Earth Syst. Sci. Data Discuss., 6, 189–222, 2013
www.earth-syst-sci-data-discuss.net/6/189/2013/
doi:10.5194/essdd-6-189-2013

Open Access Earth System Science Data Discussions

Harmonized dataset of ozone profiles from satellite limb and occultation measurements

V. F. Sofieva[1], N. Rahpoe[2], J. Tamminen[1], E. Kyrölä[1], N. Kalakoski[1], M. Weber[2], A. Laeng[3], T. von Clarmann[3], G. Stiller[3], S. Lossow[3], D. Degenstein[4], A. Bourassa[4], C. Adams[4], C. Roth[4], N. Lloyd[4], P. Bernath[5,6], R. J. Hargreaves[5], J. Urban[7], D. Murtagh[7], A. Hauchecorne[8], M. Van Roozendael[9], N. Kalb[9], and C. Zehner[10]

[1]Finnish Meteorological Institute, Helsinki, Finland
[2]Institute of Environmental Physics, University of Bremen, Bremen, Germany
[3]Karlsruhe Institute of Technology, Institute for Meteorology and Climate Research, Karlsruhe, Germany
[4]Institute for Space and Atmospheric Studies, University of Saskatchewan, Saskatoon, Saskatchewan, Canada
[5]Department of Chemistry, University of York, York, UK
[6]Department of Chemistry & Biochemistry, Old Dominion University, Norfolk, VA, USA
[7]Chalmers University of Technology, Department of Earth and Space Sciences, 41296 Gothenburg, Sweden

[8]Université Versailles St-Quentin, UPMC University Paris 06, CNRS/INSU, LATMOS-IPSL, 78280 Guyancourt, France
[9]Belgian Institute for Space Aeronomy (IASB-BIRA), Brussels, Belgium
[10]ESA/ESRIN, Frascati, Italy

Received: 30 May 2013 – Accepted: 5 June 2013 – Published: 14 June 2013

Correspondence to: V. F. Sofieva (viktoria.sofieva@fmi.fi)

Published by Copernicus Publications.

Abstract

In this paper, we present a HARMonized dataset of OZone profiles (HARMOZ) based on limb and occultation measurements from Envisat (GOMOS, MIPAS and SCIAMACHY), Odin (OSIRIS, SMR) and SCISAT (ACE-FTS) satellite instruments. These measurements provide high-vertical-resolution ozone profiles covering the altitude range from the upper troposphere up to the mesosphere in years 2001–2012. HARMOZ has been created in the framework of European Space Agency Climate Change Initiative project.

The harmonized dataset consists of original retrieved ozone profiles from each instrument, which are screened for invalid data by the instrument teams. While the original ozone profiles are presented in different units and on different vertical grids, the harmonized dataset is given on a common pressure grid in netcdf format. The pressure grid corresponds to vertical sampling of ~1 km below 20 km and 2–3 km above 20 km. The vertical range of the ozone profiles is specific for each instrument, thus all information contained in the original data is preserved. Provided altitude and temperature profiles allow the representation of ozone profiles in number density or mixing ratio on a pressure or altitude vertical grids. Geolocation, uncertainty estimates and vertical resolution are provided for each profile. For each instrument, optional parameters, which might be related to the data quality, are also included.

For convenience of users, tables of biases between each pair of instruments for each month, as well as bias uncertainties, are provided. These tables characterize the data consistency and can be used in various bias and drift analyses, which are needed, for instance, for combining several datasets to obtain a long-term climate dataset.

This user-friendly dataset can be interesting and useful for various analyses and applications, such as data merging, data validation, assimilation and scientific research.

Dataset is available at: http://www.esa-ozone-cci.org/?q=node/161.

ESSDD
6, 189–222, 2013

Title Page
Abstract | Instruments
Data Provenance & Structure
Tables | Figures
◂◂ | ▸▸
◂ | ▸
Back | Close
Full Screen / Esc
Printer-friendly Version
Interactive Discussion

1 Introduction

The creation of homogenized ozone profile datasets based on limb or occultation measurements from sensors on board the European Space Agency (ESA) Envisat satellite, as well as from ESA Third Party Missions (TPM), is one of the primary objectives of the European Space Agency Climate Change Initiative project (Ozone_cci, http://www.esa-ozone-cci.org). Six instruments that provide long-term measurements are involved in this project. Three of them are on board Envisat: Global Ozone Monitoring by Occultation of Stars (GOMOS), Michelson Interferometer for Passive Atmospheric Sounding (MIPAS), Scanning Imaging Spectrometer for Atmospheric Chartography (SCIAMACHY); two of them are on board Odin: Optical Spectrograph and InfraRed Imaging System (OSIRIS) and Sub-Millimeter Radiometer (SMR) and one is on board the SCISAT-1 satellite: Atmospheric Chemistry Experiment-Fourier Transform Spectrometer (ACE-FTS). Three of the instruments – GOMOS, SCIAMACHY and OSIRIS – retrieve ozone profiles from measurements in the UV-Visible wavelength range. MIPAS and ACE-FTS use infrared wavelengths, and SMR operates at sub-millimeter wavelengths. Two of the instruments use the occultation technique: GOMOS uses stellar occultation and ACE-FTS performs solar occultations. SCIAMACHY and OSIRIS are limb-scattering instruments; MIPAS and SMR measure thermal emission spectra. More details on individual datasets are presented in Sect. 3. The dataset cover years 2001–2012. The yearly data volume for the HARMOZ instruments is illustrated in Fig. 1. Between the various datasets, there are ozone measurements available for all seasons, various times of day, and good latitudinal coverage (as an example, Fig. 2 illustrates the latitudinal coverage in 2008).

The data from different sensors have different properties such as specific quality flags, and the data can have outliers due to problematic retrievals under some conditions. In some cases (like for GOMOS), ozone data quality strongly depends on a set of parameters, which makes using this dataset complicated for non-experts. As a first step towards data homogenization, we have created a HARMonized dataset

ESSDD
6, 189–222, 2013

of OZone profiles (HARMOZ). HARMOZ consists of independent datasets from individual instruments, which are carefully screened for outliers, interpolated to common pressure grid and saved in the common netcdf format. This database is used in various "higher-level" analyses performed within the ozone-CCI project. Convenience of using the harmonized dataset has prompted us to make this dataset available to the scientific community. This dataset contributes directly to the initiative on past changes in the vertical distribution of ozone (SI^2N, http://igaco-o3.fmi.fi/VDO/working_groups.html).

The paper is organized as follows. Section 2 presents a general description of the dataset and the data processing. Each dataset has mandatory parameters, which are the same for all instruments (discussed in Sect. 2), as well as optional, instrument-specific parameters (discussed in Sect. 3). The data format and availability are presented in Sect. 4. To characterize the data consistency, tables of biases between each pair of instruments and the bias uncertainties are created. The construction and format of the bias tables are discussed in Sect. 5. The summary concludes the paper.

2 General description of the harmonized dataset

The individual datasets from each instrument passed quality control, which has been performed by the instrument experts. The quality control procedures are described in detail in Sect. 3. Only valid data are included in HARMOZ.

Each profile has been interpolated onto a common pressure grid (ozone-CCI pressure grid hereafter), which is an extension of the SPARC Data Initiative pressure grid (Hegglin and Tegtmeier, 2010; Tegtmeier et al., 2013). The ozone-CCI pressure levels and the corresponding pressure altitudes are presented in Appendix A. The vertical spacing of the ozone-CCI grid corresponds to ~1 km below 20 km and ~2–3 km above. The number of pressure levels included in the individual datasets depends on the valid altitude range of the ozone profiles. For example, GOMOS data are provided on the ozone-CCI grid in the range 250–10^{-4} hPa, while MIPAS data are provided in the range 400–0.05 hPa. The altitude range of the individual datasets can be found in

Discussion Paper | Discussion Paper | Discussion Paper | Discussion Paper |

ESSDD

6, 189–222, 2013

Harmonized dataset of ozone profiles

V. F. Sofieva et al.

Table 1 and is illustrated in Fig. 3. The largest altitude range is achieved for occultation instruments, which cover also the lower thermosphere.

