

ON THE CONSISTENCY OF OZONE PROFILE DATA FROM ENVISAT, HISTORICAL SATELLITES AND THE NDACC NETWORK

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ABSTRACT

Atmospheric ozone is one Essential Climate Variable (ECV) for which consolidated, long-term data records are required. With its three atmospheric profilers, Envisat adds significantly to ozone profile data series initiated with the establishment of coordinated ground-based networks in the 1970s, and with solar occultation satellites in the 1980s. In this study, networks of NDACC-affiliated ozonesonde and lidar stations are used as a standard transfer to investigate the consistency of Envisat ozone profile data, of historical data records from SAGE II, HALOE and POAM II, and of more contemporary POAM III, ACE-FTS and Aura-MLS data. The comparisons reveal temporal, vertical and meridian features of interest. They highlight issues to be addressed for further harmonisation of long-term ozone profile data records. Except a few cases of long-term drifts, the agreement is stable along the respective satellite measurement periods. The analysis concludes to a mutual consistency of the data sets of $7\% \pm 10\%$ (mean \pm standard deviation) in the stratosphere. However, at some altitudes and latitudes a permanent bias is observed. Below a threshold altitude of 10 to 20 km, found to depend primarily on the measurement technique, the mean difference between satellite and ground-based data increases up to 20% and the associated standard deviation increases up to 30%. Finally, this paper confirms the efficiency of NDACC as a standard transfer to investigate the long-term and pseudo-global consistency of contiguous ozone profile data records from different instruments and platforms.

1. INTRODUCTION

During the last 25 years, several satellite instruments have recorded the vertical distribution of atmospheric ozone using limb-scanning techniques. Among them, two NASA's solar occultation missions with an orbit inclination of 56° , Stratospheric Aerosol and Gas Experiment II (SAGE-II) [1] aboard Earth Radiation Budget Satellite (ERBS) from 1984 to 2005, and Halogen Occultation Experiment (HALOE) [9] aboard Upper Atmosphere Research Satellite (UARS) from 1991 to 2005, yielded stratospheric ozone time series, with a meridian sampling from about 80°N to 80°S several times a year. Operating from a polar orbit, NRL's Polar Ozone and Aerosol Measurement II and III

(POAM II [12] and III [13]) aboard the polar orbiting French platforms SPOT-3/4, measured ozone profiles, from 1993 to 1996 and from 1998 to 2005, with a complementary coverage of the polar zones but no measurement at latitudes below about 56° . Since 2002, the atmospheric chemistry payload of Envisat, consisting of Global Ozone Monitoring by Occultation of Stars (GOMOS) [22], Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) [18], and Scanning Imaging Absorption spectrometer for Atmospheric Cartography (SCIAMACHY), provides a pole-to-pole sampling of atmospheric ozone on a daily basis thanks to the limb measurement of different radiation sources, respectively stars, infrared atmospheric emission, and scattering of UV-visible sunlight. Two other ozone profilers were launched in 2003 and 2004: CSA's Atmospheric Chemistry Experiment Fourier Transform Spectrometer (ACE-FTS) [28] onboard SCISAT-1, using the infrared solar occultation technique from an orbit at 75° inclination, thus with a latitude/time sampling between that of HALOE and that of polar orbiting instruments; and JPL's Microwave Limb Sounder (MLS) [30] onboard NASA's EOS-Aura, measuring the microwave limb emission with pole-to-pole sampling on a daily basis.

The data recorded by those nine satellites are of substantial interest for studies of atmospheric ozone and its link with climate. But current research has strong requirements on global and long-term consistency of the data records and requires a detailed characterization of their respective quality. A major issue is that data records are rarely coincident, at best contiguous, and never perfectly collocated in time and space. Different methods may be adopted to check the consistency of such different data records. Satellite-to-satellite validations have been published but they are limited to collocated measurement events; they also mix long-term degradation effects of both instruments. Ground-based validations of each satellite have also been published separately. These validations are usually based on similar principles but with implementation differences that might alter the validation results. An alternative is to use a global standard transfer. One possibility is to use satellite series with daily coverage like the American series of SBUV and SBUV/2 and the European series GOME-SCIAMACHY-GOME-2. However, nadir ozone profiling

exhibits limited vertical resolution and a sensitivity varying with altitude and time. Data assimilation has been used successfully as a global validation tool to check the internal consistency of data sets. Nevertheless, this technique can not be trusted as a validation source, as it is based on models, relying on our current understanding of atmospheric processes. Moreover, it cannot predict sporadic events like, e.g., solar proton events (SPE).

In this paper we use as a standard transfer between satellite missions, the well established ground-based networks of ozonesonde and lidar stations affiliated with the Network for the Detection of Atmospheric Composition Change (NDACC) and WMO's Global Atmosphere Watch (GAW). A common comparison method is used at all stations and for all satellites, and network-based comparisons are used to investigate variations of the data consistency with time, altitude and latitude. Previous validations of the satellite ozone data records are summarised in Section 2. Ground-based ozone data records and coincidence criteria are described briefly in Section 3. Comparison results themselves are reported in Section 4. We investigate possible long-term drifts in the satellite data records that would limit their usability for ozone trend studies. The vertical and meridian structures of the agreement between satellite and ground-based correlative measurements are also studied. A lowermost altitude under which the statistical quality of the ozone profile degrades is determined as the altitude below which the mean agreement exceeds 20% or the standard deviation exceeds 30%. Section 5 concludes with a summary of the results and with recommendations for the integrated use of satellite data.

2. SATELLITE OZONE DATA

2.1 SAGE II [1984 – 2005]

Different versions of SAGE II [1] ozone profile data have been developed and validated [2, 3]. Version 6.00 and 6.10 ozone profiles were compared to several ground-based and satellite data sets [4, 5, 6]. In general, studies conclude to a general agreement within 5 % above ozone volume mixing ratio maximum and within 10 % down to 20 km. More recent comparisons between SAGE II v6.20 ozone profiles and SAOZ and SBUV/2 data show a similar agreement [7, 8]. In this paper, we use SAGE version 6.20 ozone profiles.

2.2 HALOE [1991 – 2005]

Since its launch, three versions of HALOE [9] ozone profile data have been released and have experienced an extensive validation (i.e., [10] version 17; [11] version 18). The latest public version is version 19. Validation studies of this current version 19 show a general agreement with other satellite and ground-based instruments within 10 % [5, 8].

2.3 POAM II and POAM III [1993-1996/1998-2005]

POAM II [12] v5 ozone profiles have been compared to measurements from satellites and from ozonesondes [14, 15]. POAM II data show a typical mean agreement within 5-7% above 22 km, and are generally lower by a few percent than correlative measurements. Studies based on the current version 6 show similar results and also depict a negative bias [16]. The actual version of POAM III [13] ozone profile data is v4. Previous version v3 had been extensively validated using observations from aircrafts, balloons and satellite instruments [17]. These studies showed a typical agreement of $\pm 5\%$ from 13 to 60 km. Minor changes have been implemented in the actual version v4 for ozone retrieval and performed comparisons with correlative data show a similar agreement than for v3.

2.4 MIPAS [NR 2002 – 2004/RR 2005 –]

MIPAS [18-20] operated from 2002 till March 2004, when the instrument experienced a major anomaly. In February 2005 operations were resumed in a reduced resolution (RR) mode, not studied here. Latest versions of the profile retrievals at nominal resolution (NR), v4.61 and 4.62, were the subject of an extensive validation effort. MIPAS profiles were compared with several other satellites, balloons and ground-based instruments [21]. This coordinated study concludes to a typical agreement within $\pm 10\%$ from 20 to 50 km and highlights significant positive bias of up to +25% in the Upper Troposphere Lower Stratosphere (UTLS).

