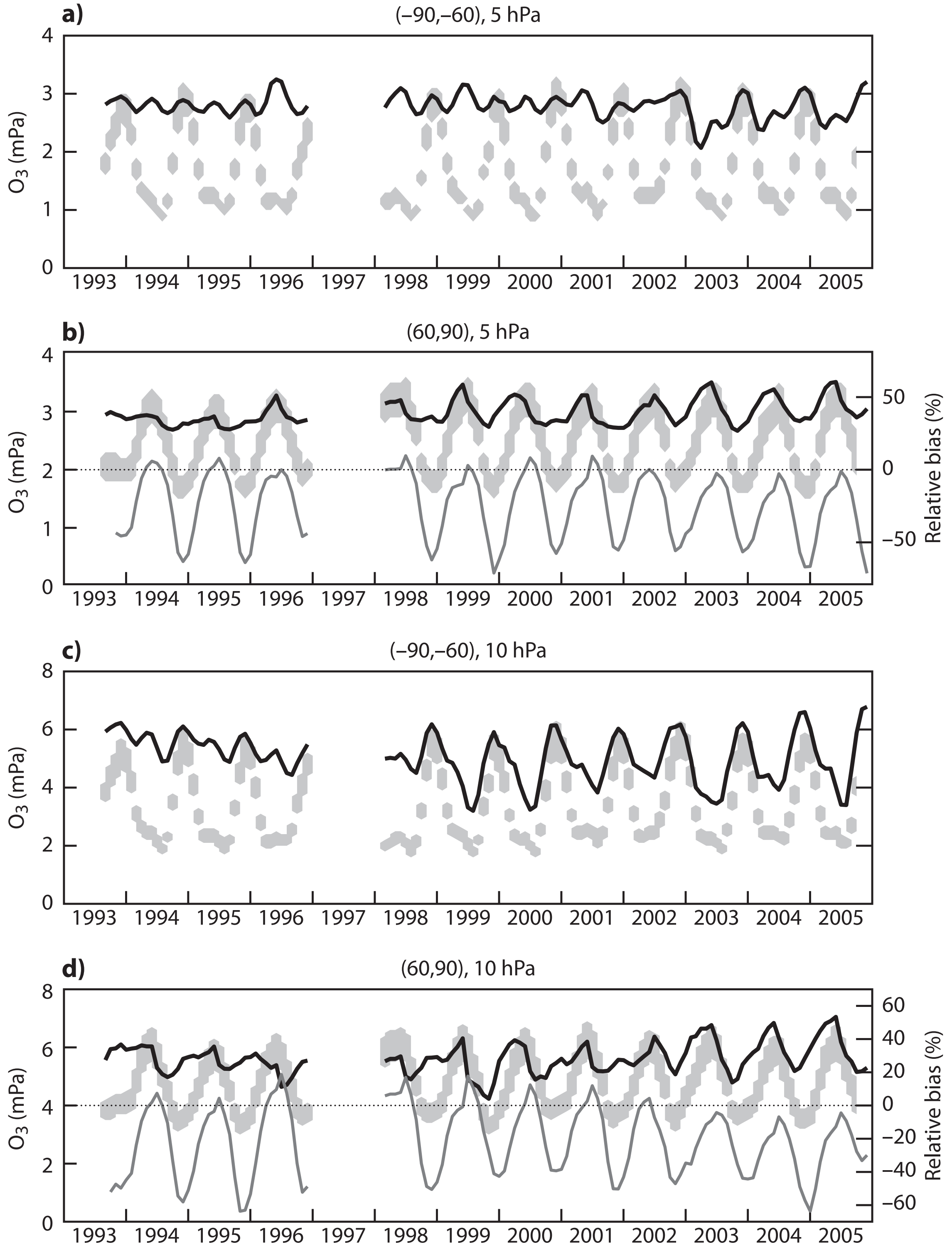

Figure 13: As in figure 4, but for POAM at 5hPa (panels a) and b)) and 10hPa (panels c) and d)). The first period from 1993 until 1996 refers to the comparisons with POAM II ozone profiles; the second period from 1998 to 2005 refers to the comparisons with POAM III. Panels a) and c) refer to the comparisons at high latitudes in the SH; panels b) and d) refer to the comparisons at high latitudes in the NH. Relative biases larger than 100% were not plotted.

