

# TOWARDS A MERGED ESSENTIAL CLIMATE VARIABLE DATA RECORD ON OZONE: STABILITY AND CONSISTENCY OF CONTRIBUTING LIMB PROFILERS

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## ABSTRACT

Various international initiatives intend to build a merged data record on the vertical profile of ozone, an Essential Climate Variable, which should allow the study of processes on the long term and at the global scale. 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. Here we use lidar and ozone-sonde network data as a transfer standard to investigate the stability and consistency of twelve satellite ozone profile data records covering altogether the 1984-2012 time period. This paper focuses on the determination of long-term drifts and of meridian and vertical features of the bias and the variability of the satellite data records.

## 1. INTRODUCTION

The vertical distribution of atmospheric ozone, an Essential Climate Variable (ECV), has been measured from space for nearly three decades by various instruments, each with their particular measurement and retrieval technique. The synergistic use of complementary ozone data records from the different satellite missions should improve our understanding of interactions between changes in ozone, ultraviolet radiation and climate on the global scale and in the long term. In this context, several international efforts were recently launched, like ESA's Climate Change Initiative project on ozone (Ozone\_cci) and the SPARC/IO<sub>3</sub>C/WMO-IGACO Initiative on Past Changes in the Vertical Distribution of Ozone (SI2N). A prerequisite to build the targeted ECV ozone data record is that the long-term stability, bias and mutual consistency of the contributing instruments meet the user requirements expressed by, e.g. the climate research community. Systematic stability and mutual consistency studies were initiated in ESA's Multi-TASTE project for Envisat and Third Party Missions (TPMs), which paved the way for network-based, multi-mission validation assessments.

In this framework of ECV construction, we investigate the suitability of current data versions of seven ESA and TPM limb/occultation ozone profilers, as well as five historical data records acquired by American satellites, namely: ERBS SAGE-II, UARS HALOE, SPOT-3

POAM-II and SPOT-4 POAM-III, Odin OSIRIS and SMR, Envisat GOMOS, MIPAS and SCIAMACHY, SCISAT-1 ACE-FTS and ACE-MAESTRO, and EOS-Aura MLS. The assessment of biases and drifts and their analysis is based on the data provided by ozonesonde and lidar networks affiliated with NDACC and WMO's GAW, used here as transfer standard. For each satellite instrument, we present the temporal, vertical and meridian structure of the consistency between co-located space- and ground-based profiles. Our results are further discussed against user requirements, in the context of the developing ozone ECV within the SPARC SI<sup>2</sup>N and Ozone\_cci initiatives.

## 2. SATELLITE OZONE DATA SETS

### 2.1 SAGE-II v6.20

[1984–2005]

The NASA Stratospheric Aerosols and Gas Experiment II (SAGE-II) aboard the ERBS satellite [1] was a solar occultation grating spectrometer and measured, from October 1984 to August 2005, atmospheric absorption spectra in the infrared. These data allowed retrieval of ozone profiles with 1 km resolution from 60 km down to cloud top level, covering from 80° N to 80° S.

Different versions of SAGE-II 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 [4-6]. 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-II version 6.20 ozone profiles.

### 2.2 HALOE v19

[1984–2005]

NASA's Halogen Occultation Experiment (HALOE) was launched on board the UARS satellite [9]. HALOE, a solar occultation grating spectrometer, measured atmospheric absorption in the infrared between October 1991 and November 2005 from 80° N to 80° S. Ozone profiles are retrieved from about 15 km up to 60-130 km with 1.6 km vertical resolution.

Since its launch, three versions of HALOE ozone profile data have been released and have experienced an extensive validation (i.e. version 17 [10],

version 18 [11]). The latest public version, version 19, is used in this work. Validation studies of this current version show a general agreement with other satellite and ground-based instruments within 10% [5, 8].