2.5 GOMOS [2002 –]

GOMOS [22] operates successfully since July 2002 except for an anomaly in 2005 that resulted in a gap in the data. Previous validation studies of successive GOMOS ozone profile data versions have shown that only data acquired on dark limb are of sufficient quality for scientific use [23, 24]. Comparisons between dark limb profiles of the latest reprocessed version 6.0cf and ground-based ozonesondes and lidars have shown a typical agreement within 10 % from 20 km up to 50 km [25]. In this paper we use GOMOS ozone data from the latest reprocessing (version 6.0cf) and its operational implementation IPF5.00. Only dark limb data have been selected.

2.6 SCIAMACHY [2002 –]

Previous SCIAMACHY [26] Ground Processor (SGP) retrievals suffered from pointing errors [27, 25, 24] and retrieved ozone VMR profiles exhibited an altitude shift of 0-1.5km. Accordingly, comparisons concluded to an altitude-dependent bias of up to $\pm 20\%$. Current SGP version 3.01 retrieves ozone number density on an altitude grid between 15 and 40 km. SGP v3.01 includes a pointing correction that should reduce the altitude uncertainty to less than 500 m, and thus the bias.

2.7 ACE-FTS [2003 –]

The latest version of ACE-FTS ozone profiles is version 2.2 updated. This data set has been the subject of a coordinated international validation [29] involving comparisons with satellite, ground- and balloon-based instruments. The study concludes to a typical agreement of the ACE-FTS profile data within 5 % between 15 and 45 km, ACE-FTS measuring ozone concentrations slightly higher than correlative data.

2.8 EOS MLS [2004 –]

Current version of EOS MLS [30] ozone profile data is 2.2x. Recent validations studies show an overall agreement with lidars, aircrafts, ozonesondes and other satellites within 5 % to 10 % in the stratosphere [31].

3 GROUND-BASED NETWORK DATA

Electrochemical cell (ECC) ozonesondes are launched regularly on board of small meteorological balloons. They measure the vertical distribution of ozone partial pressure from the ground up to burst point, the latter occurring typically around 30 km [32]. The typical vertical resolution of the ozone profile is 100-150 m and the bias is estimated to be within 5% to 7% [33].

Differential absorption lidar (DIAL) systems measure the vertical distribution of night time ozone number density at altitudes between 8-15 km and 45-50 km. The typical integration time of a stratospheric ozone measurement is between 1 and 6 hours. Vertical resolution ranges from 300 m up to 3 km depending on the altitude. Typical bias estimates range from 3 to 7 % from 15 to 40 km. Beyond 40-45 km, due to the rapid decrease in signal to noise ratio, the error bars increase and a significant bias reaching 10% may exist [35, 36].

Most ozonesonde and lidar stations perform network operation in the framework of international structures contributing to WMO's GAW, like the Network for the Detection of Atmospheric Composition Change [37,38] (NDACC, previously NDSC, <http://www.ndacc.org>), World Ozone and UV radiation Data Center (WOUDC, <http://www.woudc.org>), and Southern Hemisphere ADditional OZonesonde programme [39] (SHADOZ, <http://croc.gsfc.nasa.gov/shadoz>).

3.1 Coincidence criteria and collocations

For this preliminary study we have adopted basic coincidence criteria based on the maximum distance between the tangent point at the ozone maximum and the location of the ground-based stations. More accurate selection methods do exist, however, given the horizontal resolutions of the satellite and ground-based measurements, a maximum distance of 500 km was found as the best compromise between a sufficient coincidence of the air masses to be compared and a sufficient amount of collocated pairs of profiles. While the selection of horizontal coincidence criteria can offer some flexibility, temporal distance criteria are constrained directly by the measurement time of the data being compared, which depend on parameters like the radiation source and the orbit inclination. In this exercise, the time difference between ground-based and satellite measurements varies from 0 to maximum 12 hours. Collocations of satellite and ground-based profiles have been identified according to the above criteria for 50 ozonesonde and 10 lidar stations. Fig. 1 displays the temporal evolution and the latitude sampling of the collocations with the nine satellites, starting in 1984 with SAGE II and continuing up to recent days with Envisat, ACE-FTS and MLS.

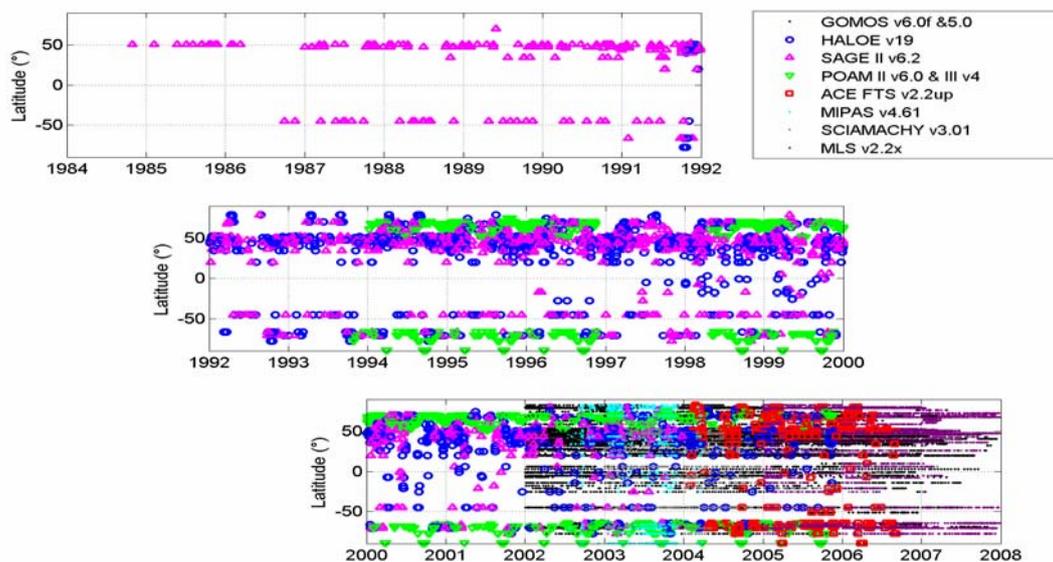


Figure 1: Latitude/time progression of collocations between nine limb-scanning satellites and ground-based network measurements of the atmospheric ozone profile, from 1984 till 2008.

4 COMPARISON RESULTS

4.1 Seasonal and long-term features

In this first part of our study, we analyse time series of the relative difference between satellite and correlative data at selected altitude levels. In particular, we look at seasonal and long-term features. To determine if a long-term drift exists, a robust linear regression¹ is undertaken. The slope of this regression is considered to be significantly different from zero if zero is not in the 95% confidence interval ($\text{slope} \pm 2 * \text{error}$) of the calculated slope. No regression is done if the standard deviation of the data set exceeds 30 %, or if the number of collocated pairs of profiles is less than 10.

The temporal analysis has been performed for each satellite at all selected ground-based stations. Figures 2, 3, 4 and 5 illustrate the results with SAGE II, HALOE, GOMOS and SCIAMACHY time series at a few European stations. Each subplot shows the relative difference at a selected altitude level (grey bullets). Mean difference (μ), standard deviation (σ) and annual slope ($\alpha \pm \sigma_\alpha$) are also written on the plots. Least squares regressions are drawn in black but are highlighted in red when significant (95% confidence).