The data files contain the mandatory variables that are the same for all sensors. The main variables are profiles of ozone concentrations (mol cm^{-3}) and their uncertainties. The auxiliary information includes temperature and altitude profiles at the measurement locations for converting ozone data to different units (mixing ratio/number density on pressure/altitude in all possible combinations), as well as geolocation, time, and vertical resolution. The full list of mandatory parameters is presented in Table 2. The optional, instrument-specific parameters, which might be related to the quality of data, can be found in Table 3; they are discussed in more detail in Sect. 3. The data are written in the netcdf format, in agreement with standard conventions (http://cf-pcmdi.llnl.gov/documents/cf-conventions/1.6). Each netcdf file contains the data from one month (see Sect. 4 for more details on data format).

For regridding of profiles, a linear interpolation in the logarithm-pressure vertical coordinate is used. For the instruments providing reliable covariance matrices of retrieval errors, the covariance matrices of uncertainties (random error) were interpolated as

$$\mathbf{C} = \mathbf{W}\mathbf{C}_{\text{orig}}\mathbf{W}^T, \tag{1}$$

where $\mathbf{C}_{\text{orig}}$ and $\mathbf{C}$ are original and interpolated matrices, respectively, and $\mathbf{W}$ is the interpolation matrix. The parameter "standard_error" contains the square roots of the diagonal elements of $\mathbf{C}$; it represents uncertainty (random error) of individual profiles. Due to the structure of $\mathbf{C}_{\text{orig}}$ and $\mathbf{W}$, diagonal elements of $\mathbf{C}$ are very slightly reduced compared to the diagonal elements of $\mathbf{C}_{\text{orig}}$. For the instruments, for which covariance matrices are not easily available or insufficiently reliable, the uncertainty estimates were simply linearly interpolated to the ozone-CCI grid (in the same way as the ozone profiles). In these cases, the reduction of uncertainties due to interpolation has been estimated based on a sample covariance matrix and the information about the vertical resolution and the original grid. This reduction is very small, of a factor ~0.85–0.95

ESSDD
6, 189–222, 2013

(Table 4). It should be stressed here that the correction factors presented in Table 4 approximate only changes in uncertainty estimates due to regridding.

Note also that the ozone-CCI grid is finer than the vertical resolution of the ozone profiles, therefore the uncertainties at adjacent layers are correlated. Without covariances provided, there is the risk to overestimate the independent information contained in the profiles. For some of the instruments, there exist "advanced" versions of HARMOZ files with full covariance matrices **C** stored. These data can be provided upon request.

3 Short descriptions of individual datasets

In this section, a brief overview of the individual datasets is presented. The general parameters of the individual datasets are collected in Table 1. They include information about the altitude range of individual datasets, typical local time, vertical resolution, original representation of ozone profiles, as well as the source of air density data, which can be used for conversion from ozone concentration to mixing ratio. Specific features of individual datasets are described below.

3.1 GOMOS

GOMOS is a stellar occultation instrument on board Envisat (Bertaux et al., 2010; Kyrölä et al., 2010). Ozone profiles are retrieved from UV-VIS spectrometer measurements at wavelengths 250–692 nm. In this study, nighttime ozone profiles (solar zenith angle larger than 105°) processed with the IPF version 6 processor are used. GOMOS provides stratospheric ozone profiles with the vertical resolution of 2–3 km and estimated precision of 0.5–5 % (Tamminen et al., 2010). GOMOS data were filtered for outliers and unreliable data using the recommendations of the readme document http://earth.eo.esa.int/pcs/envisat/gomos/documentation/RMF_0117_GOM_NL_

ESSDD
6, 189–222, 2013

_2P_Disclaimers.pdf. In addition, we have excluded occultations terminated above 40 km.

The stellar flux recorded by GOMOS, and thus signal-to-noise ratio and precision of retrieved profiles, depends on stellar magnitude and spectral class. The GOMOS optional parameters include the star identification number in the GOMOS catalogue (the smaller the star number, the brighter the star), as well as the information about the star visual magnitude and effective temperature. Note that occultations of stars with insufficient UV-flux (dim and cool stars), which cannot provide information about ozone in the upper stratosphere, are not included in the harmonized dataset, as the quality of the entire ozone profile in such occultations is still under evaluation.

The obliquity is defined as the angle between the orbital plane and the direction to the star; it is 0° for in-orbital-plane occultations. The vertical sampling is denser in oblique occultations. Thanks to the Tikhonov-type target-resolution regularization (Kyrölä et al., 2010; Sofieva et al., 2004) and accurate parameterization of modeling errors in the GOMOS v6 algorithm (Sofieva et al., 2009, 2010), the quality of GOMOS ozone profiles and uncertainty estimates practically does not depend on this parameter. Very oblique occultations (with obliquity larger than 85°) are not present in the harmonized dataset.

The profiles of the normalized χ^2 statistics indicate the quality of retrievals and the quality of error estimates (normalization is on the number of spectral channels minus the number of fitted parameters, for exact definition of this parameter see e.g. Sofieva et al., 2010). Usually, χ^2_{norm} is very close to 1, thus indicating the proper characterization of uncertainties. However, there are occultations in the GOMOS dataset that have very large χ^2_{norm} values. They usually correspond to the locations over the Southern Atlantic Anomaly (SAA), which are affected by cosmic rays. From the harmonized dataset, such data are also excluded. The SAA flag presented in the list of optional parameters has been computed based on the position of the satellite. Therefore, it does not reflect the real quality of the ozone data; it is presented for information only.

The illumination flag indicates the illumination conditions (full dark limb, straylight, twilight). The bright-limb occultations (with illumination = 1) are not present in the

ESSDD
6, 189–222, 2013

harmonized dataset. The best quality of ozone profiles and their uncertainty estimates is achieved in full dark illumination conditions. The summary of the GOMOS optional parameters is collected in Table 3.

3.2 MIPAS

MIPAS was a Fourier transform spectrometer on board Envisat for the detection of limb emission spectra in the middle and upper atmosphere, which operated in the 4.15–14.6 µm wavelength range. It measured during day and night, pole-to-pole, at an altitude range from 6 to 70 km (170 km), depending on the measurement mode, producing more than 1000 profiles/day. MIPAS provides stratospheric ozone profiles with the vertical resolution of 3–5 km and estimated precision of 1–4 %.

There exist four MIPAS Level2 processors: the operational ESA processor and three independent research processors hosted by ISAC-CNR/University of Bologna, Oxford University and KIT IMK/IAA, respectively. All four processors use the same Level 1b data, but the Level 2 algorithms are different. In the framework of Ozone_cci project, ozone profiles retrieved by the four MIPAS processors were compared. The results of this comparison are described in Laeng et al. (2013). For creating the harmonized dataset, the MIPAS data were taken from the best performing under this comparison processor, which is the KIT IMK/IAA version V5R_O3_220/221 Research Processor. The description of the processor can be found in von Clarmann et al. (2003, 2009). The dataset has been extensively validated (Laeng et al., 2012, 2013).

The following filtering was applied to the retrieved data in order to ensure the good quality of the profiles:

1. The data for which the diagonal value of the averaging kernel is less (in absolute value) than 0.03 are considered unreliable and are discarded, because this corresponds to a local altitude resolution exceeding approximately the entire altitude coverage of the profile. This filter shall guarantee that only data are used which contain at least a minimum of measurement information.

Discussion Paper | Discussion Paper | Discussion Paper | Discussion Paper |

ESSDD

6, 189–222, 2013

Harmonized dataset of ozone profiles

V. F. Sofieva et al.

2. Data in parts of the atmosphere that lie below the lowermost useful tangent altitude are discarded, as they do not contain measurement information. This applies in particular to cases when the spectra measured at low tangent altitudes are discarded due to cloud contamination.

