NDACC NETWORK BASED STUDY OF THE CONSISTENCY OF OZONE PROFILE DATA FROM ENVISAT, THIRD-PARTY MISSIONS AND HISTORICAL SATELLITES

Sophie Vandenbussche[(1)], Jean-Christopher Lambert[(1)], Coralie De Clercq[(1)], José Granville[(1)], Daan Hubert[(1)]
and the NDACC Ozone Profiling Team

(1)Belgian Institute for Space Aeronomy (IASB- BIRA), Avenue Circulaire, 3, B-1180 Brussels, Belgium,
Email: sophie.vandenbussche@aeronomie.be

ABSTRACT

Atmospheric ozone is one Essential Climate Variable (ECV) for which it is intended to build, from contiguous data records acquired by different measurement systems, a merged data record addressing long term and global scale features. With its three atmospheric limb profilers, Envisat adds significantly to the pseudo-global ozone profile monitoring initiated since 1958 with coordinated ground-based networks, and since the 1980s with limb/occultation satellites. In this work, NDACC lidar and GAW ozonesonde networks are used as a standard transfer to investigate the consistency of nine satellite ozone profile data records covering altogether the 1984-2009 time period. This paper focuses on the statistical detection of drifts and of meridian and vertical features.

1. INTRODUCTION

The consolidated, long-term data records required for atmospheric ozone could be obtained from atmospheric ozone profiles recorded since more than 25 years by satellite instruments, and through the new initiative from the European Space Agency, the Climate Change Initiative (CCI), which aims at constructing a merged dataset from different satellite records. However, this operation is not straightforward and needs to be preceded by a careful study of each data set. Indeed, each satellite instrument possesses its own characteristics like the limb-scanning technique, the vertical resolution, the geographical and time sampling, the long-term degradation of the instrument. Ozone profile data retrieved from each of these limb sounders' measurements also has its own features, like precision, accuracy, long-term drift, time cycles. Furthermore, those data records are rarely coincident, at best contiguous, and never perfectly matched in time and space.

In this study, we use data from nine different limb sounders altogether covering the time span from 1984 until now and having complementary or global geographical coverage. The two NASA's solar occultation missions with an orbit inclination of 57°, the Stratospheric Aerosol and Gas Experiment II (SAGE-II) [1] aboard Earth Radiation Budget Satellite (ERBS, 1984 to 2005), and the Halogen Occultation Experiment (HALOE) [2] aboard Upper Atmosphere Research Satellite (UARS, 1991-2005), 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 [3] and III [4]) aboard the polar orbiting French platforms SPOT-3/4, measured ozone profiles, from 1993 to 1996 and from 1998 to 2005 respectively, with coverage of the polar zones but no measurement at latitudes below about 56°. Since 2002, the atmospheric chemistry payload of Envisat, consisting of the Global Ozone Monitoring by Occultation of Stars (GOMOS) [5], the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) [6], and the SCanning Imaging Absorption spectroMeter for Atmospheric CartograpHY (SCIAMACHY [7]), 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) [8] 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) [9] onboard NASA's EOS-Aura, measuring the microwave limb emission with pole-to-pole sampling on a daily basis.

The work presented here is preliminary to the CCI work. We undertook the characterization of the datasets from these different instruments, and the check of their long-term consistency. Satellite to satellite validations may be undertaken (and some have been published), but they are limited to co-located measurements and suffer from the combined effects of the degradation of both instruments. Separate validation studies of each satellite dataset using ground-based instruments have also been published, but even though they rely on similar principles, small implementation differences may still exist, which would alter the comparisons. An alternative to this is the use of a global standard transfer to which each studied dataset is compared using one common method. This standard transfer could be satellite time series with daily coverage, like the American series SBUV and SBUV/2 or the European series GOME-

Proc. 'ESA Living Planet Symposium', Bergen, Norway
28 June – 2 July 2010 (ESA SP-686, December 2010)

SCIAMACHY-GOME-2. Nadir ozone profiling however exhibits a limited vertical resolution and its sensitivity varies with altitude and time. Data assimilation has been used successfully as a global validation tool to check the internal consistency of data sets, but this technique is based on models, relying on our current understanding of atmospheric processes, and should not be trusted as a validation source. 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 profiles 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 [10, 11]. Version 6.00 and 6.10 ozone profiles were compared to several ground-based and satellite data sets [12-14]. 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 [15, 16]. In this paper, we use SAGE-II version 6.20 ozone profiles.