The agreement between satellite and ground-based observations remains stable during the whole length of the measurement periods. For SAGE and in general, only a few small drifts are detected and they are not consistent from station to station. For HALOE the picture is a bit different. Figure 6 shows for HALOE, as a function of latitude, the slope of the regression fit performed at each ground-based station. Small negative drifts, of the order of -0.5% per year, have been found at 25 and 30km altitude at all northern middle and high latitude stations. For GOMOS and SCIAMACHY a few larger drifts are detected but are not fully consistent from one station to another. In addition to an important positive bias, SCIAMACHY comparison bears a seasonal cycle. Relative differences with ground-based data are larger in summer and lower in winter. The amplitude of this seasonal cycle is of the order of 10 % at 20 km. Figures 7 and 8 show the slope of the linear regression as a function of latitude for GOMOS and SCIAMACHY. Drift estimates are larger but also noisier (both positive and negative drifts).

¹ This method minimizes a bisquares weighted sum of squares, where the weight given to each data point depends on how far the point is from the fitted line. Points near the line get full weight. Points farther from the line get reduced weight. Points farther from the line than expected by random chance get zero weight.

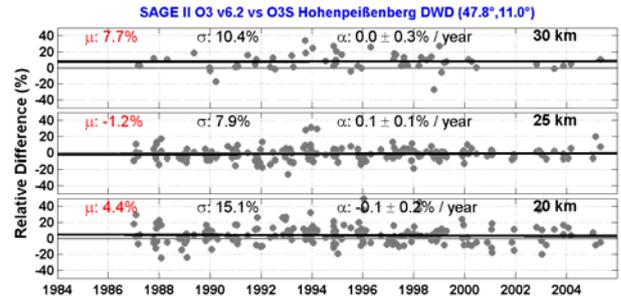


Figure 2: Time series of relative difference between SAGE II and DWD ozonesondes at Hohenpeißenberg, Germany, at selected altitude levels. When applicable a line regression is fitted to the data (black lines). Mean (μ), standard deviation (σ) and annual slope ($\alpha \pm \sigma_\alpha$) are written on each subplot.

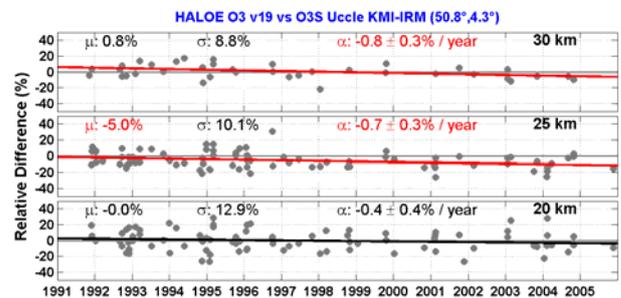


Figure 3: Same as Figure 2, but for HALOE vs. RMI ozonesondes at Uccle, Belgium.

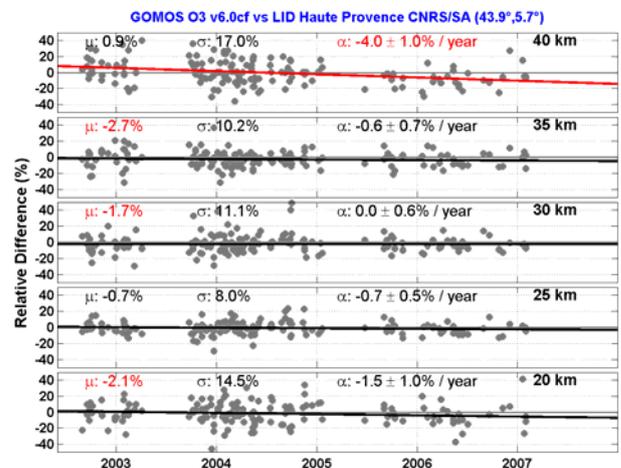


Figure 4: Same as Figure 2, but for GOMOS vs. CNRS lidar in Haute Provence, France.

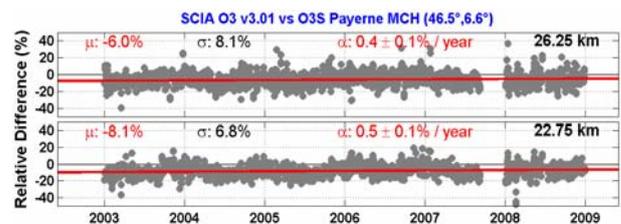


Figure 5: Same as Figure 2, but for SCIAMACHY vs. MCH ozonesondes at Payerne, Switzerland.

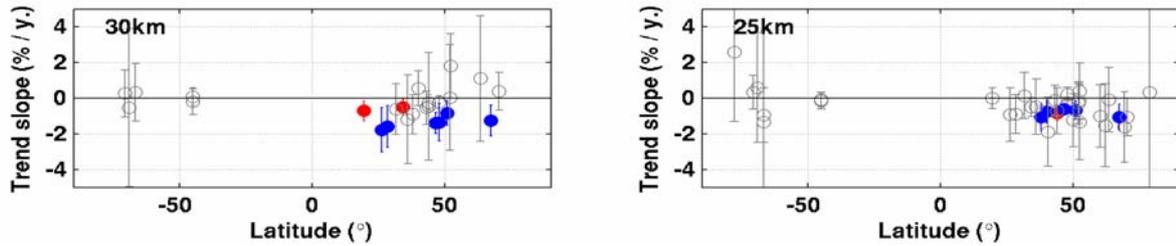


Figure 6: Slope of the multi-year linear trend fitted to time series of the relative difference between HALOE v19 and ground-based (ozonesonde and lidar) ozone measurements at each station, plotted as a function of latitude and at two altitude levels (30 and 25 km). Red dots (comparisons vs. lidars) and blue dots (comparisons vs. ozonesonde) represent trends with statistical significance (95% confidence level). Trends with no significance are shown in grey.

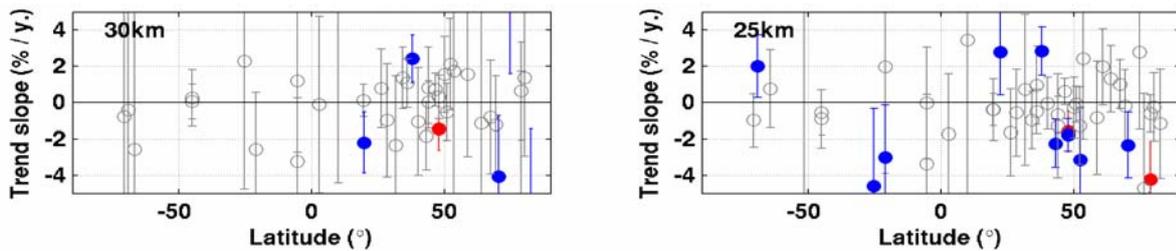


Figure 7: Same as Figure 6 but between GOMOS v6.0cf and ground-based ozone measurements at 30 km and 25 km.