3.3 SCIAMACHY

SCIAMACHY on board Envisat has three observation modes: nadir, limb and occultation (Bovensmann et al., 1999, 2004). SCIAMACHY field of view is 2.6 km in the distance of 3000 km in the flight direction. Therefore, the atmosphere is sampled vertically in 3 km steps in the limb mode. SCIAMACHY measures the backscattered, reflected and transmitted solar radiation and covers the wavelength range between 212 nm and 2386 nm divided into 8 channels. In the limb mode, the spectral backscattered radiances from UV to visible range (channels 1–2 at 212–404 nm and channels 3–4 covering 392–790 nm) are used to retrieve ozone number density profiles.

The retrieved SCIAMACHY-IUP ozone profiles from the version 2.9 are used in this study. This is an updated version of the v. 2.3 processor with four limb states, used for the measurement, which correspond to four 240 km horizontal resolution scans for covering the full 960 km swath width, instead of an average over all states. The SCIATRAN radiation transfer model (RTM) (Rozanov et al., 2001) has been implemented for use in satellite limb, nadir, and lunar/solar occultation retrievals of atmospheric trace gases and aerosols in the UV, visible, and near IR spectral regions. This RTM code is an extension of the GOMETRAN RTM (Rozanov et al., 1997) that includes an iterative spherical approximation of the atmosphere which is, in particular, required for limb scatter retrievals. To retrieve ozone profiles, the normalized radiances in the UV and triplet method in the optical wavelength ranges have been used (Mieruch et al., 2012; Rahpoe et al., 2013; von Savigny et al., 2005; Sonkaew et al., 2009). The normalized radiances from the Chappuis, Hartley and Huggins bands are combined with each other in order to retrieve the ozone number density and extend the ozone profile to altitudes up to

ESSDD
6, 189–222, 2013

80 km. SCIAMACHY provides stratospheric ozone profiles with the vertical resolution of 3–5 km and estimated precision of 10–15 % (Rahpoe et al., 2013).

Ozone data are usually of poor quality in cloudy conditions. Therefore, data at altitudes contaminated by the clouds are filtered out in the harmonized dataset.

3.4 OSIRIS

OSIRIS on board the Odin satellite has been taking limb-scattered measurements of the atmosphere from 2001 to present. It operates at wavelengths 280–810 nm. For the harmonized dataset, the OSIRIS SaskMART v5.0x ozone data (Degenstein et al., 2009; Roth et al., 2007), which is retrieved using the SASKTRAN spherical radiative transfer model (Bourassa et al., 2008), have been filtered for outliers according to the techniques described by Adams et al. (2013a). OSIRIS provides stratospheric ozone profiles with the vertical resolution of 2–3 km and estimated precision of 2–10 % (Bourassa et al., 2012).

During inter-comparisons with other satellite and in-situ measurements (Adams et al., 2013a, b), it was found that agreement between OSIRIS and the validation datasets depends on OSIRIS optics temperature, retrieved aerosols and albedo. These are included as optional parameters in the OSIRIS harmonized dataset.

3.5 SMR

SMR on board the Odin satellite has been measuring thermal emissions from 2001 to the present. For SMR, the version 2.1 501.8 GHz band retrievals are presently (April 2013) recommended for use. These level-2 products provide ozone data in the $\sim$ 12–60 km altitude range (above 17–18 km at mid-latitudes) with a 2.5–3.5 km vertical resolution and a single-profile precision of about 20 %. The systematic error is estimated to be smaller than 0.75 ppmv (e.g., Urban et al., 2005, 2006). Note that measurements in this observation mode were carried out on every third day until April 2007 and on every other day thereafter. The thermal emission technique allows ozone to be measured

ESSDD
6, 189–222, 2013

Harmonized dataset of ozone profiles

V. F. Sofieva et al.

during day and night. Global fields between ~83° S and ~83° N are typically produced from 14–15 orbits per observation day based on up to 65 limb-scans per orbit. Since they are derived from a relatively weak spectral line, individual ozone profiles are quite noisy but averages agree reasonably well with correlative measurements (e.g., Dupuy et al., 2009; Jégou et al., 2008; Jones et al., 2007).

For HARMOZ, SMR data with a quality flag equal to 0 or 4 and a measurement response larger than 0.67 have been used. A filtering of outliers (also using data from other simultaneously retrieved species such as N_2O and ClO) has also been applied. For SMR, vertical resolution is estimated from the full-width-at-half-maximum (FWHM) of averaging kernel functions calculated (off-line by the retrieval algorithm) for 4 observation days in 2010 (mid-March, mid-June, mid-September, mid-December). The FWHM profiles were interpolated on the HARMOZ pressure grid and zonal means were calculated in 10° wide latitude zones. The derived FWHM climatology indicates thus typical values of the altitude resolution as a function of latitude and pressure.

The most important optional parameter is the measurement response, which indicates the fraction of measurement information in the retrieved profiles. In the case of a very weak influence of the a priori, the measurement response is close to 1. User may apply an additional data filtering depending on application.

3.6 ACE-FTS

ACE-FTS is a solar occultation instrument that records spectra between 2.2 and 13.3 µm (750–4400 cm^{-1}) at a high spectral resolution of 0.02 cm^{-1} (Bernath et al., 2005). ACE-FTS provides retrieved altitude profiles of the volume mixing ratio (vmr) of ozone on a 1 km native grid. Each measurement is made at the time of local sunrise/sunset. ACE-FTS provides stratospheric ozone profiles with the vertical resolution of ~3 km and estimated precision of 1–3 %.

For HARMOZ, the version 3.0 processed data from March 2004 to September 2010 have been used. These data have been filtered to only include data points, which are

ESSDD
6, 189–222, 2013

within 5 median absolute deviations (MADs) from the vmr median. Additionally, any data point for which the vmr error exceeds the measurement has also been excluded.

The temperature profiles, which are included in the netcdf files, are determined in two parts. Between 0–15 km, values from the GEM operational weather model of Environment Canada are used. Between 15 and 125 km, CO_2 lines are used for direct temperature retrievals (Boone et al., 2005).

For this study, it is useful to include the beta angle (angle between orbital plane and the sun-earth vector) as an optional parameter for each profile, as this can give an indication of the vertical spacing. ACE initially takes measurements on a tangent-altitude grid and the vertical spacing of this grid varies depending on the beta angle. When the beta angle is at a minimum (zero degrees), the vertical spacing can be as high as 6 km at high altitude, which means that the occultation is almost perpendicular to the Earth's surface. However, when the beta angle is at a maximum (set to about 65 degrees) the vertical spacing can be as low as 2 km (at high altitudes) because now ACE measurements are at an oblique angle to the Earth's surface. It is not a straightforward problem to determine the vertical resolution of each occultation because this is dependent on a number of factors including the beta angle. It is best to estimate the vertical resolution as an average of 3 km for all points and the beta angle is provided to indicate the quality of this estimate. A vertical resolution of 3 km is typically used when validating ACE-FTS measurements (Dupuy et al., 2009).

4 Data format and availability

The harmonized dataset is provided in netcdf format (with README file) and can be found at the ozone-CCI web-page http://www.esa-ozone-cci.org/?q=node/161. It consists of folders corresponding to each instrument. Each folder contains monthly data files with self-explanatory names. For example, the file ESACCI-OZONE-L2-LP-GOMOS_ENVISAT_IPF_V6_200801_fv0003.nc contains GOMOS ozone profiles for January 2008. The parameters in the files are compliant with CF-1.5 convention.

Sample scripts to read the netcdf files with MATLAB and IDL are also available on the web page.