2.2. HALOE [1991 – 2005]

Since its launch, three versions of HALOE [2] ozone profile data have been released and have experienced an extensive validation (i.e. version 17 [17]; version 18 [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% [13, 16].

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

POAM-II [3] v5 ozone profiles have been compared to measurements from satellites and from ozonesondes [19, 20]. POAM-II data shows a typical mean agreement within 5-7% above 22 km, with in general a negative bias of a few percents with respect to correlative measurements. Studies based on the current version 6 show similar results and also depict a negative bias [21]. The current version of POAM-III [4] ozone profile data is v4. Previous version v3 had been extensively validated using observations from aircrafts, balloons and satellite instruments [22]. These studies showed a typical agreement of ±5% from 13 to 60 km. Minor changes have been implemented in the current version v4 for ozone retrieval and comparisons with correlative data show a similar agreement than for v3.

2.4. MIPAS [NR 2002 - 2004/OR 2005 -]

MIPAS [6, 23, 24] operated from 2002 till March 2004, when the instrument experienced a major anomaly. In February 2005 operations were resumed in an optimised reduced resolution (OR) mode, not studied here. Latest versions of the profile retrievals at nominal resolution (NR), IPF 4.61 and 4.62, were the subject of an extensive validation effort. MIPAS profiles were compared with several other satellites, balloons and ground-based instruments [25]. This coordinated study concludes to a typical agreement within ±10% from 20 to 50 km and highlights significant positive bias of up to +25% in the Upper Troposphere Lower Stratosphere (UTLS). In this study, we used ozone data from both versions IPF 4.61 and IPF 4.62.

2.5. GOMOS [2002 -]

GOMOS [5] 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 [26, 27]. 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 [28]. 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 (including straylight data).

2.6. SCIAMACHY [2002 -]

Previous SCIAMACHY [7] Ground Processor (SGP) retrievals suffered from pointing errors [27-29] and retrieved ozone profiles exhibited an altitude shift of 0 to 1.5 km. Accordingly, comparisons concluded to an altitude-dependent bias of up to ±20%. The current SGP version 3.01 retrieves ozone profiles on an altitude grid between 15 and 40 km. SGP 3.01 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 [8] ozone profiles is version 2.2 updated. This data set has been the subject of a coordinated international validation [30] 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, with a small positive bias in ACE-FTS data with respect to correlative data.

2.8. EOS MLS [2004 -]

The current version of EOS MLS [9] ozone profile data is 2.2x. Recent validations studies show an overall agreement with lidars, aircrafts, ozone sondes and other satellites within 5% to 10% in the stratosphere [31]. In this work, we used only data with the status flag at zero (no problem occurred during the retrieval and no clouds in the field of view).

3. CORRELATIVE GROUND-BASED DATA AND CO-LOCATION CRITERIA

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 [34, 35].

Most ozone sonde 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 [36, 37] (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 [38] (SHADOZ, http://croc.gsfc.nasa.gov/shadoz).

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. Even if more accurate selection methods do exist, 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 co-located 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. Co-locations of satellite and ground-based profiles have been identified according to the above criteria for 50 ozonesonde and 10 lidar stations.

4. COMPARISON RESULTS

4.1. Seasonal and long-term features

In this first part of our study, we analyze time series of the relative differences between satellite and correlative data at selected altitude/pressure levels. In particular, we look for any seasonal feature or long-term drift.

Seasonal features were observed only in SCIAMACHY comparison data, over the whole altitude range. The relative differences with ground-based data are more positive (or less negative where there is a negative bias) in the summer, and more negative in the winter. The amplitude of the cycle is of about 10%. These features will maybe be corrected in the new SGP algorithm, version 5.01, currently under delta validation.