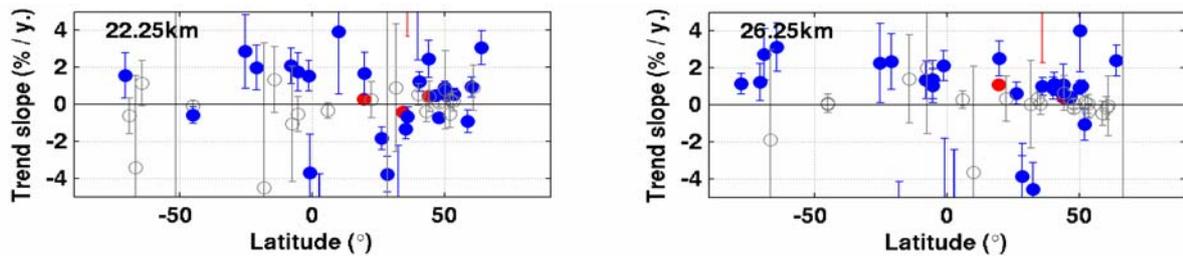


Figure 8: Same as Figure 6 but between SCIAMACHY v3.01 and ground-based measurements at 26.25 and 22.25 km.

4.2 Meridian structure

While the agreement between satellite and ground-based data varies with altitude and latitude, it does not vary between stations close in latitude and it shows long-term stability for most satellites. These findings allow us to derive multi-year and zonal statistics, which we use hereafter to study meridian and vertical features of the consistency between the nine satellites. Figures 9 to 17 show, as a function of latitude and altitude, the mean relative difference (upper panels) and standard deviation (lower panels) between the nine satellites and correlative ground-based data, averaged into 5°-wide latitude bins.

4.2.1 SAGE II

Figure 9 illustrates SAGE II results. In the stratosphere the mean agreement is of 7 % and even better with a standard deviation of 10 %. In Antarctica, we observe larger differences and standard deviations than at other latitudes that can be associated with the high dynamics of the ozone hole. Below 10-15 km at high latitude and

20 km in the tropics, the quality of the ozone profile degrades severely. Mean differences reach more than 20 % and standard deviations are larger than 30 %.

4.2.2 HALOE

Figure 10 displays HALOE meridian and vertical features. Results are similar than those obtained for SAGE II with a mean agreement within 7 % \pm 10 %. The standard deviation in the inter-tropical troposphere is surprisingly low and even close to zero. This might indicate a retrieval problem and certainly a lack of measured information in this region.

4.2.3 POAM II and POAM III

Figure 11 and 12 show, respectively, POAM II and POAM III comparisons with ozonesondes data. Due to their polar orbits, these satellites cover the polar regions only. At these latitudes there are not enough collocations with lidar data to derive meaningful statistics, therefore only comparisons with ozonesondes are shown. Although the mean agreement with

ozonesonde profiles is within 7 % for both POAM II and III, the use of ground-based networks as standard transfer confirms a 5 % bias between the two satellites.

4.2.4 MIPAS

Figure 13 displays MIPAS results. MIPAS altitude pointing suffers from a known but not corrected inaccuracy. Fortunately, pressure is also retrieved from the measurement and can be used as reference height scale (an approximate altitude scale is indicated on the plot to facilitate comparisons with other satellites). In the middle and high latitude stratosphere, as for other instruments, the mean agreement between MIPAS and correlative ozone profiles is usually better than $7\% \pm 10\%$. Here the main point is a permanent bias of +10 to +15 % observed in the inter-tropical upper troposphere and lower stratosphere.

4.2.5 GOMOS

Figure 14 displays GOMOS comparison results from July 2002 to December 2005. The general agreement is similar to that obtained for the other satellites except in the Arctic where there is a mean negative bias of -5 %. The GOMOS Quality Working Group (QWG) is investigating possible links between this bias and the contamination of GOMOS spectra by auroral light.

4.2.6 SCIAMACHY

Figure 15 shows SCIAMACHY comparison results. At all altitudes SCIAMACHY ozone number densities are about 10% lower than values reported by the ozonesondes and lidars. The stability of the bias with altitude indicates that the altitude pointing correction is working properly.

4.2.7 ACE-FTS

Figure 16 summarises ACE-FTS comparison results. The orbital inclination of ACE is such that the amount of collocations with ground-based data at tropical sites is too weak to derive statistics. Consequently, only polar and mid-latitude regions have been considered in this meridian analysis. The mean agreement is similar as that for other satellite data sets: within $7\% \pm 10\%$. There is no particular issue to discuss.

4.2.8 EOS MLS

Finally, Figure 17 summarises MLS comparison results. The mean agreement is within $5\% \pm 10\%$ from the tropopause up to the stratopause. Below 200hPa at middle latitudes and 100hPa in the inter-tropical zone, mean relative differences increase to up to 20 %. MLS data were not used at pressure above 215 hPa as recommended in the MLS metadata files.

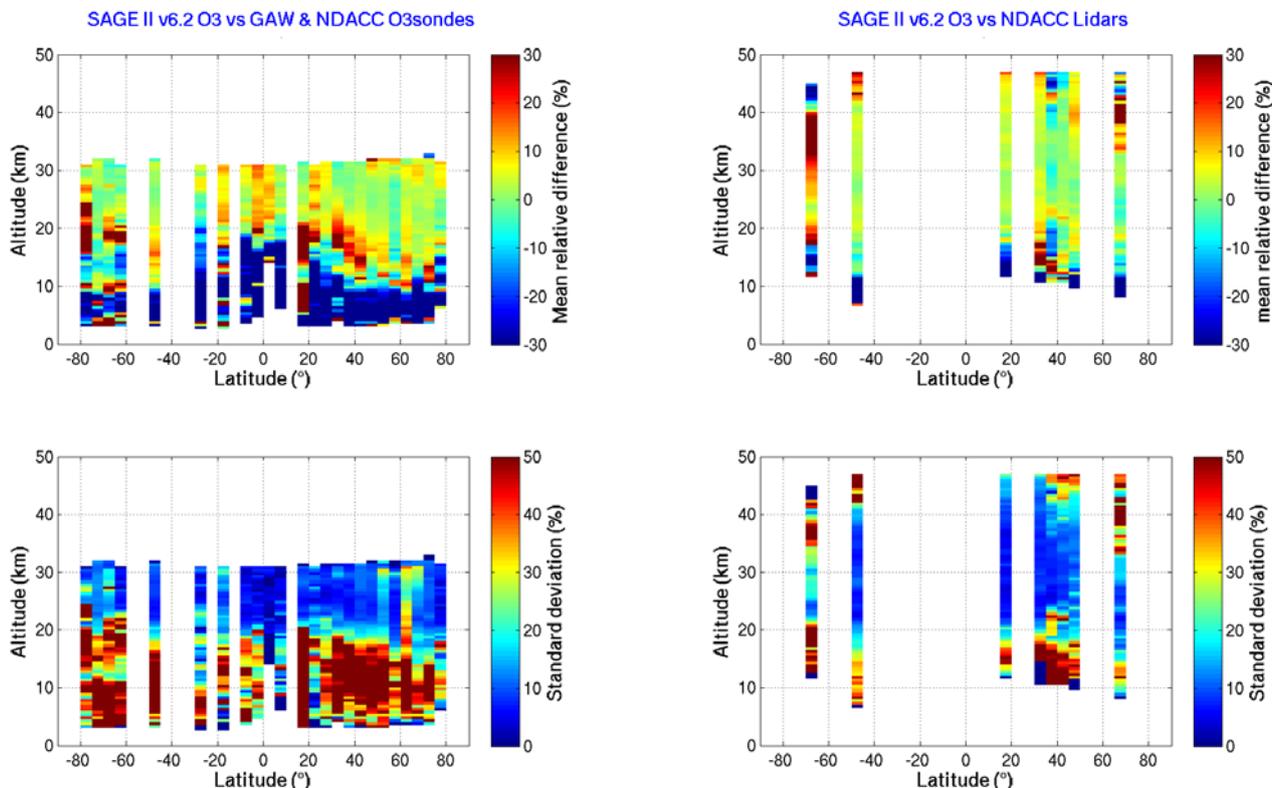


Figure 9: Mean relative differences between SAGE II v6.2 and ozonesonde (top left) and lidar (top right) ozone profile data, as a function of altitude and latitude, and corresponding standard deviation (bottom left and right).