### **2.3 POAM-II v6 / [1993–1996 POAM-III v4 / 1998–2005]**

The American Polar Ozone and Aerosol Measurement II (POAM-II) [12] was launched aboard the French SPOT-3 platform. It observed solar occultations in the UV/VIS/NIR range from September 1993 to November 1996, at mid to high latitudes. The slightly improved follow-up instrument, Polar Ozone and Aerosol Measurement III (POAM-III) [13], was launched on the SPOT-4 satellite in March 1998 and remained operational until December 2005.

POAM-II v5 ozone profiles have been compared to measurements from satellites and from ozone-sondes [14, 15], which indicate a typical mean underestimation of 5-7% above 22 km. Studies based on the current version 6, used in this work, show similar results and also depict a negative bias [16]. The previous POAM-III data version v3 has been extensively validated using observations from aircrafts, balloons and satellite instruments [17]. These studies showed typical agreement of  $\pm 5\%$  from 13 to 60 km. Minor changes have been implemented for the ozone retrieval in the current version v4, used in this work, and comparisons studies show a similar agreement as for v3.

### **2.4 OSIRIS v5.07 [2001– ]**

The Swedish-Canadian-French-Finnish Optical Spectrograph and InfraRed Imager System (OSIRIS) [18] aboard the Odin spacecraft records limb-radiance profiles between  $82^\circ$  N and  $82^\circ$  S since February 2001. The UV/VIS/NIR spectra allow the retrieval of ozone from cloud top to 60 km, with a vertical resolution of about 2 km.

In this paper we investigate the recently released v5.07 data set. Studies of a preceding data set concluded to a 2% mean agreement with SAGE-II between 18-53 km [19], and a 3% agreement of the 14-52 km partial columns with ACE-FTS and ACE-MAESTRO [20].

### **2.5 SMR v2.1 [2001– ]**

The Sub-Millimetre Radiometer (SMR) [21] is the second Swedish-Canadian-French-Finnish instrument on the Odin platform, sharing its time equally between astronomy and aeronomy observations from February 2001 to April 2007. From then on, the five receivers were exclusively pointed towards Earth's limb to record thermal emission. These data allow the retrieval of ozone from about 18 to 65 km, with a vertical resolution of about 3 km in middle atmosphere.

In this study we investigate the Chalmers v2.1 data set retrieved from the 501.8GHz band. Earlier studies comparing SMR to ground-based, balloon and satellite data pointed to the existence of large vertical oscillations and an agreement within 0.15 to 0.30 ppmv, depending on the validating instrument [22].

### **2.6 GOMOS IPF 5.01 / GOPR 6.0cf [2002–2012]**

The instrument Global Ozone Monitoring by Occultation of Stars (GOMOS) [23], part of the European Envisat payload, operated from July 2002 until the loss of the platform in April 2012. Its medium resolution spectrometer observed up to 40 stellar occultations per orbit in the ultraviolet, visible and infrared. Ozone is retrieved from 15-80 km, with a resolution of  $\sim 1.5$  km.

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 [24, 25]. Comparisons between ground-based data and dark limb profiles of the processor IPF 5.01 and its scientific implementation version 6.0cf have shown a typical agreement below 5-10% from 20 km up to 40 km [26, 27]. In this work, we used the dark limb and stray light profiles of this version.

### **2.7 MIPAS IPF 5.05 [2002–2012]**

Another Envisat instrument, the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) [28], operated from July 2002 to April 2012. This Fourier Transform Spectrometer measured the infrared emission at the limb during day and night, from Pole to Pole. In March 2004 the instrument experienced a major anomaly, but operations could be resumed in January 2005 in an optimized resolution mode (with reduced spectral but increased vertical sampling). Ozone profiles are retrieved from 68 to 6 km with a vertical resolution of about 3 km [29, 30].

Earlier data versions, IPF 4.61 and 4.62, could only process the nominal resolution spectra recorded prior to March 2004. The resulting ozone profiles were extensively compared to data from other satellites and ground-based instruments [31]. A typical agreement within  $\pm 10\%$  was found from 20 to 50 km and a significant positive bias of up to +25% in the Upper Troposphere Lower Stratosphere (UTLS). Here, we study the IPF 5.05 data set which contains profiles from the full mission. First comparisons to ground-based data showed similar results as for the profiles measured before the instrument anomaly [32].