Long-term drifts of satellite data are searched for using a robust linear regression method, iteratively minimizing a 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. No regression is undertaken if the standard deviation of the dataset exceeds 30%, or if the time series comprises less than 20 co-located pairs of profiles. The slope of the regression is considered to be significantly different from zero if zero is not in the 95% confidence interval (slope ± 2*error) of the calculated slope. The error on the calculated slope is obtained using standard statistics, to which the effect of noise autocorrelation is added as described in Eq.1 (where σ_x: standard deviation on the dates; σ_N; standard deviation on the regression residuals; N: number of data entries; ϕ: noise autocorrelation).

$$\sigma = \frac{\sigma_N}{\sigma_x * \sqrt{N-1}} \sqrt{\frac{1+\phi}{1-\phi}} \tag{1}$$

This temporal analysis has been performed for each satellite at each selected ground-based station. Graphs representing these drift results as a function of the latitude, for different altitude levels, are shown in Figs 1 to 5. Significant drifts are plotted in red (for comparisons with lidar data) or blue (for comparisons with ozonesonde data) while non-significant drifts are plotted in grey. The 95% confidence intervals are also displayed as a bar of the same colour as the drift.

In order for the presence of drifts to be detected, a sufficiently long time series of data and a sufficient number of coincident pairs of profiles is required. For this reason, the analysis is inconclusive for POAM-II/III, MIPAS, ACE-FTS and EOS MLS. For these instruments, drifts are indeed detected, but they are not significant and/or not consistent at all from station to station (see for example Fig. 1 for MIPAS). This analysis will probably improve for ACE-FTS and EOS MLS when the time series get longer. For MIPAS, the upcoming OR data will allow for a new drift analysis to be undertaken, on a longer time series also.

For SAGE-II and HALOE, the time series and the sampling are largely sufficient to obtain a reliable drift analysis. SAGE-II comparison data (Fig. 2) shows a stable agreement with ground-based data during the whole life of the instrument. HALOE comparison data (Fig. 3) bears negative drifts of about 0.5 to 1% per year at about 25 km altitude (22.6 hPa), for Northern mid-latitude stations.

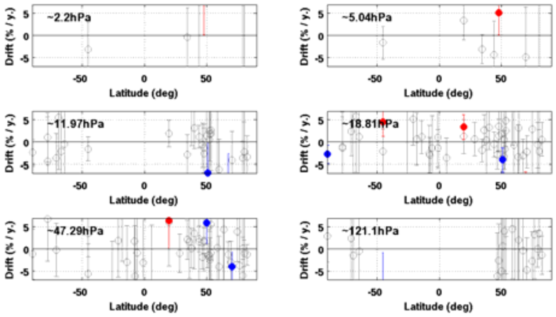

Figure 1: Slope of the multi-year linear trend fitted to time series of the relative differences between MIPAS IPF 4.61/4.62 and ground-based (ozonesonde and lidar) ozone measurements at each station, plotted as a function of latitude and at different pressure levels. Red dots (comparisons vs. lidars) and blue dots (comparisons vs. ozonesondes) represent trends with statistical significance (95% confidence level). Trends with no significance are shown in grey.

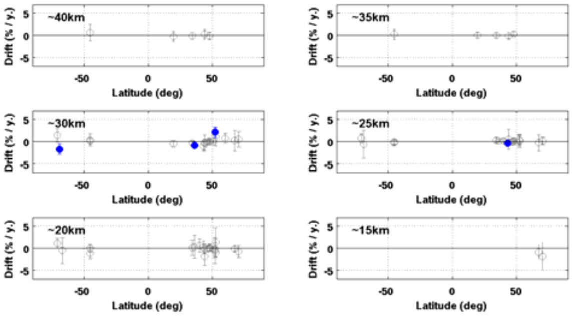

Figure 2: Same as Fig. 1Figure 3, for SAGE-II v6.2 at different altitude levels.

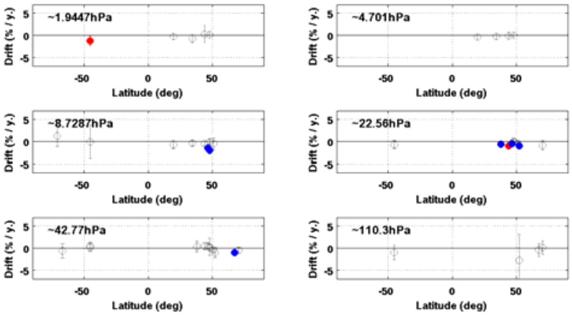

Figure 3: Same as Fig. 1Figure 3, for HALOE v19.