5 Data agreement tables

To quantify the agreement between the individual datasets in HARMOZ, tables of experimental biases between each pair of instruments are provided, as well as the uncertainty of the bias estimates. The data agreement tables are computed using collocated measurements with the following restrictions on time difference Δt, distance between tangent points Δd, and latitude difference $\Delta\theta$:

i. standard collocation: $|\Delta t| \leq 24$ h, $|\Delta d| \leq 1000$ km, $|\Delta\theta| \leq 2^\circ$.

ii. tight collocation: $|\Delta t| \leq 4$ h, $|\Delta d| \leq 400$ km.

The tight collocation criterion is based on the effective horizontal resolution of the considered limb/occultation measurements, and can be considered therefore as the "natural" collocation criterion. The standard criterion ensures a sufficient number of collocated measurements and thus provides reliable bias estimates with better seasonal and latitudinal coverage. Analogous criteria have previously been successfully applied in satellite inter-comparisons (Adams et al., 2013a, b; Kyrölä et al., 2013). In the case of multiple collocated measurements, only the nearest in time is selected.

For all pairs of instruments, the bias tables are provided for the standard collocation criterion. When possible, the bias tables for tight collocation criterion are also provided; these are for pairs involving the dense samplers MIPAS and SCIAMACHY.

The vertical resolution is ~ 3 km for all instruments (slightly smaller for GOMOS and OSIRIS, slightly larger for MIPAS and SCIAMACHY). The difference in vertical resolution between the HARMOZ instruments cannot generate significant systematic differences in ozone profiles (they can be as large as ~ 1–2 % in the worst cases). Therefore, we ignored the difference in vertical resolution in the bias analysis.

ESSDD
6, 189–222, 2013

The analysis of ozone differences between ozone-CCI limb instruments has shown that biases are additive rather than multiplicative. Therefore, we calculate the relative bias b as:

$$b = 2\frac{\langle x_1 - x_2 \rangle}{\langle x_1 \rangle + \langle x_2 \rangle}, \quad (2)$$

where x_1 and x_2 are collocated measurements from two instruments at a given altitude and $\langle . \rangle$ denotes mean/median estimates (both are provided). The relative uncertainty of b is estimated as:

$$\sigma_b = \frac{2}{\langle x_1 \rangle + \langle x_2 \rangle} \cdot \frac{\sigma_{(x_1 - x_2)}}{\sqrt{N}}, \quad (3)$$

where $\sigma_{(x_1-x_2)}$ is the sample standard deviation of the difference distribution computed in a standard or in a robust way as $\sigma = 0.5(P_{84} - P_{16})$, P_{84} and P_{16} are 84th and 16th percentiles, respectively, and N is the number of collocated measurements. In the agreement tables, both parameters b and σ_b are presented in %. The estimates using the median and percentiles are referred to as "robust" in created files. The bias is evaluated over the common altitude range of the pair of instruments.

The bias is evaluated for each month in 20° latitude zones from 90° S to 90° N. The bias tables are structured in 15 folders corresponding to the instrument pairs, e.g., "GOMOS_OSIRIS". They can be found at the same web-page http://www.esa-ozone-cci.org/?q=node/161. The folders contain bias tables corresponding to each month in netcdf format. The file names contain information about the year and the month, as well as the instruments and the collocation type. For example, the file "ESACCI-OZONE-AgreementTable_GOMOS_OSIRIS_200801.nc" contains the bias table between GOMOS (x_1) and OSIRIS (x_2) for January 2008, for the standard collocation criterion. The files for tight collocation criterion are ended with "_tight.nc". The parameters included in the netcdf files are presented in Table 5. An example visual representation of the main bias parameters is shown in Fig. 4.

ESSDD
6, 189–222, 2013

The data agreement tables present experimental estimates of biases and their uncertainties. At some locations and seasons, the estimated biases can be not statistically significant. Furthermore, discrepancies at upper altitudes are expected (and observed), because of diurnal ozone variations (e.g., Sakazaki et al., 2013 and references therein). The created bias tables are convenient for higher-level analyses, which might aim at detecting statistically significant biases, their latitudinal dependence, and possible drift in time. Examples of such higher-level analyses are presented in Figs. 5 and 6. A detailed analysis of biases and drifts between the instruments will be presented in a separate paper.

Figure 5 shows the time-latitude dependence of biases for "GOMOS minus MIPAS" at 15 hPa ($\sim$ 30 km), for standard and tight collocation criteria. As seen in Fig. 5, the wider collocation criteria do not significantly change the observed biases. At the majority of locations, GOMOS reports slightly smaller ozone values, and this difference is stable in time.

Figure 6 shows mean (over all seasons) biases for 2007–2008 with respect to MIPAS, as a function of latitude and altitude (subplots show relative differences for "instrument minus MIPAS"). The weighted mean (with uncertainties of individual biases) is used for averaging of monthly bias values. Two features can be easily noticed in Fig. 6. First, MIPAS is biased high at altitudes 40–45 km with respect to all instruments. This feature has also been noticed in MIPAS validation studies (Laeng et al., 2012, 2013). Second, a visible enhancement in SCIAMACHY data in the equatorial atmosphere at $\sim$ 30 km is observed. This feature is unique for SCIAMACHY and also has been observed previously (Mieruch et al., 2012). The presented examples are only simple illustrations of possible analyses using the harmonized data set and the data agreement tables.

6 Summary

We have described the HARMonized dataset of OZone profiles (HARMOZ) based on limb and occultation data from six satellite instruments: GOMOS, MIPAS, SCIAMACHY,

ESSDD
6, 189–222, 2013

OSIRIS, SMR and ACE-FTS. The main strength of HARMOZ is that it is user-friendly: the independent datasets from individual instruments, which passed thorough quality control, are presented in the same form as far as possible (common vertical grid, common parameters, and a common data format). Although the datasets are simple and user-friendly, they are also comprehensive: all important parameters attributed to individual datasets are presented. Quality of ozone profiles in HARMOZ is characterized by uncertainty estimates and the vertical resolution. The created data agreement tables provide ready information for various bias and drift analyses. This information is of high importance in joint data analyses and in data merging. A detailed analysis of biases and drifts between the Ozone_cci instruments will be the subject of a future publication.

Between the various datasets, there are ozone measurements available for all seasons, various times of day, and good latitudinal coverage. This user-friendly dataset can be very interesting and useful for different analyses and applications, such as data merging, data validation, different inter-comparisons, data assimilation and scientific research. The system has been designed in a flexible and open way in order to facilitate the ingestion of additional data sets from other instruments and/or from other processors, when these become available.

Appendix A

The pressure levels (P, hPa) of the ozone-CCI grid are:

450, 400, 350, 300, 250, 200, 170, 150, 130, 115, 100, 90, 80, 70, 50, 40, 30, 20, 15, 10, 7, 5, 4, 3, 2, 1, 1.5, 1, 0.7, 0.5, 0.4, 0.3, 0.2, 0.15, 0.1, 0.07, 0.05, 0.04, 0.03, 0.02, 0.015, 0.01, 0.007, 0.005, 0.004, 0.003, 0.002, 0.0015, 0.001, 0.0007, 0.0005, 0.0004, 0.0003, 0.0002, 0.00015, 0.0001.

ESSDD
6, 189–222, 2013

The corresponding pressure altitudes $z = 16 \log_{10}(1013/P)$ in km are:

5.64, 6.46, 7.38, 8.46, 9.72, 11.27, 12.4, 13.27, 14.27, 15.12, 16.09, 16.82, 17.64, 18.57, 20.91, 22.46, 24.46, 27.27, 29.27, 32.09, 34.57, 36.91, 38.46, 40.46, 43.27, 48.09, 45.27, 48.09, 50.57, 52.91, 54.46, 56.46, 59.27, 61.27, 64.09, 66.57, 68.91, 70.46, 72.46, 75.27, 77.27, 80.09, 82.57, 84.91, 86.46, 88.46, 91.27, 93.27, 96.09, 98.57, 100.91, 102.46, 104.46, 107.27, 109.27, 112.09.