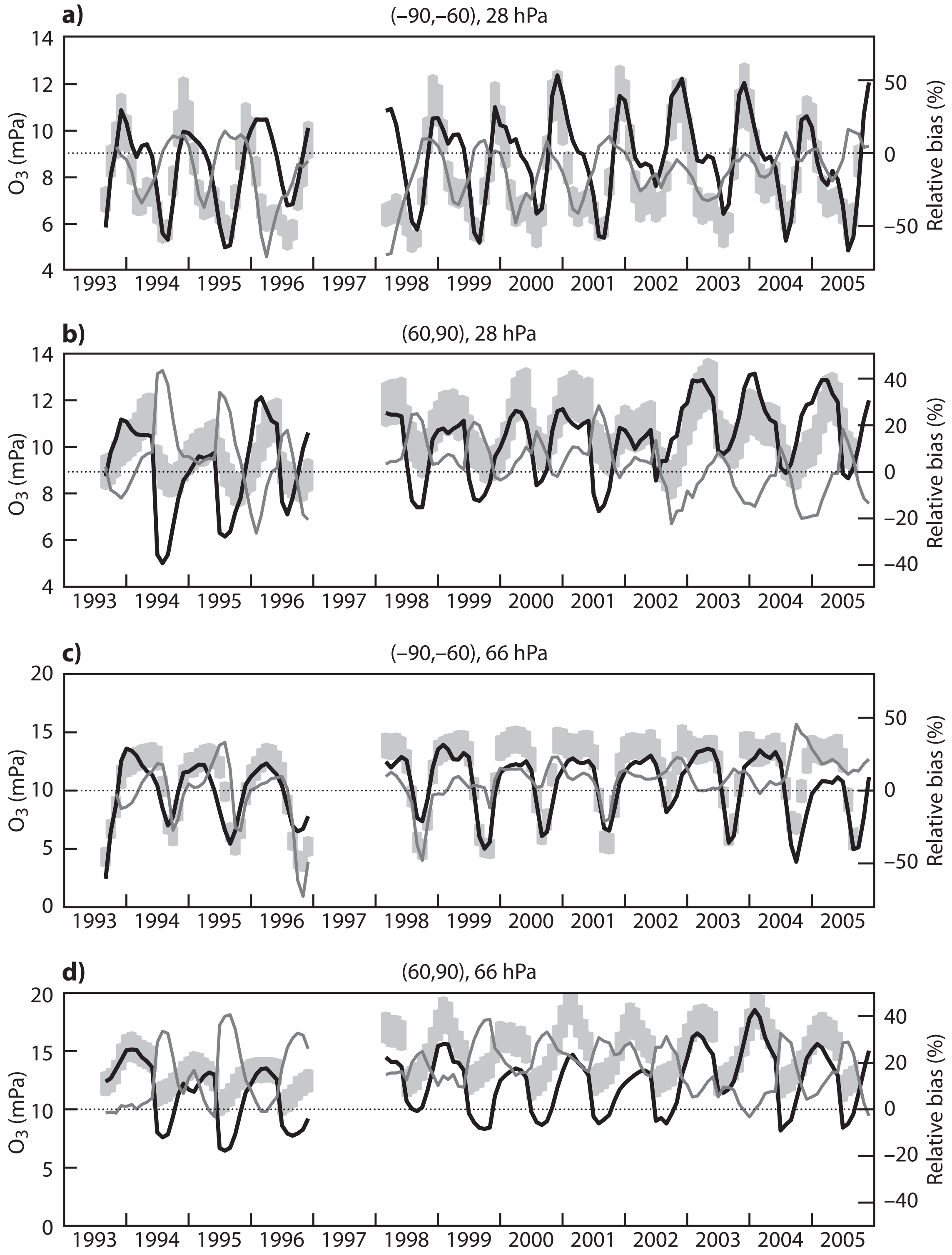

Figure 14: As in figure 13, but at 28hPa (panels a) and b)) and 66hPa (panels c) and d)).