### **2.8 SCIAMACHY SGP 3.01 [2002–2012]**

The SCanning Imaging Absorption spectroMeter for Atmospheric CHartography (SCIAMACHY) [33] completes the atmospheric chemistry payload of

Envisat. This grating spectrometer recorded from July 2002 to April 2012 UV/VIS/NIR light in the limb, nadir and occultation viewing mode. The limb data permit near-global retrieval of ozone between 15 and 40 km, with a vertical resolution of roughly 3 km.

In this paper we study the SGP 3.01 ozone profile data. Even though this version reduced the altitude shift noticed for earlier processors [25, 34, 35], a small shift remains and a negative bias of about 10% with respect to ground-based measurements is present at all altitudes [26, 36].

### 2.9 ACE-FTS v3.0 [2003– ]

The Atmospheric Chemistry Experiment Fourier Transform Spectrometer (ACE-FTS) instrument [37] is part of the Canadian SCISAT-1 platform, carrying out routine measurements since February 2004. Its Michelson interferometer observes solar occultations from 85° N to 85° S in the mid-infrared. Ozone profiles are retrieved from the cloud top level up to about 95 km with a vertical resolution of about 3-4 km.

An earlier version of ACE-FTS ozone profiles, version 2.2 update, was extensively compared to satellite, ground and balloon-based instruments [38]. Between 15 and 45 km a typical positive bias of 5% was found, increasing to 20% in the upper stratosphere. This paper uses the latest v3.0 data set, which seems to reduce the positive bias by about 5% above 40 km.

### 2.10 ACE-MAESTRO v1.2 [2003– ]

A second solar occultation instrument on-board SCISAT-1 is Measurements of Aerosol Extinction in the Stratosphere and Troposphere Retrieved by Occultation (MAESTRO) [39]. Its dual spectrophotometer, operational since February 2004, covers the UV-visible and the visible-near-IR domain. Ozone profiles are retrieved from 85° N to 85° S and from cloud top to 100 km with a resolution of about 1.5 km.

Here we study the latest version 1.2 of ozone profiles from the visible spectrometer, which were compared to ozonesonde and satellite measurements in [40]. The general agreement is about 5-10% from 15-40 km, but with opposing signs for sunrise and sunset observations. Above 40 km the sunset profiles overestimate the correlative data by 20-30%. The UV data lead to reduced quality above 30 km [39].

### 2.11 Aura-MLS v3.3 [2004– ]

NASA's Microwave Limb Sounder (MLS) [41], on-board EOS-Aura, observes thermal emission in the (sub)millimeter region during day and night since August 2004. Vertical profiles of ozone are retrieved

between 82° N and 82° S and from 10 to 75 km, with a resolution of about 3 km.

The previous release of Aura-MLS ozone profiles, version 2.2, showed in the stratosphere a 5-10% agreement with other satellite, aircraft, balloon and ground-based data [42, 43]. The latest data version 3.3 introduces a finer pressure grid and extends the vertical range for ozone. However, first studies reveal cloud-induced vertical oscillations in the Tropical UTLS [44].

## 3. CORRELATIVE GROUND-BASED 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, which typically occurs around 30 km [45]. The vertical resolution of the ozone profile is usually 100-150 m and the bias is estimated to be within 5% to 7% [46].

Differential absorption lidar (DIAL) systems measure the vertical distribution of night-time ozone number density at altitudes from 8-15 km to 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 [47, 48].

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 [49, 50] (NDACC), World Ozone and UV radiation Data Center (WOUDC), and Southern Hemisphere ADditional OZonesonde programme [51] (SHADOZ).

## 4. DATA PREPROCESSING

The satellite and correlative ozone profiles entering the comparison analysis are screened according to the guidelines of the responsible data provider. Depending on the recommendations data are removed for single vertical levels or for the entire profile.