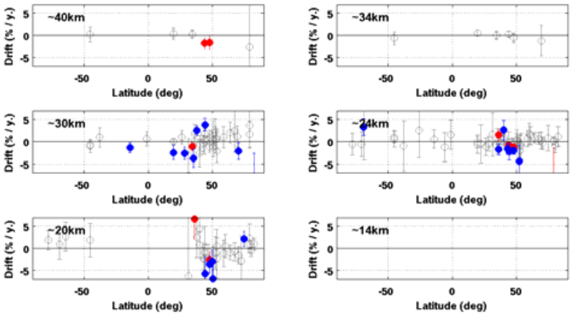

Figure 4: Same as Fig. 1Figure 3, for GOMOS IPF 5.00 / GOPR 6.0cf at different altitude levels.

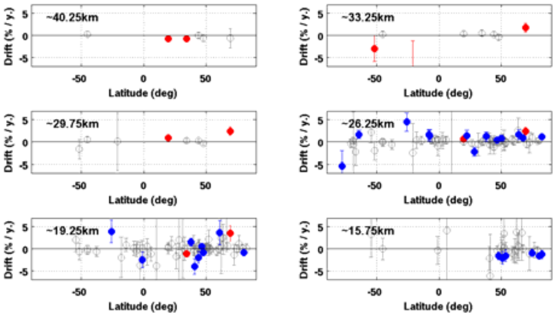

Figure 5: Same as Fig.1, for SCIAMACHY SGP 3.01 at different altitude levels.

For GOMOS (Fig. 4) and SCIAMACHY (Fig. 5), the analysis concludes in the detection of significant drifts, even if they are not fully consistent from station to station. GOMOS data shows negative drifts of 1 to 2% per year at Northern mid-latitudes, from 20 to 30 km altitude. SCIAMACHY data presents, in addition to the seasonal cycle already mentioned, positive drifts of 1 to 2% per year at 26 km altitude, all latitudes, and negative drifts of 1 to 2% per year at 19 km altitude, high Northern latitudes. This analysis will certainly enhance with the lengthening of the time series, and maybe for SCIAMACHY with the new version of the algorithm (SGP 5.01), currently under delta validation.

4.2. Meridian and vertical structures

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. Figs 6 to 11 show, as a function of latitude and altitude, the median relative difference between satellite and correlative ground-based data, averaged into 5°-wide latitude bins.

In general, the mean agreement between satellite and ground-based data in the stratosphere is of 7% or better, with a standard deviation of about 10%. For each instrument, there is also an altitude below which the statistical quality of the data degrades rapidly. This point will be addressed in the next section. In the following paragraphs we will discuss features which differ from the general ones.

SAGE-II comparison data (Fig. 6) shows slightly larger differences and standard deviations in Antarctica than at other latitudes. This can be associated with the high dynamics of the ozone hole, and therefore does not point to a lower quality of the satellite data.

In HALOE comparison data (Fig. 7), 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.

Our analysis using the ground-based networks as standard transfer confirms a 5% bias between POAM-II and POAM-III datasets, even though both agree with ground-based data within about 7% like the other instruments.

For MIPAS (Fig. 8), data shows a permanent positive bias of 10 to 15% in the inter-tropical upper troposphere and lower stratosphere.

For GOMOS (Fig. 9), a mean negative bias of 10% is observed at Arctic stations. The GOMOS Quality Working Group (QWG) is investigating possible links between this bias and the contamination of GOMOS spectra by auroral light.

SCIAMACHY comparison data (Fig. 10) bear a negative bias of about 10% at all altitudes. The stability of this bias with altitude indicates that the altitude pointing correction implemented in SGP 3.01 is working properly.

ACE-FTS (Fig. 11) and EOS MLS data do not show any feature different from those of all satellite datasets described before.

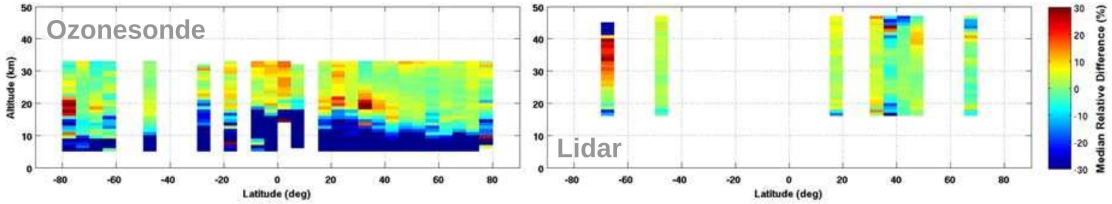

Figure 6: Median relative differences between SAGE-II v6.2 and ozonesonde (left) or lidar (right) ozone profile data, as a function of altitude and latitude.