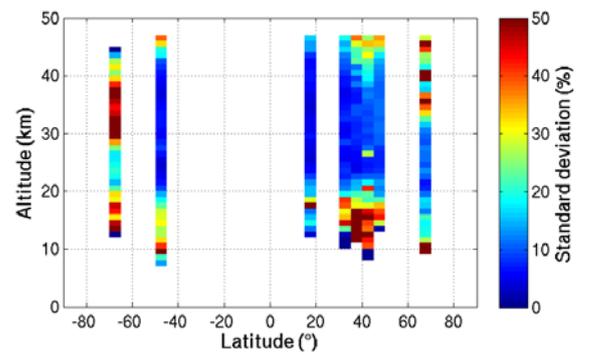
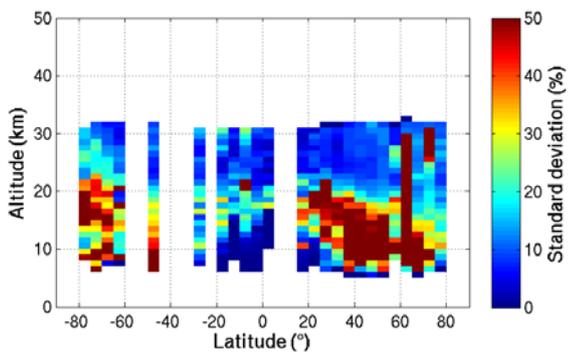
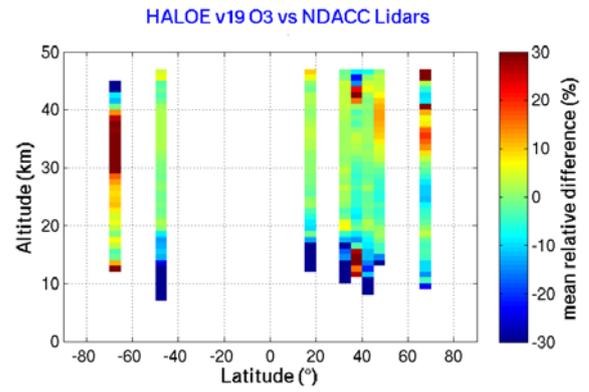
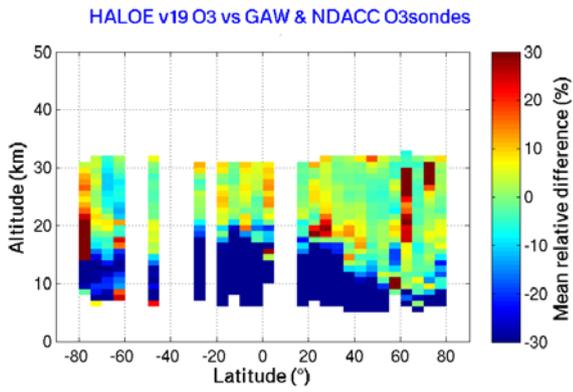


Figure 10: Same as Figure 9 but for HALOE v19.

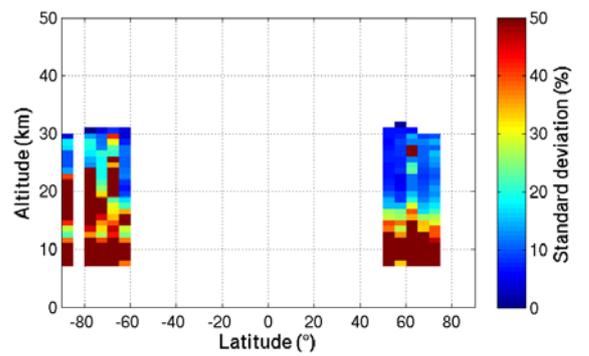
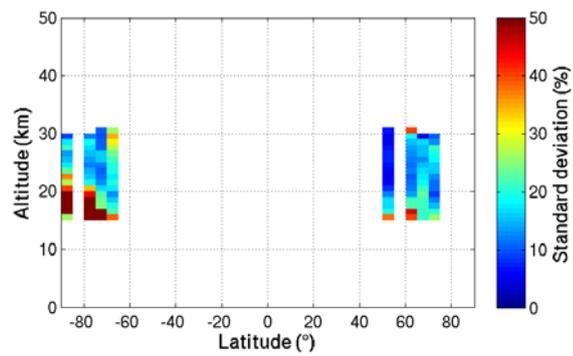
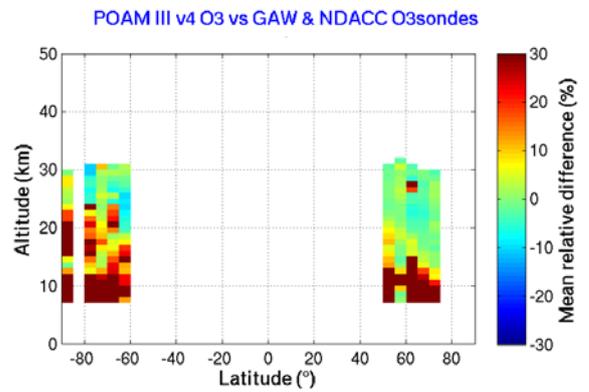
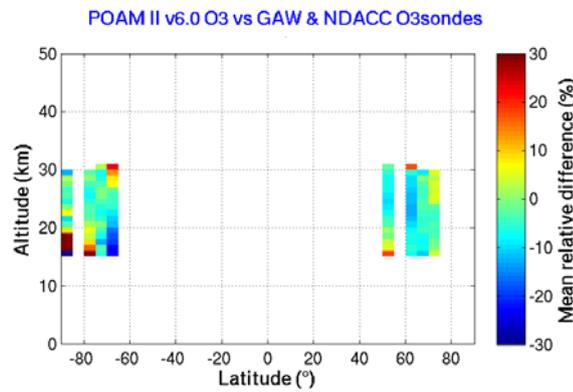


Figure 11: Same as Figure 9 but for POAM II v 6.0.

Figure 12: Same as Figure 9 but for POAM III v4.