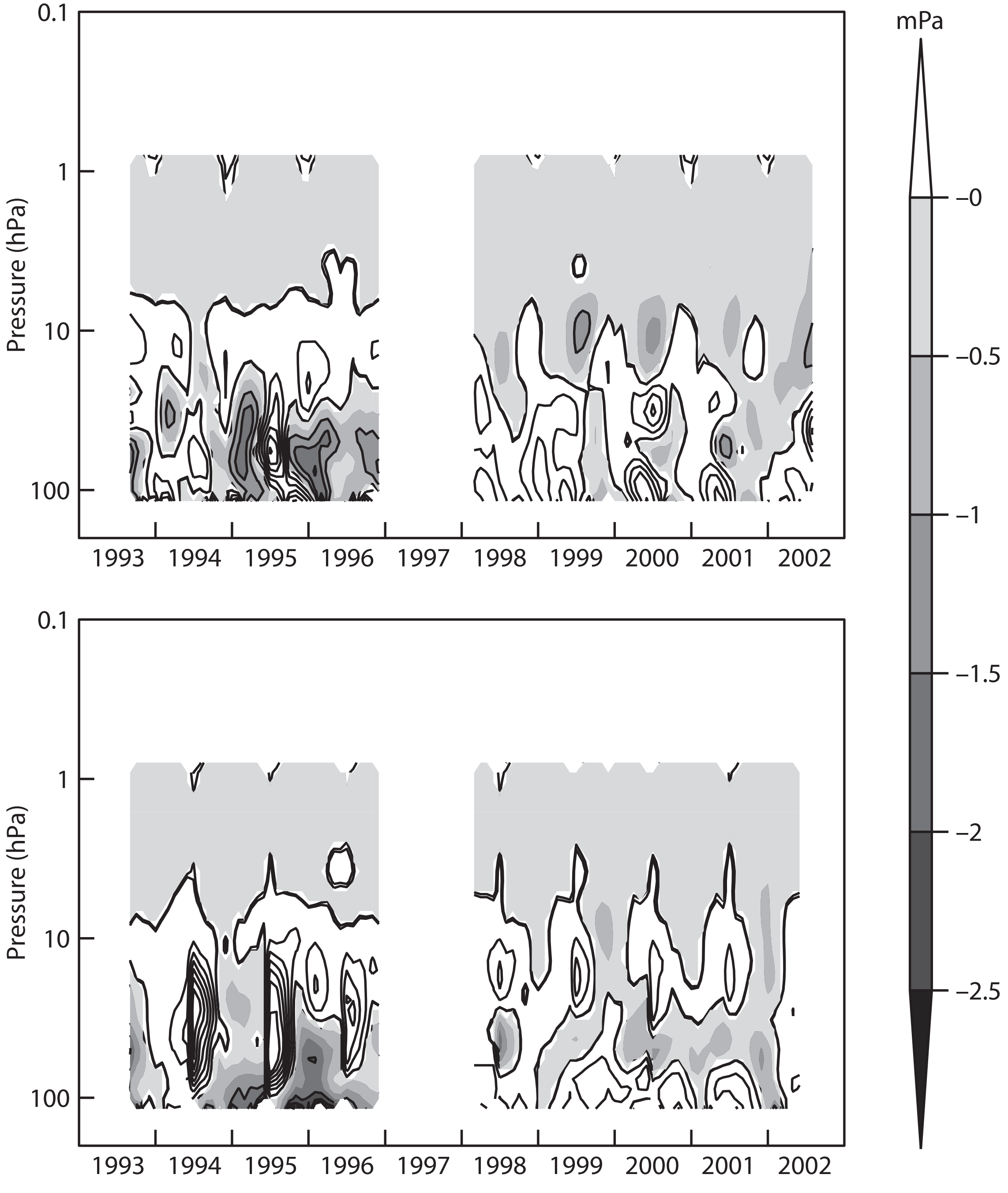

Figure 15: As in figure 6, but for the comparisons with POAM II and POAM III. Because of the POAM data coverage, the y-axes are limited to the region of the atmosphere between 200 and 0.1 hPa; the top panel shows the comparisons averaged over the high latitudes in the NH ([60,90]N); the bottom panel shows the comparisons averaged over the high latitudes in the SH ([60,90]S).

(panel **a** of figure 14).

The comparison between POAM data and the two reanalysis datasets (ERA-40 and ERA-Interim) shows differences and it is not immediately clear which dataset fits POAM observations better at these high latitudes. However, there seems to be a rather different response during the two periods 1993-1996 and 1998-2002, suggesting probably some non-negligible differences in the POAM II and III retrievals. Some inter-hemispheric differences can also be detected. Compared with POAM II (1993-1996), ERA-Interim showed a generally better agreement with the data than ERA-40 in the NH lower stratosphere typically for pressures larger than 30hPa during winter/spring time, but ERA-40 seems to perform better during summer. Conversely, in the SH (bottom panel of figure 15), the ERA-40 ozone reanalyses agree better with POAM II than those from ERA-Interim in winter time, and less in summer. The comparisons with POAM III (1998-2002) are somehow controversial, and it is not immediately clear which reanalysis agrees better with these dataset.