We adopt 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 though more accurate selection methods exist, given the horizontal resolutions of the satellite and ground-based measurements, a maximum distance of 500 km was found to be the best compromise between a sufficient coincidence of the sampled air masses and a sufficient number of collocated pairs of profiles.

While the selection of horizontal coincidence criteria offers some flexibility, temporal distance criteria are constrained directly by the measurement time of the data being compared, which depends on parameters like the radiation source and the orbit inclination. In this study, 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 88 ozonesonde and 13 lidar stations.

All profiles are regridded, using [52], on a common grid that reflects the vertical range and resolution of the satellite data. The comparison results presented below are in the nominal coordinate system of the satellite instrument. However, additional consistency checks were performed, in the alternative vertical (altitude or log pressure) and/or ozone (volume mixing ratio or number density) coordinates.

## 5. COMPARISON RESULTS

### 5.1 Long-term stability

Long-term drifts of the satellite data w.r.t. correlative data are determined from the regression of the daily averaged time series of the relative ozone differences at each station, and for each vertical level in the grid.

We used a robust regression method that iteratively minimizes the Tukey bisquares weighted sum of the squared residuals. The baseline fit model includes a linear term, where the slope represents the long-term drift. The standard deviation of the fitted drift was computed with the standard statistical formula, to which the factor  $\sqrt{[1 + \phi(z)]/[1 - \phi(z)]}$  is added to account for autocorrelations  $\phi(z)$ . The usual  $2\sigma$  significance threshold is adopted to reject the no-drift hypothesis.

Since a good estimate of the drift error is essential; it was computed with an alternative, bootstrap method as well. The drift errors presented below however are not those of the bootstrap method, since these are in general smaller and we prefer to quote the conservative edge of our results at the moment. A second consistency check was to feed the regression with monthly averaged and non-averaged time series. These settings produced a very consistent picture, even though e.g. the monthly averages lead to larger drift errors because of the smaller sample size. Adding a seasonal term to the model did not alter the results either, nor were our conclusions different when changing coordinate system.

The drift results at individual stations are shown in Fig. 1 as a function of the latitude, for different vertical levels. The drift results vary strongly from station to station, in sign, magnitude and significance. Since no

clear meridian structure is visible, our further conclusions are based on the global weighted mean and its standard deviation. These are shown as the solid black line and dashed red line.

In general, significant drifts at single stations remain below 20% per decade; the global average is typically not larger than 5% per decade. Fig. 1 demonstrates that the SAGE-II, OSIRIS and Aura-MLS instruments are very stable with respect to correlative data, with insignificant drifts of 1-2% / dec. These data records are long and the comparison time series sufficiently sampled to be sensitive to global 3-5% / dec. drifts.

For other instruments, like HALOE, POAM-III, GOMOS, MIPAS and SCIAMACHY we do find significant global drifts at certain altitude levels. HALOE drifts with -5% / dec. between 25-30 km. POAM-III probably has a -5% / dec. drift at 30 km. GOMOS seems to drift -(5-10)% / dec. below 25 km, possibly due to the uncorrected for increase in dark current with time. MIPAS drifts are +10% / dec. at 30 km and -5% / dec at 20 km, which is quite surprising and currently not understood. It might be caused by an altitude-dependent difference in bias between the full and optimized resolution part of the mission. SCIAMACHY has a drift at 30km, of about +5% / dec.

For the remaining instruments (POAM-II, SMR, ACE-FTS, ACE-MAESTRO), the comparison time series are too short or too sparsely sampled for an accurate detection of drifts. However, drifts are likely below the  $\sim 10\%$  / dec. level.

### 5.2 Meridian and vertical structure

In general the agreement between satellite and ground-based data does not vary strongly between stations close in latitude, which allows us to derive zonal statistics. These are then used to investigate the vertical and meridian structure of the bias and variability (not shown here) of the satellite data. Fig. 2 shows, as a function of latitude and altitude, the median relative difference between satellite and correlative ground-based data, averaged into  $5^\circ$ -wide latitude bins.