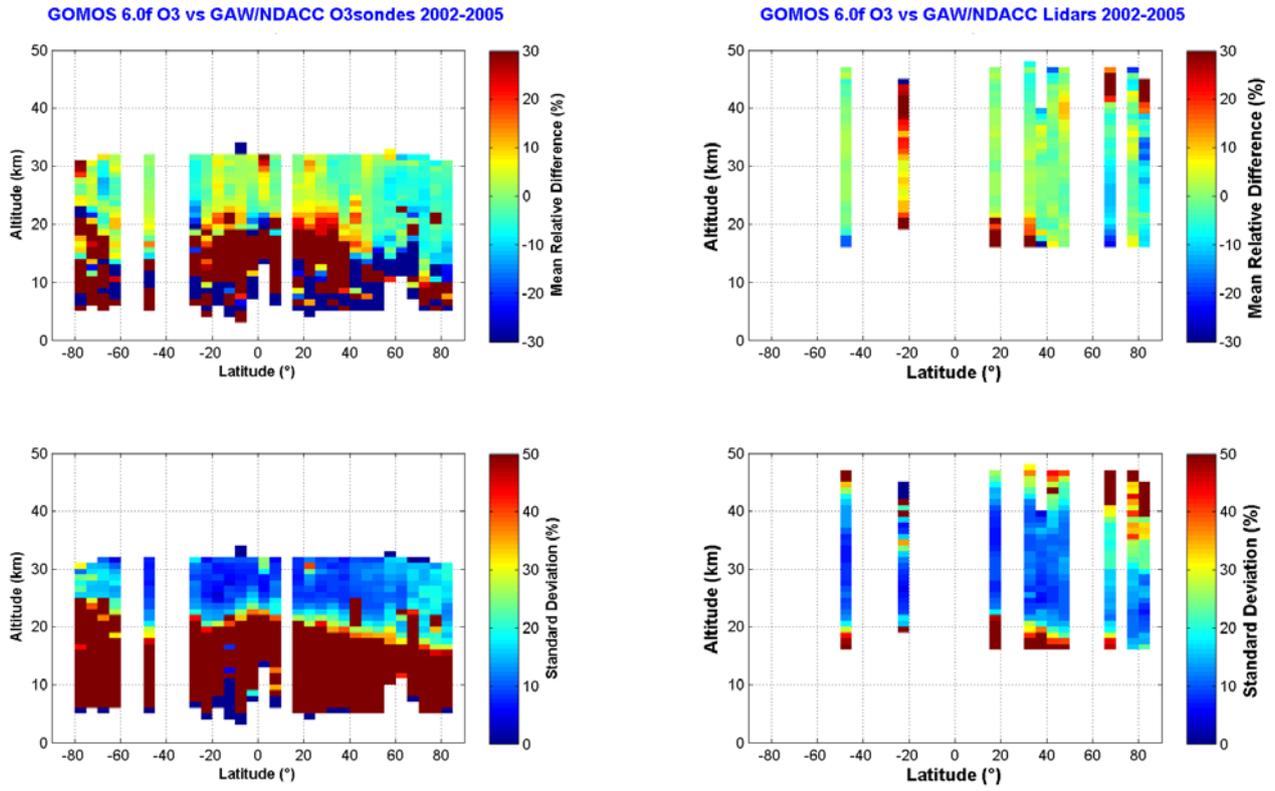


Figure 13: Same as Figure 9 but for GOMOS v6.0cf.

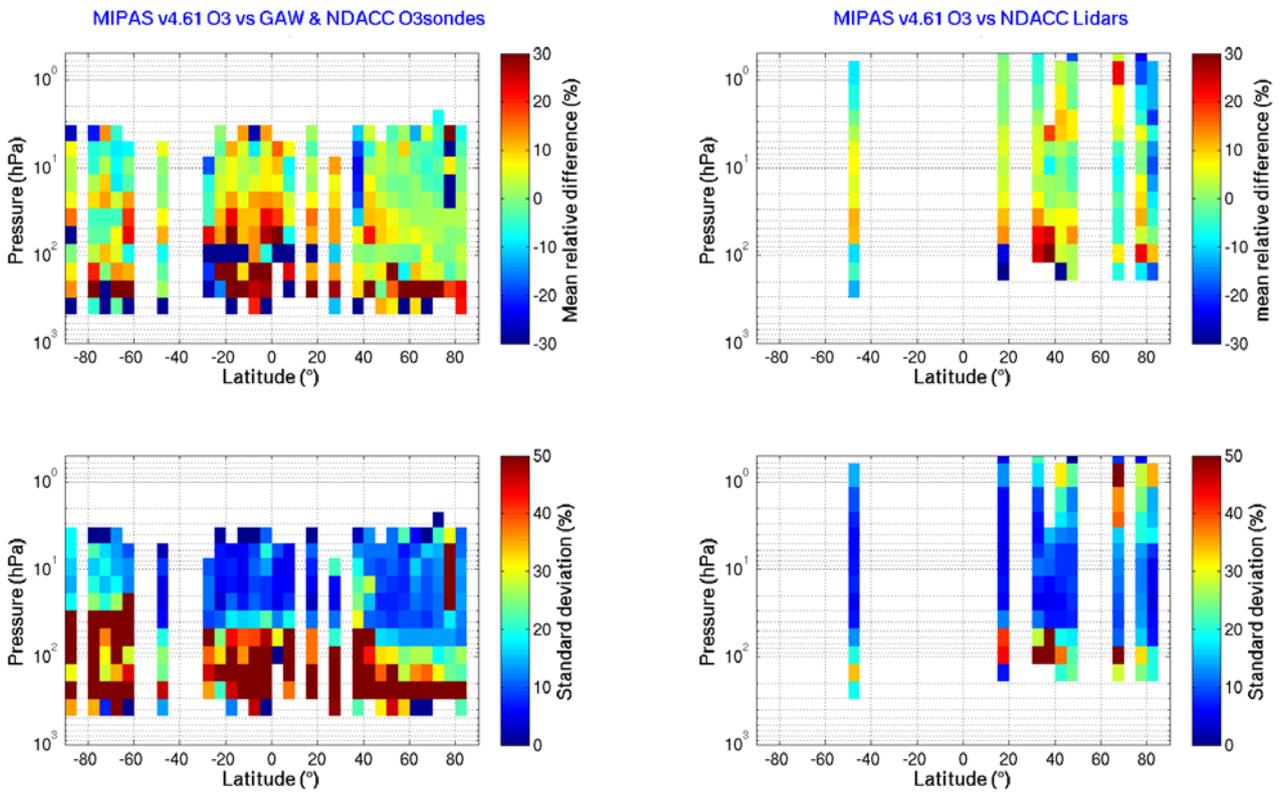


Figure 14: Same as Figure 9 but for MIPAS v4.61.