3 Analysis of the trends

As done in section 5 of Dragani (2010), we now investigate the existence of possible trends in the residuals between the satellite observations used in the validation study and the ERA-Interim ozone reanalyses, as a function of pressure. An indication of the possible trends could already be derived from the discussion in section 2 for specific stratospheric levels. Here, this analysis tries to fill the gaps between those vertical levels to provide conclusions valid over the entire vertical range spanned by both the data and the reanalyses. A weighted least squares fit to the monthly mean departures was used to derive the annual variations at different vertical levels, and to identify statistically significant changes. As mentioned inDragani (2010), because neither the ECMWF system (e.g. model version and various parameterizations) nor the version of the assimilated and independent data changed during the period of the reanalysis production, any temporal dependence of the residuals can only be associated to changes in the actual amount of data and data type actively assimilated in the system. This investigation neither made use of the POAM data, due to the large differences found in the comparisons with the ERA-Interim ozone analyses and its seasonal variability already discussed, nor of the Aura MLS data, because of the short period available. It should be noted that the periods considered to estimate the temporal trends were the entire availability period of each independent instrument, and therefore it differs from one sensor to another and may lead to differences in the results. Nonetheless, the trends in the residuals with the three satellite sensors often show some degree of agreement. Because of the lower accuracy of the independent data in the troposphere than that at stratospheric levels, this discussion is limited to the stratosphere.

Figure 16 shows the slope profile of the time series for the ERA-Interim residuals from SAGE, HALOE, and UARS MLS data computed over six thirty-degree latitudinal bins, the error bar provides the range of variability for each estimate with a confidence level of 95%. In general, the variations are within ±0.5%/year at all vertical levels and latitudinal bands, and in most cases, the residuals for the three instruments show similar changes (i.e. positive/negative trends). Above 10hPa in the stratosphere, there are small, and generally not statistically significant trends in the difference between the independent ozone retrievals and their ERA-Interim equivalent both at midlatitudes and in the tropics. Conversely, statistically significant changes can be observed at high latitudes, particularly in the SH, and in the tropical UTLS.

To understand whether these changes can be associated with an improved or degraded level of agreement between satellite ozone data and the ozone reanalyses, we can relate the information provided in figure16 with the timeseries presented at four selected pressure levels in section 2, and from there derive some indications at different vertical levels. In general, the timeseries discussed in section 2 showed that the ERA-Interim ozone reanalyses exhibited lower ozone values than measured by the three instruments in most of the lower stratosphere. For example at 30hPa in the tropics the comparisons with SAGE, HALOE and UARS MLS (panels **b)** in figures 5, 8 and 11, respectively) showed positive observation minus analysis residuals, and these are associated with negative slopes, that overall imply an improved agreement with time. We can then extrapolate information on the temporal evolution of that agreement at different levels, and say, for example, that also the negative slopes at 20hPa and 40hPa in the tropics are likely to be associated with an improved level of agreement between the independent observations and their co-located ERA-Interim ozone analyses. Two exceptions are noticeable. The first at 10hPa at high latitudes in the SH (panel **a)**). Here, the slope is positive for all the instruments. However, in these cases the ERA-Interim ozone analyses are higher than the independent data (panels **d)** in figures 4, 7, and 10). Therefore, the positive sign in the trend still means an improved agreement with time. The second exception is represented by the comparisons with MLS around 70hPa at midlatitudes in the NH, where a positive MLS minus ERA-Interim bias (panel **f)** in figure 11) is associated with a small (0.2%/year) but statistically significant positive slope (panel **e)** in figure16) leading to an overall degraded agreement with time.