For most instruments, the median agreement between satellite and ground-based data is 5-10% or better between 20-40 km, with a spread of about 10%. Around the UTLS all instruments show increased bias ( $\pm 30\%$ ) and variability (50%). Here the relative differences become more pronounced due to lower ozone abundances, but clouds and aerosols play an important role as well. Although each data set fits the above picture rather well, the comparisons uncover particular qualitative and quantitative features. This increases the complexity of building a merged ECV data record.

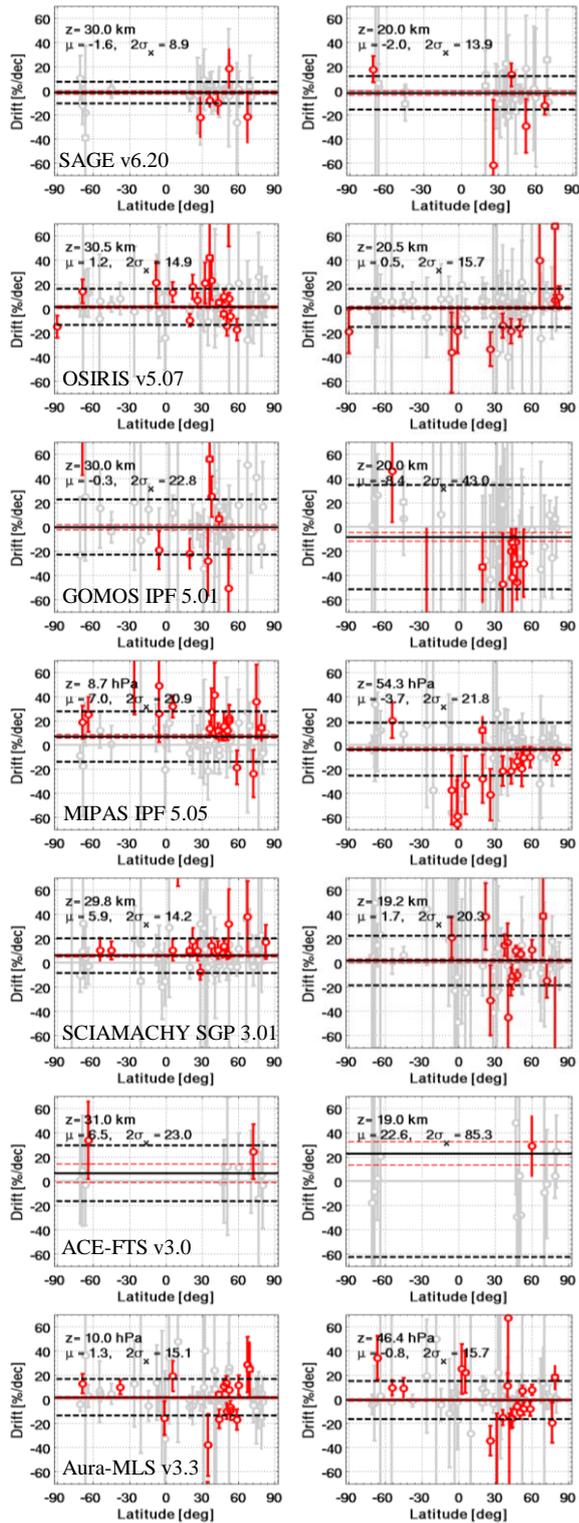


Figure 1: latitude cross-section of drift estimates for various satellite data records at 30 km (left) and 20 km (right), at ozonesonde (o) and lidar (□) stations. Error bars represent  $2\sigma$ ; red symbols show significant drifts. The text shows the global weighted mean (solid black) and spread of the drifts (dashed black). Less visible is the standard error of the weighted mean (red dashed).