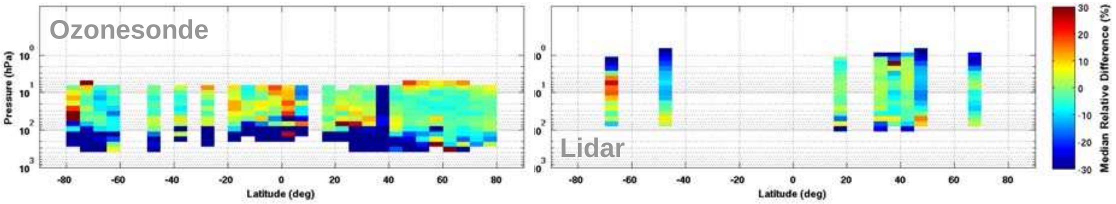

Figure 7: Same as Fig. 6, for HALOE v19 data

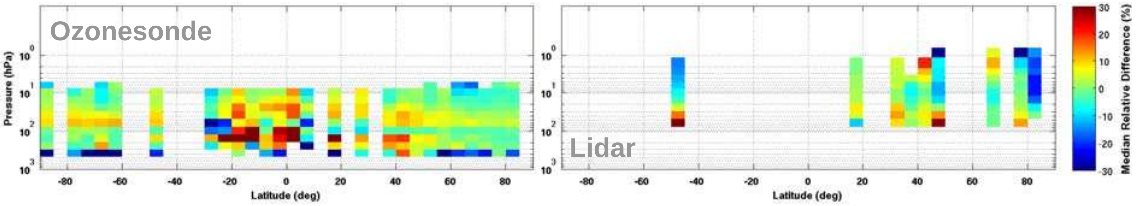

Figure 8: Same as Fig. 6, for MIPAS IPF 4.61/4.62 data

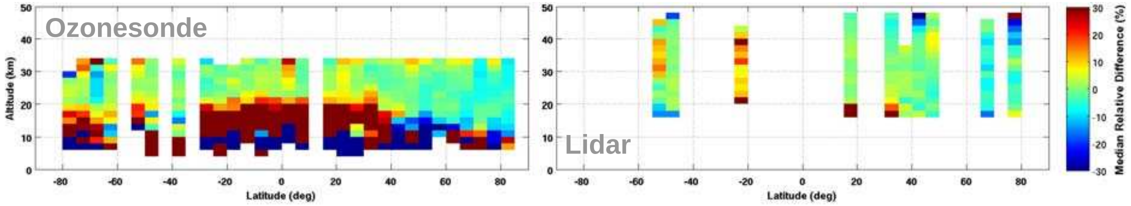

Figure 9: Same as Fig. 6, for GOMOS IPF 5.00 / GOPR 6.0cf data

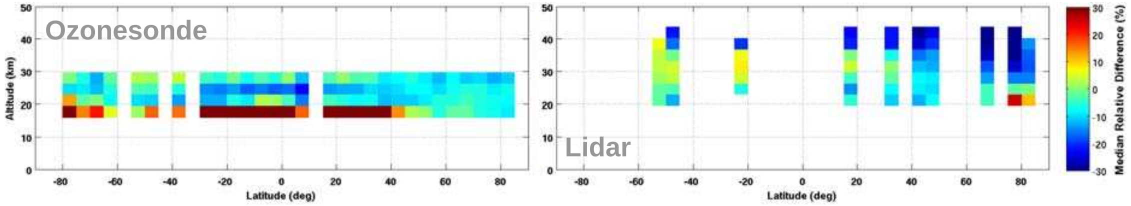

Figure 10: Same as Fig. 6, for SCIAMACHY SGP 3.01 data

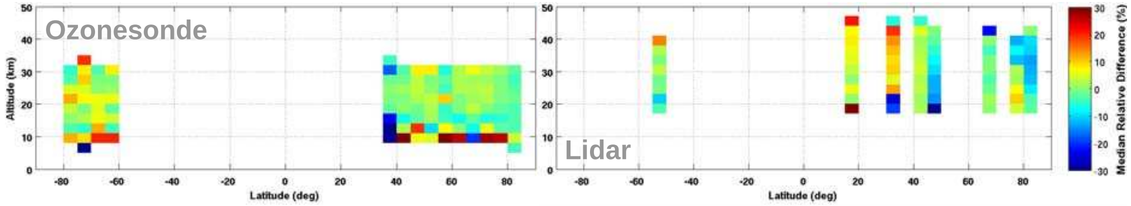

Figure 11: Same as Fig. 6, for ACE-FTS v2.2 data

4.3. Lowest altitude with statistical quality

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 studied sounders by two different means. The upper panel of Fig. 12 shows the altitude below which the median relative difference exceeds 20%. The lower panel shows the altitude below which the half 68% inter-percentile exceeds 30%. These two criteria give similar results.

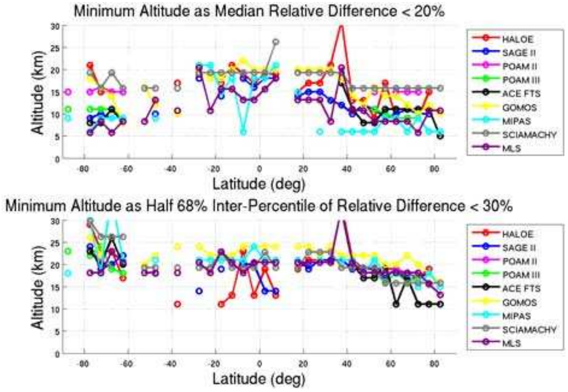

Figure 12: Threshold altitude of satellite measurements, above which median relative differences exceed systematically 20% (top panel) and above which half 68% inter-percentiles exceed systematically 30% (bottom panel).

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 (5 to 15 km) and the highest for UV-visible scattering and star occultation (15 to 20 km). In the star occultation 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 EOS 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. This work is preliminary to the work to be done in the ESA Climate Change Initiative program. To study the consistency of these nine satellite data sets characterized 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'sGAW. 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%±10%. However, a few exceptions and peculiarities have been detected and reported:

(i) Over the entire altitude range, SCIAMACHY SGP 3.01 underestimates ozone densities by 10%.
(ii) GOMOS IPF 5.00 / GOPR 6.0cf ozone profiles have a negative bias of 10% in the Arctic.
(iii) MIPAS IPF 4.61/4.62 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 ±7%, we confirm a 5% bias between POAM-II and POAM-III ozone data.