4 Summary and conclusions

We presented an evaluation of the quality of the ECMWF ERA-Interim ozone analyses for the period January 1989 through December 2008 by comparisons with remote independent ozone observations. Total column ozone from OMI and a global TCO reference, created from the NASA's merged satellite dataset, were used to assess the quality of the ozone column analyses; ozone profiles from SAGE, HALOE, UARS and Aura MLS, and POAM II and III were used to validate the ozone vertical distribution. Three periods, over which changes in the level of agreement between the ERA-Interim ozone analyses and the independent ozone observations could be identified, were found and related to changes in the ozone observing system used in ERA-Interim, mainly related to the assimilation of GOME ozone profiles. Thereby, these periods were definied as follows: 1) the pre-GOME assimilation period (January 1989 through December 1995); the GOME assimilation period (January 1996 until December 2002); and 3) the post-GOME/SCIAMACHY assimilation period (January 2003 through December 2008). The results discussed in the present paper complement those presented in a companion validation paper (Dragani, 2010), based on the comparisons of the ECMWF ozone reanalyses with in-situ measurements.

In terms of the total column ozone, comparisons with OMI data for the most recent years of the ERA-Interim production show a good level of agreement. The TCO analyses typically exhibited lower ozone values than measured by the OMI instrument, though the relative residuals are less than 2% over the latitudinal band 50°S-50°N. In addition, comparisons with an ad-hoc created global mean TCO reference, created from the NASA's merged satellite dataset, showed residuals generally within ±2% during most of the twenty-year period under study.

The comparisons with the retrieved ozone profiles showed a generally well represented seasonal variability of the stratospheric ozone in the ERA-Interim ozone analyses, with a few exceptions, e.g. in the comparisons with POAM data (high latitudes) where not only was the amplitude of such a variability not fully captured, but also the occurrence of the ozone minima and maxima appeared lagged in time of about one month. All the comparisons showed some degree of consistency in the results. In general, the ozone amount is underestimated in the lowermost stratosphere (below 30hPa), and generally slightly overestimated in the middle stratosphere (5 and 10hPa), regardless of the latitudinal band. Both in the tropics and in the extra-tropics, the analysis departures (observation minus analyses) above 10hPa were within ±10% in the case of SAGE and HALOE, and within ±5% in the case of MLS. In the region of the ozone maximum at 30hPa, larger positive departures up to +25% in the case of SAGE and up to +35% in the case of HALOE and MLS were found at all latitudinal bands before January 1996.