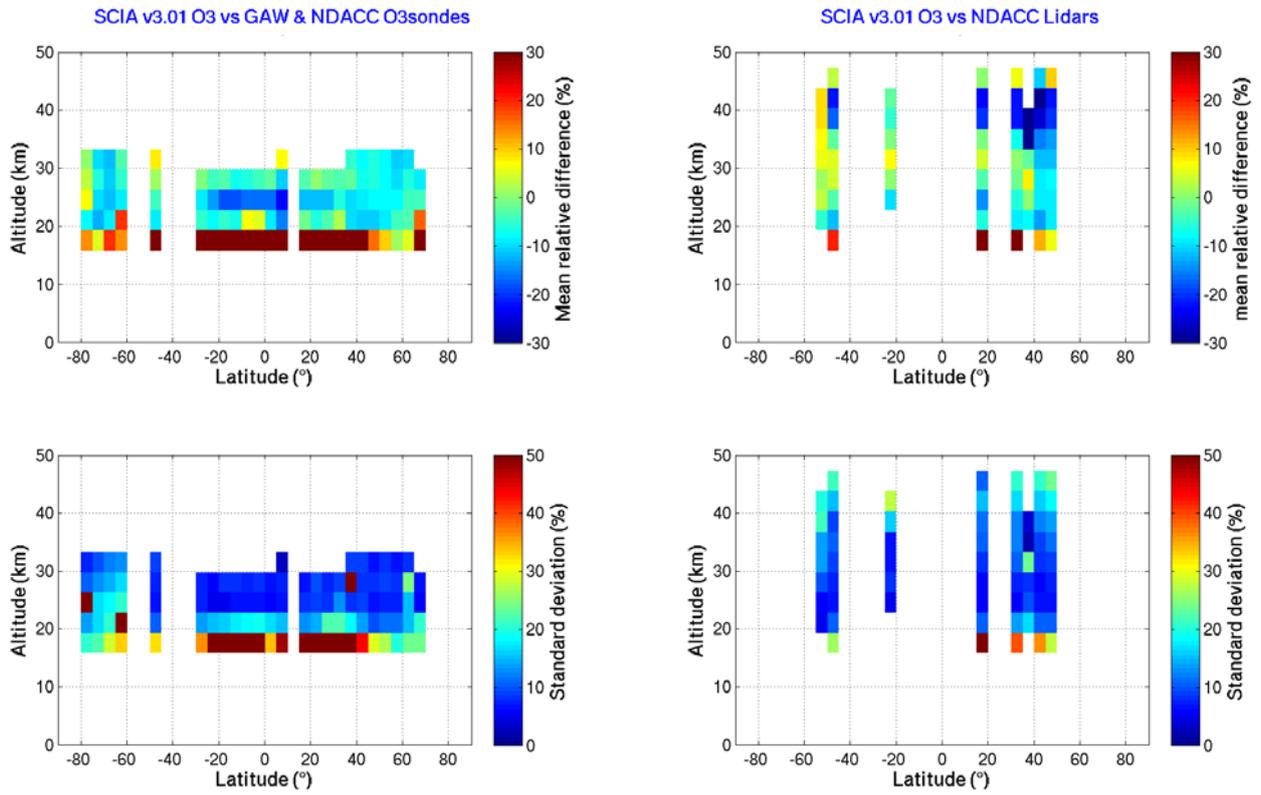


Figure 15: Same as Figure 9 but for SCIAMACHY v3.01.

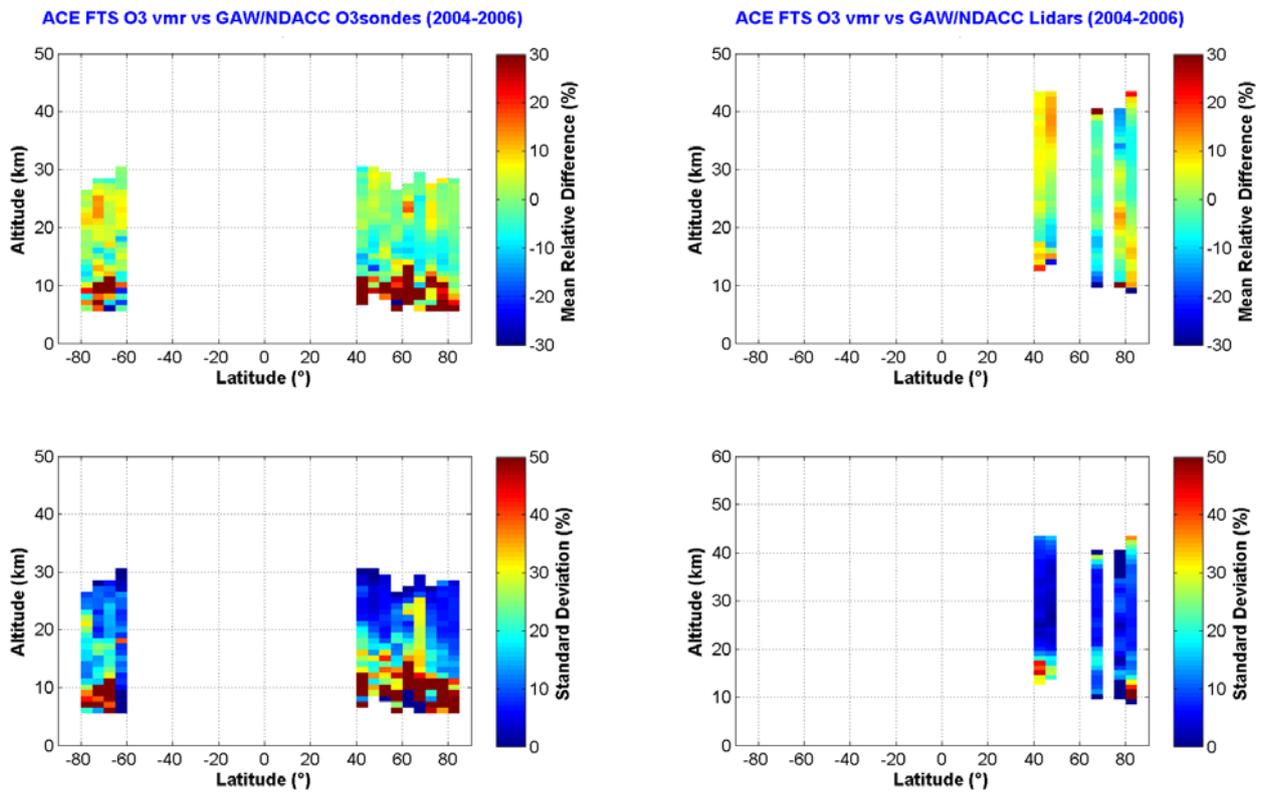


Figure 16: Same as Figure 9 but for ACE-FTS.