For most of the data sets, the observed agreement seems to remain stable along the satellite measurement period. However, except for SAGE-II where the dataset has sufficient length and sampling to allow concluding that no drift indeed occurs, the absence of drift detection is not a certainty that the dataset is stable in time. Indeed, it may be only due to the short time series of data available and/or the low time sampling. Exceptions to this absence of drifts are HALOE, GOMOS and SCIAMACHY. HALOE profiles suffer from a small negative drift of 0.5 to 1% per year at 25 km altitude, Northern mid latitudes. GOMOS bears a negative drift of 1 to 2% per year from 20 to 30 km altitude at Northern mid-latitudes. SCIAMACHY, in addition to a seasonal behaviour, shows positive drifts of 1 to 2% per year at 26 km altitude at all latitudes and negative drifts of 1 to 2% per year at 19 km altitude at high Northern latitudes. However, for both GOMOS and SCIAMACHY, the analysis is not fully consistent from station to station and would greatly benefit from the extension of the time series. The use of these three datasets for the establishment of long-term ozone profile time series is limited by the presence of drifts.

Below 10-20 km, the ozone profile data quality of any limb sounding instrument degrades rapidly, and should not be used in the establishment of long-term ozone profile records. 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 18-20 km for the GOMOS star occultation instrument and scattering limits this altitude to 15-20 km for the SCIAMACHY UV visible 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 wit 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.

6. ACKNOWLEDGEMENTS

This work has been funded by ESA's multi-mission validation project Multi-TASTE, by the Belgian Science Policy Office and ESA via the ProDEX project SECPEA, and by EC FP6 GEOmon. Ozonesonde and lidar data were obtained as part of the Network for the Detection of Atmospheric Composition Change (NDACC) and WMO's Global Atmosphere Watch (GAW), and are publicly available via *www.ndacc.org* and *www.woudc.org*. We acknowledge the scientific and technical support of lidar and ozonesonde PIs and the staff at the stations, as well as the science and processing teams of the various satellite data.

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