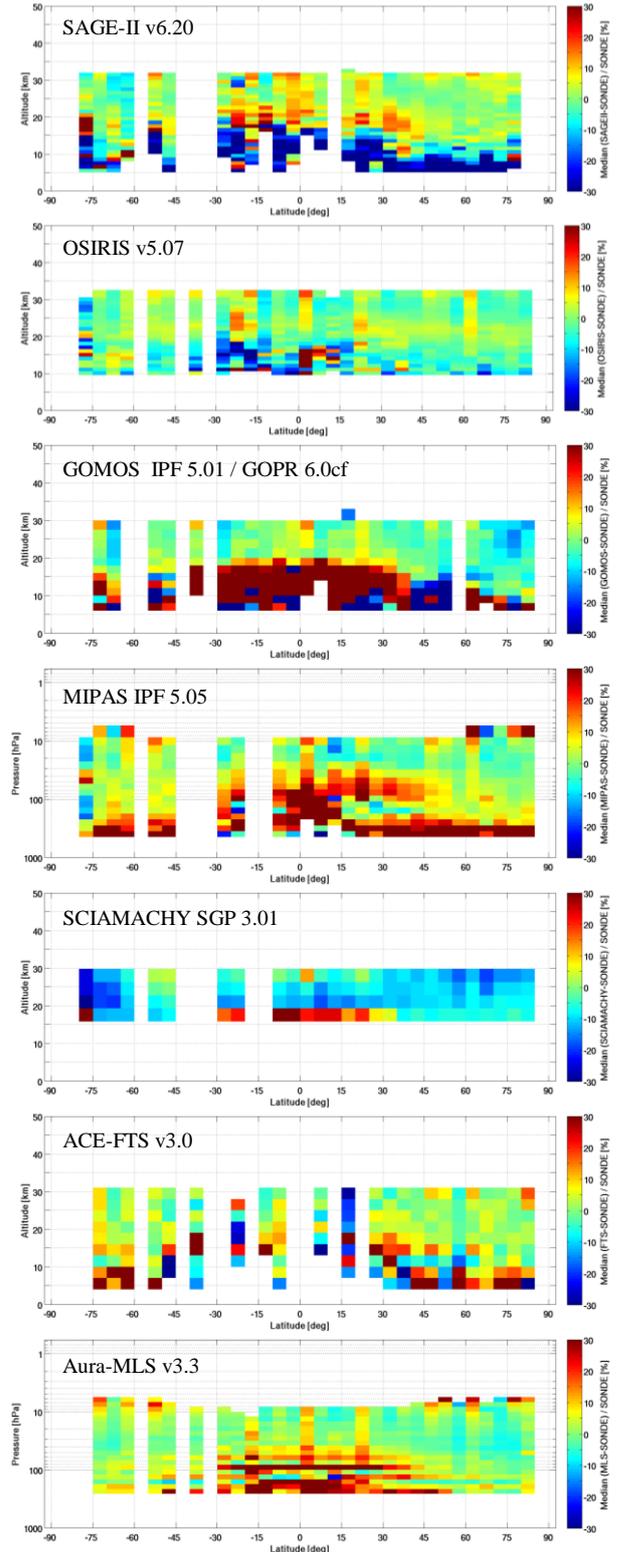


Figure 2: vertical-latitude cross section of the median relative difference between various satellite data records and NDACC-WOUDC ozonesonde data.

Fig. 2 shows that while SAGE-II and HALOE underestimate ozone in the UTLS, GOMOS, MIPAS and Aura-MLS tend to have a positive bias in the same region. The recommended data screening is hence either not intended to or insufficient to remove cloud/aerosol induced biases and variability.

The MIPAS data have an alternating positive and negative bias below the tropopause, from the equator extending to northern mid-latitudes. Very pronounced vertical oscillations were found for the Aura-MLS v3.3 data set, from pole to pole and independent of season.

A global altitude-independent bias of -10% is seen for SCIAMACHY. GOMOS data is cold biased by about -5% at high northern latitudes (possibly induced by stray light) and by -20% in the UTLS at mid northern latitudes. SMR is low biased by 5% with respect to correlative data, between 20-30 km. OSIRIS profiles overestimate ozone by 5-10% between 20-25 km, nearly independent of latitude and season. The MAESTRO VIS data also seem persistently low biased by 5-10% in the stratosphere.