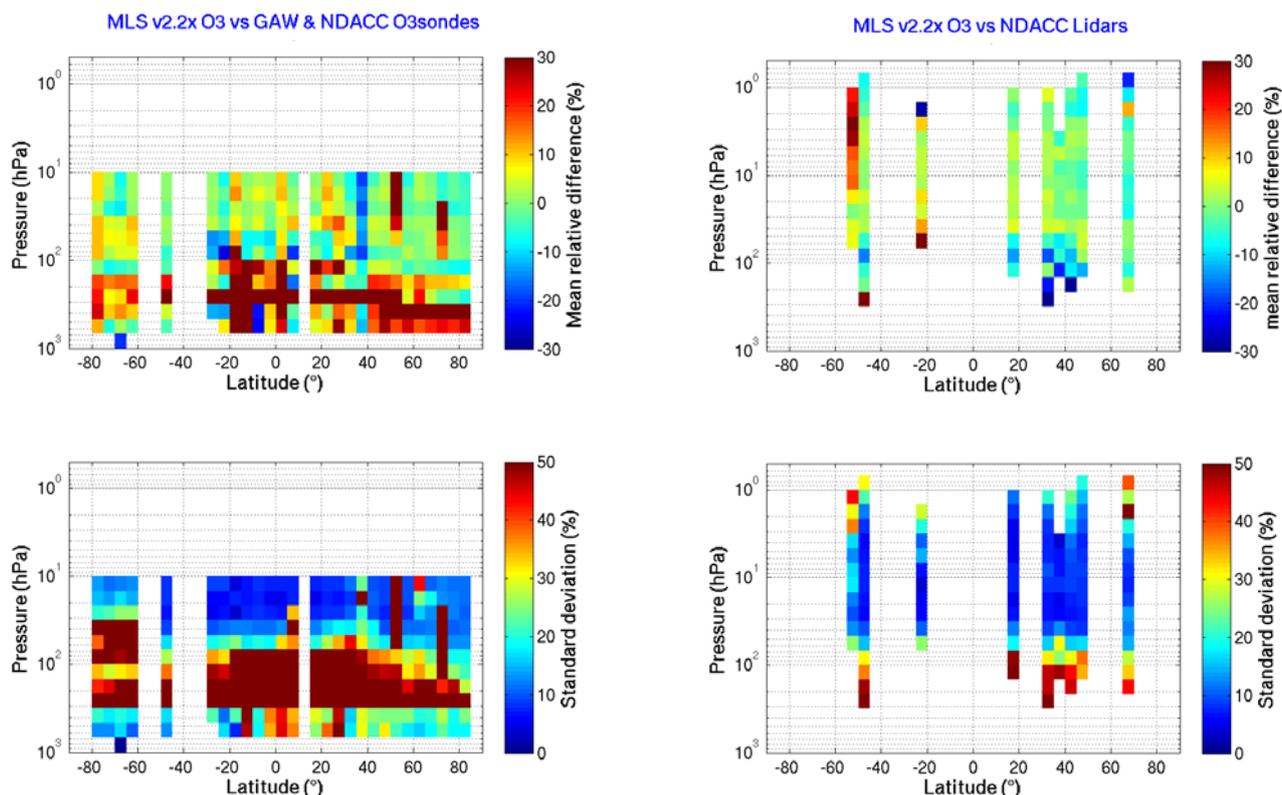


Figure 17: Same as Figure 9 but for MLS v2.2x.

4.3 Lowermost altitude

Interferences with aerosols and clouds limit the access of limb sounding to accurate information on the troposphere and UTLS [2]. As consequence, below an altitude threshold usually varying between 10 and 20 km as a function of the instrument measurement technique and the aerosol load, the quality of individual profiles can differ significantly from the quality estimates derived statistically from comparisons with correlative data. Above this threshold altitude the ozone profiles agree statistically with ground-based network data; below this altitude data quality varies strongly from one profile to another. Using the meridian and vertical analysis results reported above, we estimate here the respective threshold altitude of the nine satellites by two different means. The upper panel of Figure 18 shows the altitude below which the mean relative difference exceeds 20 %. The lower panel shows the altitude below which the standard deviation exceeds 30 %. These two criteria give similar results. The threshold altitude is found to vary as a function of latitude – following likely the meridian variation of the tropopause height – from 8 km in the Arctic to 20 km at low latitudes. It varies also primarily with the viewing technique and its radiation source: it is the lowest for infrared sounding and the highest for UV-visible star occultation. In the latter case,

atmospheric scintillation, which increases as the atmosphere becomes denser, add to the radiative transfer perturbations caused by aerosols and clouds.

5 CONCLUSION

In this paper we have studied ozone profile data records delivered by nine limb-viewing satellite instruments (SAGE II, HALOE, POAM II, POAM III, GOMOS, MIPAS, SCIAMACHY, ACE-FTS, and Aura MLS), forming all together a 25-year time series of substantial interest for scientific studies of ozone trends and of the links between ozone and climate. To study the consistency of these satellite data sets characterised by different latitude/time sampling and coverage, and to verify their compliance with data requirements for trend studies, we have compared them to the pseudo-global standard reference offered by ground-based networks of ozonesondes and lidars affiliated with NDACC and WMO's GAW. The studies reported here focus on time, altitude and latitude variations of the agreement between satellite and ground-based network data.

In the stratosphere, the analysis concludes to a mutual consistency of the nine ozone profile data records, to within 7 % \pm 10 %. However, a few exceptions and peculiarities have been detected and reported:

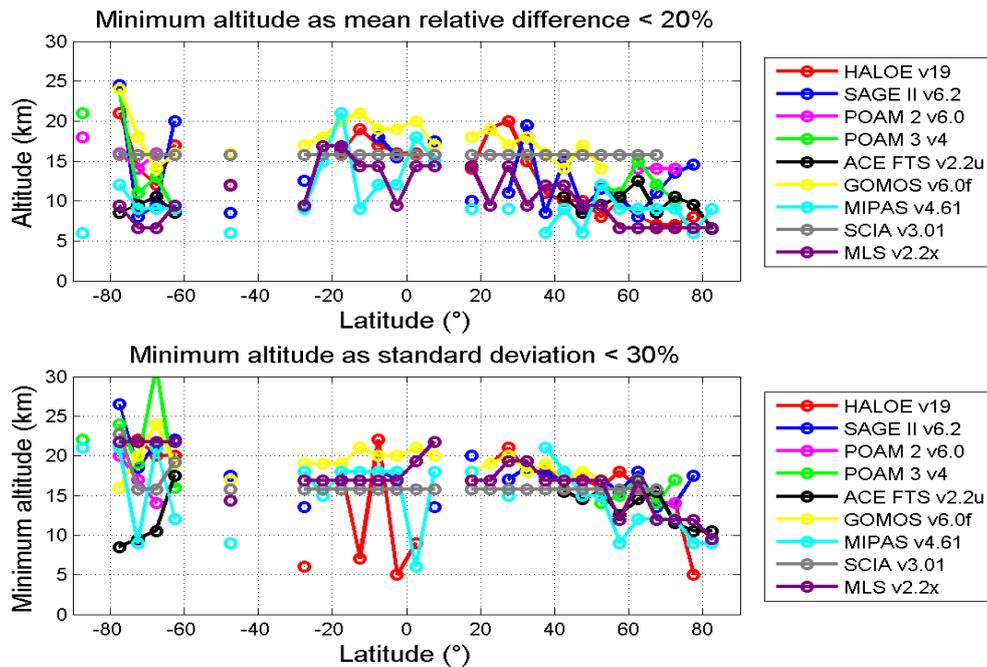


Figure 18: Lowermost altitude of satellite measurements as a function of latitude, defined as the threshold altitude above which the mean relative difference exceeds systematically 20 % (top panel) and the threshold altitude above which the 1σ standard deviation exceeds systematically 30 % (bottom panel).

- (i) Over nearly the entire altitude range, SCIAMACHY SGP 3.01 underestimates ozone densities by 10 %.
- (ii) GOMOS 6.0cf ozone profiles have a negative bias of -10 % in the Arctic.
- (iii) MIPAS v4.61 ozone profiles have a positive bias of 10 % in the inter-tropical UTLS.
- (iv) Although both agree with ground-based data with a mean difference within $\pm 7\%$, we confirm a 5 % bias between POAM II and POAM III ozone data.

For most of the data sets, the observed agreement remains stable along the satellite measurement period. However, HALOE profiles seem to suffer from a small drift of -0.5 % per year between 20 and 30 km altitude. This drift will limit the usability of HALOE data for long-term ozone trends study.

Below 10-20 km, the ozone profile data quality of any limb sounding instrument degrades rapidly. Our study shows that the threshold altitude (defined here as the lowermost altitude below which the mean difference with ground-based data exceeds 20 % or the standard deviation exceeds 30 %) varies with the latitude and the measurement technique. Lowest altitudes (10 km at the poles and 15 km at the tropics) are reached by infrared sounders like ACE-FTS, MIPAS, and HALOE, while scintillation limits this altitude to 20-25 km for the GOMOS star occultation instrument.

This work shows that ground-based networks can be used successfully as a standard transfer to investigate the consistency of ozone profile data records from (very) different satellites. However, we should remark that the station-to-station homogeneity of network data sets can depend on a variety of factors, like differences in instrument maintenance, operation, calibration, data retrieval, as well as the range of measured atmospheric states, which also varies from one station to another. Therefore, statistical studies should always be carried out with the greatest care. Considering the accuracy achieved currently by satellite ozone profilers, after appropriate selection of ground-based stations, the internal consistency of the networks seems to be sufficient for multi-mission analysis.

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