Acknowledgements. This work has been performed in the framework of the ESA Ozone_cci project.

References

Adams, C., Bourassa, A. E., Bathgate, A. F., McLinden, C. A., Lloyd, N. D., Roth, C. Z., Llewellyn, E. J., Zawodny, J. M., Flittner, D. E., Manney, G. L., Daffer, W. H., and Degenstein, D. A.: Characterization of Odin-OSIRIS ozone profiles with the SAGE II dataset, Atmos. Meas. Tech. Discuss., 6, 1033–1065, doi:10.5194/amtd-6-1033-2013, 2013a.

Adams, C., Bourassa, A. E., Sofieva, V., Froidevaux, L., McLinden, C. A., Hubert, D., Lambert, J.-C., Sioris, C. E., and Degenstein, D. A.: Assessment of Odin-OSIRIS ozone measurements from 2001 to the present using MLS, GOMOS, and ozone sondes, Atmos. Meas. Tech. Discuss., 6, 3819–3857, doi:10.5194/amtd-6-3819-2013, 2013b.

Bernath, P. F., McElroy, C. T., Abrams, M. C., Boone, C. D., Butler, M., Camy-Peyret, C., Carleer, M., Clerbaux, C., Coheur, P.-F., Colin, R., DeCola, P., DeMazière, M., Drummond, J. R., Dufour, D., Evans, W. F. J., Fast, H., Fussen, D., Gilbert, K., Jennings, D. E., Llewellyn, E. J., Lowe, R. P., Mahieu, E., McConnell, J. C., McHugh, M., McLeod, S. D., Michaud, R., Midwinter, C., Nassar, R., Nichitiu, F., Nowlan, C., Rinsland, C. P., Rochon, Y. J., Rowlands, N., Semeniuk, K., Simon, P., Skelton, R., Sloan, J. J., Soucy, M.-A., Strong, K., Tremblay, P., Turnbull, D., Walker, K. A., Walkty, I., Wardle, D. A., Wehrle, V., Zander, R., and Zou, J.: Atmospheric Chemistry Experiment (ACE): Mission overview, Geophys. Res. Lett., 32, L15S01, doi:10.1029/2005GL022386, 2005.

Bertaux, J. L., Kyrölä, E., Fussen, D., Hauchecorne, A., Dalaudier, F., Sofieva, V., Tamminen, J., Vanhellemont, F., Fanton d'Andon, O., Barrot, G., Mangin, A., Blanot, L., Lebrun, J. C., Pérot, K., Fehr, T., Saavedra, L., Leppelmeier, G. W., and Fraisse, R.: Global ozone monitoring by occultation of stars: an overview of GOMOS measurements on ENVISAT, Atmos. Chem. Phys., 10, 12091–12148, doi:10.5194/acp-10-12091-2010, 2010.

Boone, C. D., Nassar, R., Walker, K. A., Rochon, Y., McLeod, S. D., Rinsland, C. P., and Bernath, P. F.: Retrievals for the atmospheric chemistry experiment Fourier-transform spectrometer, Appl. Opt., 44, 7218–7231, doi:10.1364/AO.44.007218, 2005.

Bourassa, A. E., Degenstein, D. A., and Llewellyn, E. J.: SASKTRAN: A spherical geometry radiative transfer code for efficient estimation of limb scattered sunlight, J. Quant. Spectrosc. Ra., 109, 52–73, doi:10.1016/j.jqsrt.2007.07.007, 2008.

Bourassa, A. E., McLinden, C. A., Bathgate, A. F., Elash, B. J., and Degenstein, D. A.: Precision estimate for Odin-OSIRIS limb scatter retrievals, J. Geophys. Res., 117, D04303, doi:10.1029/2011JD016976, 2012.

Bovensmann, H., Burrows, J. P., Buchwitz, M., Frerick, J., Noël, S., Rozanov, V. V., Chance, K. V., and Goede, A. P. H.: SCIAMACHY: Mission Objectives and Measurement Modes, J. Atmos. Sci., 56, 127–150, doi:10.1175/1520-0469(1999)056<0127:SMOAMM>2.0.CO;2, 1999.

Bovensmann, H., Buchwitz, M., Frerick, J., Hoogeveen, R. W. M., Kleipool, Q., Lichtenberg, G., Noel, S., Richter, A., Rozanov, A., Rozanov, V. V., Skupin, J., Von Savigny, C., Wuttke, M. W., and Burrows, J. P.: SCIAMACHY on ENVISAT: in-flight optical performance and first results, in: Remote Sensing of Clouds and the Atmosphere VIII, edited by: Schaefer, K., Comeron, A., Carleer, M. R., and Picard, R. H., Proceedings of the SPIE, 5235, 160–173, 2004.

Degenstein, D. A., Bourassa, A. E., Roth, C. Z., and Llewellyn, E. J.: Limb scatter ozone retrieval from 10 to 60 km using a multiplicative algebraic reconstruction technique, Atmos. Chem. Phys., 9, 6521–6529, doi:10.5194/acp-9-6521-2009, 2009.

Dupuy, E., Walker, K. A., Kar, J., Boone, C. D., McElroy, C. T., Bernath, P. F., Drummond, J. R., Skelton, R., McLeod, S. D., Hughes, R. C., Nowlan, C. R., Dufour, D. G., Zou, J., Nichitiu, F., Strong, K., Baron, P., Bevilacqua, R. M., Blumenstock, T., Bodeker, G. E., Borsdorff, T., Bourassa, A. E., Bovensmann, H., Boyd, I. S., Bracher, A., Brogniez, C., Burrows, J. P., Catoire, V., Ceccherini, S., Chabrillat, S., Christensen, T., Coffey, M. T., Cortesi, U., Davies, J., De Clercq, C., Degenstein, D. A., De Mazière, M., Demoulin, P., Dodion, J., Firanski, B., Fischer, H., Forbes, G., Froidevaux, L., Fussen, D., Gerard, P., Godin-Beekmann, S., Goutail, F., Granville, J., Griffith, D., Haley, C. S., Hannigan, J. W., Höpfner, M., Jin, J. J., Jones, A., Jones, N. B., Jucks, K., Kagawa, A., Kasai, Y., Kerzenmacher, T. E., Kleinböhl, A., Klekociuk,

A. R., Kramer, I., Küllmann, H., Kuttippurath, J., Kyrölä, E., Lambert, J.-C., Livesey, N. J., Llewellyn, E. J., Lloyd, N. D., Mahieu, E., Manney, G. L., Marshall, B. T., McConnell, J. C., McCormick, M. P., McDermid, I. S., McHugh, M., McLinden, C. A., Mellqvist, J., Mizutani, K., Murayama, Y., Murtagh, D. P., Oelhaf, H., Parrish, A., Petelina, S. V., Piccolo, C., Pommereau, J.-P., Randall, C. E., Robert, C., Roth, C., Schneider, M., Senten, C., Steck, T., Strandberg, A., Strawbridge, K. B., Sussmann, R., Swart, D. P. J., Tarasick, D. W., Taylor, J. R., Tétard, C., Thomason, L. W., Thompson, A. M., Tully, M. B., Urban, J., Vanhellemont, F., Vigouroux, C., von Clarmann, T., von der Gathen, P., von Savigny, C., Waters, J. W., Witte, J. C., Wolff, M., and Zawodny, J. M.: Validation of ozone measurements from the Atmospheric Chemistry Experiment (ACE), Atmos. Chem. Phys., 9, 287–343, doi:10.5194/acp-9-287-2009, 2009.

Hegglin, M. I. and Tegtmeier, S.: The SPARC Data Initiative, SPARC Newsletter No. 36, 22, 2010.