Although not shown, the results of the comparison variability also reveal particular features. E.g. for SMR the variability is 30% over the entire stratosphere, which is three times larger than for any other instrument. This is a known feature of the data set [22]. A rather small spread is seen for SAGE-II and HALOE in the UTLS, indicating the lack of measured information.

Our results also permit the determination of a threshold altitude below which the statistical quality of the data degrades rapidly, based on bias and/or precision requirements. This threshold altitude depends on instrument. E.g. at mid-latitudes the MIPAS data quality remains good down to about 10 km, while for GOMOS and SCIAMACHY the threshold lies a few km higher.

## 6. DISCUSSION AND CONCLUSION

We studied ozone profile data records delivered by twelve limb/occultation satellite instruments (SAGE-II, HALOE, POAM-II, POAM-III, SMR, OSIRIS, GOMOS, MIPAS, SCIAMACHY, ACE-FTS, ACE-MAESTRO and Aura-MLS), forming all together a nearly 30-year time series of substantial interest for scientific studies of ozone trends and of the links between ozone and climate. This work is carried out in the context of various recent international efforts, like ESA's Climate Change Initiative program and the SI<sup>2</sup>N initiative of SPARC/IO<sub>3</sub>C/WMO-IGACO. The altitude and meridian structure of the long-term stability and consistency of the satellite data sets was evaluated in terms of drift, bias and variability with respect to correlative data from ground-based ozonesonde and lidar networks, affiliated with NDACC and WMO's GAW.

Our results indicate that, in general, the stratospheric part of the twelve ozone profile data records agree within 5-10%, with a spread of about 10%, with the ground-based data. Even though this suggests a good general mutual consistency, the various data records do exhibit particular features in some latitude and vertical ranges which must be considered when merging data records. E.g. in the UTLS large biases are seen, but with different signs and threshold altitudes depending on the instrument. Neglecting these differences might lead to artificial ozone trends in the lower stratosphere. Differences are also visible in other parts of the atmosphere. GOMOS is -5% low biased in the Arctic, while OSIRIS has a global +5-10% high bias between 20-25 km. The SCIAMACHY profiles are low by -10% at all latitudes and altitudes. Aura-MLS exhibits strong vertical oscillations below the tropopause, and MIPAS has a particular vertical structure at northern mid-latitudes as well. The spread in the comparisons is large for SMR in the stratosphere, and small for SAGE and HALOE in the UTLS.

The analysis of the comparison time series revealed that from 20-40 km most records are stable within about 5% per decade, and that there is not clear meridian structure of the drifts. We therefore based our conclusions on the globally weighted average. For SAGE-II, OSIRIS and Aura-MLS no significant drift was detected. The comparison time series are sufficiently long and well-sampled to achieve a 3-5% per decade detection limit. Time series of other data records are either too noisy (SMR) or too sparsely sampled (POAM-II/III, ACE-FTS/MAESTRO) to be sensitive below the 5% per decade level. Significant drifts are detected at some altitudes for HALOE (-5% / dec. at 25-30 km), GOMOS (-5% / dec. below 25 km), MIPAS (-5% / dec. at 20 km, +10% / dec. at 30 km.) and SCIAMACHY (+5% / dec. at 30 km). The instability must be accounted for when these data sets contribute to a merged record.

The climate users within ESA's Ozone\_cci project expressed an upper limit of 8-15% uncertainty on stratospheric ozone, in order to study the evolution of the ozone layer, seasonal cycle, interannual and short-term variability. Such a requirement can indeed be verified, and is met by most instruments. However, the requested stability of 1-3% per decade is very challenging to verify. This level of precision can only be obtained for certain satellite and ground-based data records. At the moment the 5% per decade level is realistic, and 2-3% per decade at selected stations. Only SAGE-II, OSIRIS and Aura-MLS seem to meet the user requirements at the moment.

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