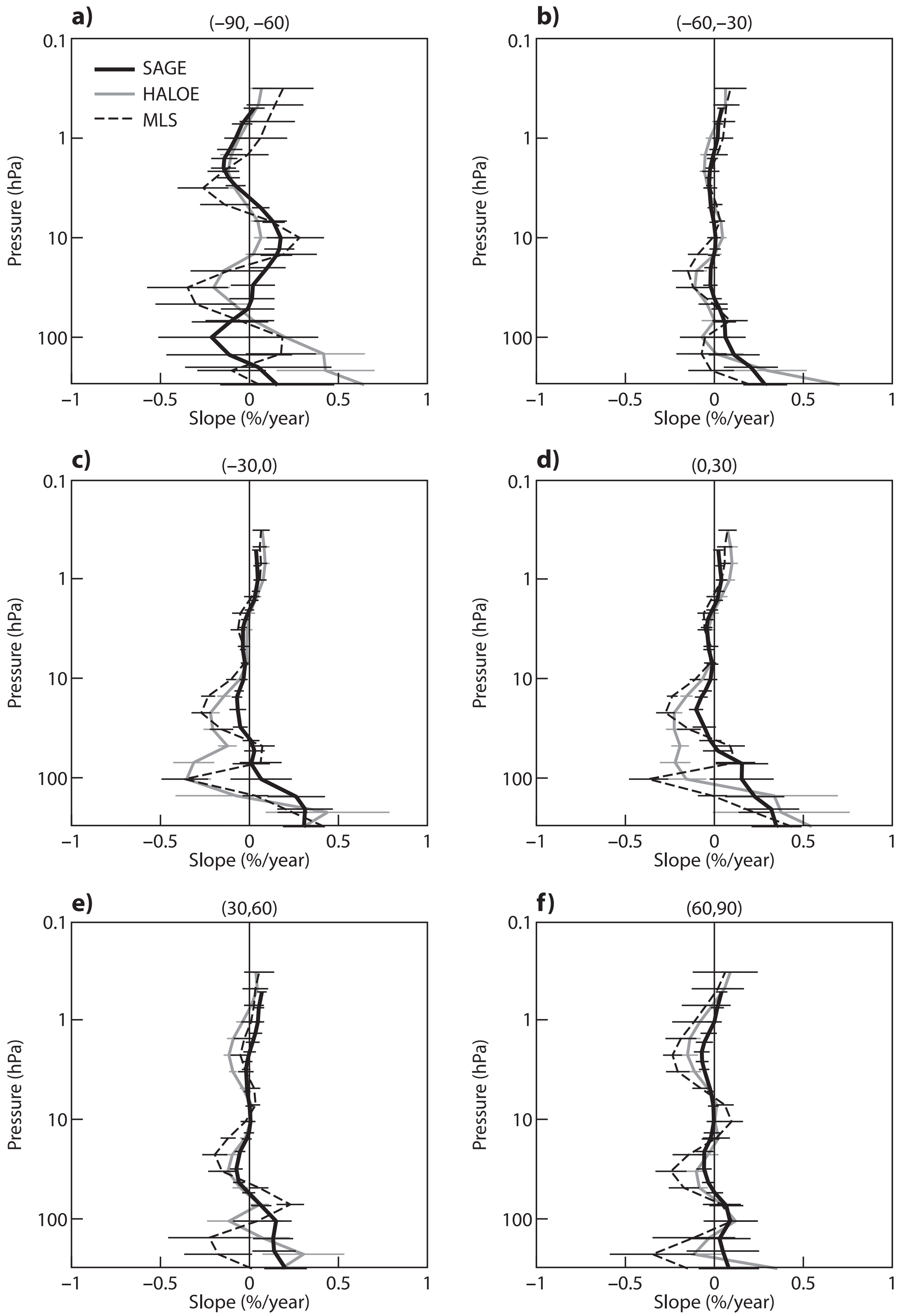

Figure 16: Slopes of time series differences between independent data sets and the co-located ERA-Interim ozone analyses as function of pressure (from 0.1 to 300hPa) and over 30° latitudinal bins as reported in each panel title. The closed circles refer to SAGE; the star symbols were used for HALOE; finally, the diamonds refer to UARS MLS. The error bars refer to twice the error in the slope estimate.

With the active assimilation of GOME ozone profiles, the level of agreement typically improved leading to positive residuals up to about +20%. Despite the improvements at all latitudes and with respect to three instruments, the discrepancies between the independent ozone observations and their ERA-Interim equivalent around the ozone peak still appear to be large. These differences can be partly understood and explained by accounting for the limitation of the assimilated ozone products as well as the characteristics of the various validating instruments. In the ERA-Interim data assimilation system, most of the assimilated ozone products were in the form of either total columns or partial columns like the SBUVs. To avoid problems related to unaccounted vertical correlations, the operational NOAA SBUV ozone profile - that yielded twelve levels in version 6, used until 21 January 2008, and twenty levels in version 8, used from 22 January 2008 onwards - was converted into a six layer partial column profile for which the bottom layer spans from the surface up to about 15hPa. In this situation, the ozone vertical distribution is mainly determined by the assumed errors in the model first guess as the ozone increments are distributed and placed by the variational data assimilation system in the region of the atmosphere where least constrained. This region, which depends on the structure of the model background, is normally located between 20 and 70hPa in the ECMWF case. Even when the ozone information is provided in the form of a multi-level profile, like in the case of GOME, improvements can be obtained within the typical limitations of a UV nadir instrument. Despite their good horizontal resolution, nadir instruments normally have a poor vertical resolution that prevent them from characterizing properly the ozone maximum, and this reflects into the ozone analyses. Conversely, the three independent instruments used here made use of a limb viewing geometry that provides highly accurate vertical information at the expense of a poorer horizontal resolution. The same arguments also apply to the region below the ozone peak.

The results discussed in this paper for the lower stratosphere around 70hPa showed that the ERA-Interim ozone analyses had lower ozone values than SAGE, HALOE, and MLS, with differences up to 20%, except in the case of UARS MLS, for which they were slightly higher. Some improvements were seen in the tropics during the GOME assimilation period, particularly in the comparisons with HALOE (residuals were within -5 and +10%). The ERA-Interim ozone analyses at high latitudes were also compared with POAM II and III ozone observations. By considering the comparisons with both instruments together, the residuals were typically negative (i.e. ozone values in ERA-Interim larger than the POAM observations) and larger than 50% at 5 and 10 hPa. At 30hPa, the analyses departures were within ±20% in the NH and within -30 and +10% in the SH. Finally, in the lowermost stratosphere (70hPa), the residuals were positive and up to 30% in the NH, and within ±25% in the SH. In the latter case, the better agreement with POAM III data, that was normally within -5 and 10%, is noticeable.