Jégou, F., Urban, J., de La Noë, J., Ricaud, P., Le Flochmoën, E., Murtagh, D. P., Eriksson, P., Jones, A., Petelina, S., Llewellyn, E. J., Lloyd, N. D., Haley, C., Lumpe, J., Randall, C., Bevilacqua, R. M., Catoire, V., Huret, N., Berthet, G., Renard, J. B., Strong, K., Davies, J., Mc Elroy, C. T., Goutail, F., and Pommereau, J. P.: Technical Note: Validation of Odin/SMR limb observations of ozone, comparisons with OSIRIS, POAM III, ground-based and balloon-borne instruments, Atmos. Chem. Phys., 8, 3385–3409, doi:10.5194/acp-8-3385-2008, 2008.

Jones, A., Murtagh, D., Urban, J., Eriksson, P., and Rösevall, J.: Intercomparison of Odin/SMR ozone measurements with MIPAS and balloon sonde data, Can. J. Phys., 85, 1111–1123, doi:10.1139/p07-118, 2007.

Kyrölä, E., Tamminen, J., Sofieva, V., Bertaux, J. L., Hauchecorne, A., Dalaudier, F., Fussen, D., Vanhellemont, F., Fanton d'Andon, O., Barrot, G., Guirlet, M., Mangin, A., Blanot, L., Fehr, T., Saavedra de Miguel, L., and Fraisse, R.: Retrieval of atmospheric parameters from GOMOS data, Atmos. Chem. Phys., 10, 11881–11903, doi:10.5194/acp-10-11881-2010, 2010.

Kyrölä, E., Laine, M., Sofieva, V., Tamminen, J., Päivärinta, S.-M., Tukiainen, S., Zawodny, J., and Thomason, L.: Combined SAGE II-GOMOS ozone profile data set 1984–2011 and trend analysis of the vertical distribution of ozone, Atmos. Chem. Phys. Discuss., 13, 10661–10700, doi:10.5194/acpd-13-10661-2013, 2013.

Laeng, A., Grabowski, U., Von Clarmann, T., Stiller, G., Kellmann, S., Kiefer, M., Linden, A., Lossow, S. T. B., Bernath, P., Boone, C., Clerbaux, C., Degenstein, D., Fritz, S., Froidevaux, L., Hervig, M. K., Hoppel, J. L., McHugh, M., Sano, T., Sofieva, V., Suzuki, M.,

Tamminen, J., Urban, J., Walker, K., Weber, M., and Zawodny, J.: Validation of MIPAS IMK/IAA ozone profiles, Quadrennial Ozone Symposium, available at: http://larss.science.yorku.ca/QOS2012pdf/5935.pdf, 2012.
Laeng, A., Hubert, D., Verhoelst, T., Von Clarmann, T., Dinelli, B. M., Dudhia, A., Raspollini, P., Stiller, G., Grabowski, U., Keppens, A., Kiefer, M., Sofieva, V., Froideveaux, L., Walker, K. A., Lambert, J.-C., and Zehner, C.: The Ozone Climate Change Initiative: Comparison of four Level 2 Processors for the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS), Remote Sens. Environ., submitted, 2013.
Mieruch, S., Weber, M., von Savigny, C., Rozanov, A., Bovensmann, H., Burrows, J. P., Bernath, P. F., Boone, C. D., Froidevaux, L., Gordley, L. L., Mlynczak, M. G., Russell III, J. M., Thomason, L. W., Walker, K. A., and Zawodny, J. M.: Global and long-term comparison of SCIAMACHY limb ozone profiles with correlative satellite data (2002–2008), Atmos. Meas. Tech., 5, 771–788, doi:10.5194/amt-5-771-2012, 2012.
Rahpoe, N., von Savigny, C., Weber, M., Rozanov, A. V., Bovensmann, H., and Burrows, J. P.: Error budget analysis of SCIAMACHY limb ozone profile retrievals using the SCIATRAN model, Atmos. Meas. Tech. Discuss., 6, 4645–4676, doi:10.5194/amtd-6-4645-2013, 2013.
Roth, C. Z., Degenstein, D. A., Bourassa, A. E., and Llewellyn, E. J.: The retrieval of vertical profiles of the ozone number density using Chappuis band absorption information and a multiplicative algebraic reconstruction technique, Can. J. Phys., 85, 1225–1243, doi:10.1139/P07-130, 2007.
Rozanov, A., Rozanov, V., and Burrows, J. P.: A numerical radiative transfer model for a spherical planetary atmosphere: combined differential–integral approach involving the Picard iterative approximation, J. Quant. Spectrosc. Ra., 69, 491–512, doi:10.1016/S0022-4073(00)00100-X, 2001.
Rozanov, V. V., Diebel, D., Spurr, R. J. D., and Burrows, J. P.: GOMETRAN: A radiative transfer model for the satellite project GOME, the plane-parallel version, J. Geophys. Res.-Atmos., 102, 16683–16695, doi:10.1029/96JD01535, 1997.
Sakazaki, T., Fujiwara, M., Mitsuda, C., Imai, K., Manago, N., Naito, Y., Nakamura, T., Akiyoshi, H., Kinnison, D., Sano, T., Suzuki, M., and Shiotani, M.: Diurnal ozone variations in the stratosphere revealed in observations from the Superconducting Submillimeter-Wave Limb-Emission Sounder (SMILES) on board the International Space Station (ISS), J. Geophys. Res.-Atmos., 118, 2991–3006, doi:10.1002/jgrd.50220, 2013.

Sofieva, V. F., Tamminen, J., Haario, H., Kyrölä, E., and Lehtinen, M.: Ozone profile smoothness as a priori information in the inversion of limb measurements, Ann. Geophys., 22, 3411–3420, doi:10.5194/angeo-22-3411-2004, 2004.

Sofieva, V. F., Kan, V., Dalaudier, F., Kyrölä, E., Tamminen, J., Bertaux, J.-L., Hauchecorne, A., Fussen, D., and Vanhellemont, F.: Influence of scintillation on quality of ozone monitoring by GOMOS, Atmos. Chem. Phys., 9, 9197–9207, doi:10.5194/acp-9-9197-2009, 2009.

Sofieva, V. F., Vira, J., Kyrölä, E., Tamminen, J., Kan, V., Dalaudier, F., Hauchecorne, A., Bertaux, J.-L., Fussen, D., Vanhellemont, F., Barrot, G., and Fanton d'Andon, O.: Retrievals from GOMOS stellar occultation measurements using characterization of modeling errors, Atmos. Meas. Tech., 3, 1019–1027, doi:10.5194/amt-3-1019-2010, 2010.

Sonkaew, T., Rozanov, V. V., von Savigny, C., Rozanov, A., Bovensmann, H., and Burrows, J. P.: Cloud sensitivity studies for stratospheric and lower mesospheric ozone profile retrievals from measurements of limb-scattered solar radiation, Atmos. Meas. Tech., 2, 653–678, doi:10.5194/amt-2-653-2009, 2009.

Tamminen, J., Kyrölä, E., Sofieva, V. F., Laine, M., Bertaux, J.-L., Hauchecorne, A., Dalaudier, F., Fussen, D., Vanhellemont, F., Fanton-d'Andon, O., Barrot, G., Mangin, A., Guirlet, M., Blanot, L., Fehr, T., Saavedra de Miguel, L., and Fraisse, R.: GOMOS data characterisation and error estimation, Atmos. Chem. Phys., 10, 9505–9519, doi:10.5194/acp-10-9505-2010, 2010.

Tegtmeier, S., Hegglin, M. I., Anderson, J., Bourassa, A., Brohede, S., Degenstein, D., Froidevaux, L., Fuller, R., Funke, B., Gille, J., Jones, A., Kasai, Y., Kyrölä, E., Lingenfelser, G., Lumpe, J., Nardi, B., Neu, J., Pendlebury, D., Remsberg, E., Rozanov, A., Smith, L., Toohey, M., Urban, J., von Clarmann, T., Walker, K. A., and Wang, R.: A comparison of ozone climatologies from international limb satellite sounders, J. Geophys. Res., submitted, 2013.

Urban, J., Murtagh, D., Lautié, N., Barret, B., Dupuy, E., De La Noë, J., Eriksson, P., Frisk, U., Jones, A., Le Flochmoë, E., Olberg, M., Piccolo, C., Ricaud, P. and Rösevall, J.: Odin/SMR Limb Observations of Trace Gases in the Polar Lower Stratosphere during 2004–2005, in: ESA Atmospheric Science Conference, 8-12 May 2006, Frascati, Italy, European Space Agency publications ESA-SP-628, ISBN-92-9092-939-1, ISSN-1609-042X., 2006.

Urban, J., Lautié, N., Le Flochmoën, E., Jiménez, C., Eriksson, P., De La Noë, J., Dupuy, E., Ekström, M., El Amraoui, L., Frisk, U., Murtagh, D., Olberg, M., and Ricaud, P.: Odin/SMR limb observations of stratospheric trace gases: Level 2 processing of ClO, N_2O, HNO_3, and O_3, J. Geophys. Res.-Atmos., 110, D14307, doi:10.1029/2004JD005741, 2005.

von Clarmann, T., Glatthor, N., Grabowski, U., Höpfner, M., Kellmann, S., Kiefer, M., Linden, A., Mengistu Tsidu, G., Milz, M., Steck, T., Stiller, G. P., Wang, D. Y., Fischer, H., Funke, B., Gil-López, S., and López-Puertas, M.: Retrieval of temperature and tangent altitude pointing from limb emission spectra recorded from space by the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS), J. Geophys. Res., 108, 4736, doi:10.1029/2003JD003602, 2003.

von Clarmann, T., Höpfner, M., Kellmann, S., Linden, A., Chauhan, S., Funke, B., Grabowski, U., Glatthor, N., Kiefer, M., Schieferdecker, T., Stiller, G. P., and Versick, S.: Retrieval of temperature, H_2O, O_3, HNO_3, CH_4, N_2O, $ClONO_2$ and ClO from MIPAS reduced resolution nominal mode limb emission measurements, Atmos. Meas. Tech., 2, 159–175, doi:10.5194/amt-2-159-2009, 2009.

Von Savigny, C., Rozanov, A., Bovensmann, H., Eichmann, K.-U., Noël, S., Rozanov, V., Sinnhuber, B.-M., Weber, M., Burrows, J. P., and Kaiser, J. W.: The Ozone Hole Breakup in September 2002 as Seen by SCIAMACHY on ENVISAT, J. Atmos. Sci., 62, 721–734, doi:10.1175/JAS-3328.1, 2005.

Table 1. General information about the datasets.

	HARMOZ altitude range	Local time	Vertical resolution	Original ozone unit and Level 2 vertical grid	Source of temperature data
GOMOS	250–10^{-4} hPa	~ 10 p.m.	2 km below 30 km and 3 km above 40 km	number density on tangent altitudes	ECMWF analysis
MIPAS	400–0.05 hPa	~ 10 p.m. and ~ 10 a.m.	profile-dependent, 3–5 km	vmr on fixed altitude grid	Retrieved temperature
SCIAMACHY	250–0.05 hPa	~ 10 a.m.	profile-dependent, 3–5 km	number density on fixed altitude grid	ECMWF analysis
OSIRIS	450–0.1 hPa	~ 6 a.m. and ~ 6 p.m.	~ 2–3 km	number density on fixed altitude grid	ECMWF analysis
SMR	300–0.05 hPa	~ 6 a.m. and ~ 6 p.m.	profile-dependent, ~ 2.5–3.5 km	vmr on fixed alt/pressure grid	ECMWF analysis
ACE-FTS	450–2×10^{-4} hPa	Sunrise and sunset	~ 3 km	vmr on fixed altitude grid	Retrieved (15–120 km) +GEM model (0–15 km)

ESSDD
6, 189–222, 2013

Table 2. Mandatory parameters in the HARMOZ netcdf files. N_{alt} and N_{prof} denote the number of pressure levels and the number of profiles, respectively.

Parameter and unit	Dimensions	Description
time (days since 1900-01-01 00:00:00)	$N_{prof} \times 1$	The parameter to index the profiles
air_pressure (hPa)	$N_{alt} \times 1$	The vertical coordinate
altitude (km)	$N_{alt} \times N_{prof}$	The geometric altitude above the mean sea-level
latitude (degree_north)	$N_{prof} \times 1$	Latitude of each profile (given at altitude ~35 km)
longitude (degree_east)	$N_{prof} \times 1$	Longitude of each profile (given at altitude ~35 km)
mole_concentration_of_ozone _in_air (mol cm^{-3})	$N_{alt} \times N_{prof}$	Vertical profiles of ozone. Number density (cm^{-3}) is acquired by multiplying the variable with Avogadro constant $N_A = 6.02214e23$ mol^{-1}
mole_concentration_of_ozone_in_air standard_error (mol cm^{-3})	$N_{alt} \times N_{prof}$	Uncertainty (random error) associated with the ozone profiles
vertical_resolution (km)	$N_{alt} \times N_{prof}$ or $N_{alt} \times 1$	FWHM of the averaging kernel
air_temperature (K)	$N_{alt} \times N_{prof}$	Temperature profiles at the locations of measurements, for conversion from concentration to mixing ratio

ESSDD
6, 189–222, 2013

Table 3. Optional parameters in the HARMOZ netcdf files. N_{alt} and N_{prof} denote the number of pressure levels and the number of profiles, respectively.

Parameter and unit	Dimensions	Description/comment
		GOMOS
star_number	$N_{prof} \times 1$	Star number in GOMOS catalogue
star_magnitude	$N_{prof} \times 1$	Star visual magnitude
star_temperature (K)	$N_{prof} \times 1$	Star effective temperature
obliquity (deg)	$N_{prof} \times 1$	Obliquity of occultation: the angle between the orbital plane and the line of sight
sza (deg)	$N_{prof} \times 1$	solar zenith angle at tangent point
Chi2	$N_{prof} \times N_{alt}$	Profiles of χ^2-statistics. χ^2 is usually close to 1; large values indicate problems with retrievals
illumination_condition _flag	$N_{prof} \times 1$	0 – full dark, 3 – straylight, 2 – twilight, 4 – straylight & twilight.
SAA_flag	$N_{prof} \times 1$	The indicator showing that the data might be affected by the Southern Atlantic Anomaly (cosmic rays); 0 – no, 1 – yes
		SCIAMACHY
orbit_number	$N_{prof} \times 1$	Envisat orbit number
state_id	$N_{prof} \times 1$	State ID of the SCIA measurement
height_sat (km)	$N_{prof} \times 1$	Satellite altitude above the sea-level, for each profile
radius_earth (km)	$N_{prof} \times 1$	The Earth radius at locations above the tangent points
sza_tanpnt (deg)	$N_{prof} \times 1$	solar zenith angle at tangent point
pixel_lat (degree_north)	$N_{prof} \times 4$	the ground latitudes of the four corners of the limb scan pixel
pixel_lon (degree)	$N_{prof} \times 4$	the ground longitude of the four corners of the limb scan pixel
total_ozone_column (mm)	$N_{prof} \times 1$	Total ozone column for each profile; 1 mm = 100 DU (Dobson Unit)
systematic_error (%)	$N_{alt} \times N_{prof}$	Systematic errors derived from parameter deviation simulation
		MIPAS
apriori_temperature (K)	$N_{alt} \times N_{prof}$	temperature profiles at locations of measurements based on ECMWF and MSIS data
geo_id	$N_{prof} \times 22$	MIPAS geolocation identifier formatted as XXXXX_YYYYMMDDThhmmssZ where XXXXX=orbit, YYYY=year, MM=month, DD=day, hh=hour, mm=minute, ss=second
orbit_number	$N_{prof} \times 1$	Orbit number
sza (deg)	$N_{prof} \times 1$	Solar zenith angle
chi2	$N_{prof} \times 1$	χ^2-value of retrievals
dof	$N_{prof} \times 1$	degrees of freedom of target retrieval
rms (nW cm^{-1} sr^{-1})	$N_{prof} \times 1$	root mean square of residual spectra
		OSIRIS
scan_number	$N_{prof} \times 1$	OSIRIS scan number
albedo	$N_{prof} \times 1$	Retrieved albedo
ssa (deg)	$N_{prof} \times 1$	Solar scattering angle
sza (deg)	$N_{prof} \times 1$	Solar zenith angle
optics_temperature (K)	$N_{prof} \times 1$	Average optics box temperature
		SMR
quality	$N_{prof} \times 1$	Quality flag 0: best quality, 4: tolerable
solar_zenith_angle (deg)	$N_{prof} \times 1$	
local_solar_time (h)	$N_{prof} \times 1$	
measurement_response	$N_{alt} \times N_{prof}$	Proportion of measurement; measurements with weak influence of a priori have measurement response close to 1.
scaled_potential_ vorticity (K m^2 kg^{-1} s^{-1})	$N_{alt} \times N_{prof}$	Profiles of potential vorticity (Lait, 1994) scaled at 475 K potential temperature level
equivalent_latitude (deg)	$N_{alt} \times N_{prof}$	Profiles of equivalent latitude at locations of measurements
		ACE-FTS
beta_angle (deg)	$N_{prof} \times 1$	β-angle is defined as the angle between the orbit plane of ACE-FTS and the vector from the Sun. It is a proxy for vertical resolution.