The combined information from the time series of the observation minus analysis residuals at given stratospheric pressure levels and the evaluation of their trends led to the conclusion that the level of agreement between the ERA-Interim ozone reanalyses and the independent ozone profiles improved with time at most vertical levels in the stratosphere.

Throughout this paper, we also discussed the quality of the ERA-Interim ozone analyses with respect to those produced in ERA-40. The comparisons with satellite data showed generally a better fit of the ERA-Interim ozone analyses to the independent data than their ERA-40 equivalent. In particular, the improvement gathered by the active assimilation of GOME ozone profiles in the lower stratosphere was clearly demonstrated in the tropics and to a smaller extent in the extra-tropics. Dragani (2010) came to similar conclusions based on the comparisons with ozone sondes. Our analysis has also pointed out the regions of the atmosphere and the areas of the globe where these improvements mainly occurred. Indeed, it was also shown that a number of deficiencies still remain and need to be addressed in the future. An area where it is notoriously difficult to accurately model the ozone distribution is represented by the high latitudes at the beginning of spring, particularly in the SH. Without a proper characterization of the chemical processes involving ozone, as done for example within Chemical Transport Models (CTMs), simple parameterizations of the homogeneous and heterogeneous chemical processes cannot provide accurate responses in those areas, and phenomena, such as the ozone depletion, are sometimes not well represented. In these cases, the assimilation of accurate ozone information, especially in the form of a profile, can lead to substantial improvements. Here, for example, it was mentioned several times the impact on the quality of the ERA-Interim ozone analyses produced by the assimilation of GOME ozone profiles.

5 Recommendations for future reanalysis

Although, at the time of the writing, the ERA-Interim project is still providing global analyses with about two month time lag from real time, ECMWF has already started planning the next reanalysis project anticipated to cover an even longer period than that spanned by ERA-40. Several scientific and technical improvements could already be identified to fully justify the effort for a new extended reanalysis.

Besides covering a longer period and using a much improved and a more up-to-date model than ERA-Interim, the new suite will likely benefit from an increased spatial resolution. Much work and effort were already anticipated to be devoted to improving the data assimilation system and better exploiting the available observing system, e.g. by including more accurate, reprocessed observations whenever possible. In addition, the ozone retrievals used as independent observations in this study could also be considered, subject to accurate assimilation impact studies. In addition, the use of a variational bias correction (VarBC) scheme for retrieval products in general and ozone data in particular is already foreseen. Such a scheme was successfully implemented in the ECMWF operational system in September 2009 (operational cycle CY35R3), and represented an extention to retrieval products of the VarBC scheme used in ERA-Interim for radiance data (Dee and Uppala, 2009).

The parameterization of the homogeneous and heterogeneous processes that regulates the ozone chemistry is under periodic revisions and updates. Undoubtedly the ozone analyses will benefit from any further improvement in its accuracy.

Other improvements could also be implemented, but are still subject to further testing to assess their potential impact on the ozone field as well as on the other meteorological variables. As anticipated in section 2 of Dragani (2010), because of unrealistic feedbacks on the temperature and wind products generated by 4D-Var in an attempt to accommodate unrealistic observed local changes in ozone, the sensitivity of the mass and wind variables to ozone observations during the assimilation minimisation was switched off. In this way, the dynamical link between ozone and the other meteorological variables was effectively removed. As these feedbacks are mainly due to deficiences in the assimilated tracer field, the use of a bias correction scheme could in principle be beneficial to, at least partly, address the problem. However, it is noted that the degree of success of a bias correction scheme in addressing this issue will depend on the quality of the ozone products as well as on the bias predictors used.

A further link that is not yet exploited, as in need of further attention, concerns the coupling between the ozone field and the shortwave radiation package. The current radiation scheme used at ECMWF includes the absorption of shortwave radiation by uniformly mixed gases (such as oxygen, CO_2, CH_4, CO_2, NO and O_3 itself), aerosol, and cloud particles. Although the ozone absorption is accounted for, the current formulation of the radiation scheme only makes use of an ozone climatology rather than the full prognostic ozone field, so that there are no actual feedbacks between ozone and radiation (Morcrette, 2003). The contribution of all these changes, if successfully implemented, have the potential to produce a much improved global ozone reanalyses.

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