ESSDD
6, 189–222, 2013

Harmonized dataset of ozone profiles

V. F. Sofieva et al.

Table 4. The approximate reduction factors for uncertainty estimates due to regridding (the reported values of uncertainties should be multiplied with the factor from the table).

GOMOS	MIPAS	SCIAMACHY	OSIRIS	SMR	ACE-FTS
1	1	0.94	0.9	0.85	0.92

ESSDD
6, 189–222, 2013

Harmonized dataset of ozone profiles

V. F. Sofieva et al.

Table 5. Main parameters of bias tables in the netcdf format.

Parameter and unit	Dimensions	Description/comment
air_pressure (hPa)	$N_{alt} \times 1$	The vertical coordinate
approximate_altitude (km)	$N_{alt} \times 1$	Approximate altitude at pressure levels computed as $z = 16 \log_{10}(1013/P)$, P is pressure in hPa
latitude_centers (degree_north)	$N_{lat} \times 1$	Centers of latitude bins: 80° S, 60° S, 40° S, 20° S, 0° S, 20° N, 40° N, 60° N, 80° N
bias (%)	$N_{lat} \times N_{alt}$	Bias between instrument#1 and instrument#2 estimated as the mean of differences, Eq. (2)
robust_bias (%)	$N_{lat} \times N_{alt}$	As "bias", but the median estimates are used
bias_uncertainty (%)	$N_{lat} \times N_{alt}$	Uncertainty of the bias estimated using the standard sample std of differences, Eq. (3)
robust_bias_uncertainty (%)	$N_{lat} \times N_{alt}$	Uncertainty of the bias estimated using the robust sample std of differences, Eq. (3)
number_of _collocated_data	$N_{lat} \times N_{alt}$	number of collocated data in each latitude bin and at each pressure level

ESSDD
6, 189–222, 2013
Harmonized dataset of ozone profiles
V. F. Sofieva et al.

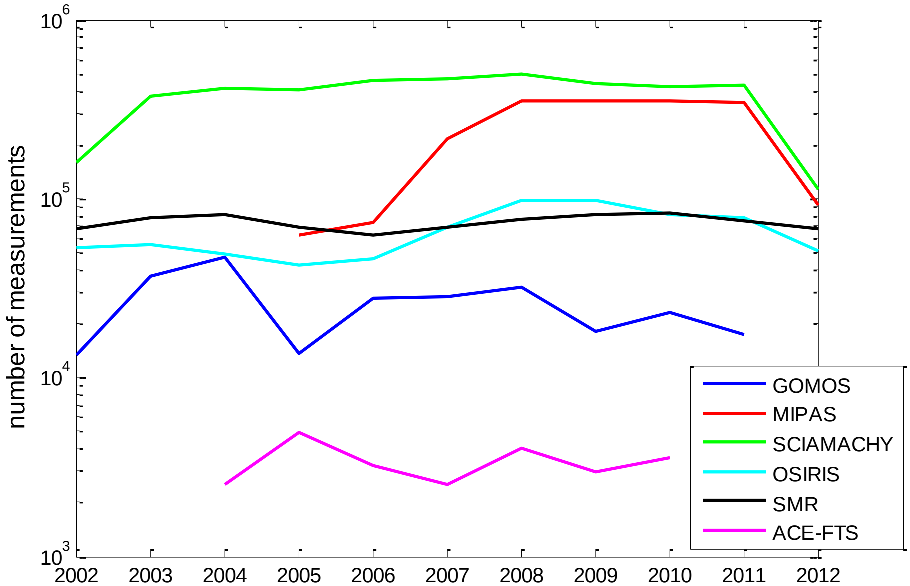

Fig. 1. Number of measurements in each year and for each instrument.

ESSDD
6, 189–222, 2013

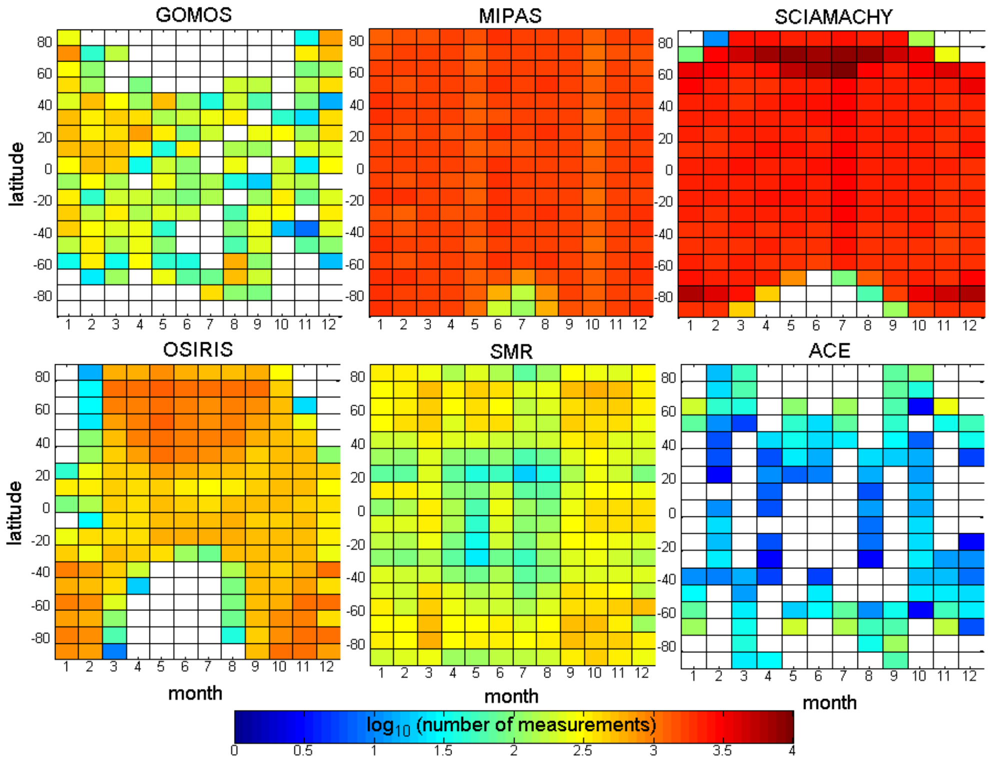

Fig. 2. Logarithm of number of measurements in 10° latitude zones and in each month of year 2008.

ESSDD
6, 189–222, 2013

Harmonized dataset of ozone profiles

V. F. Sofieva et al.

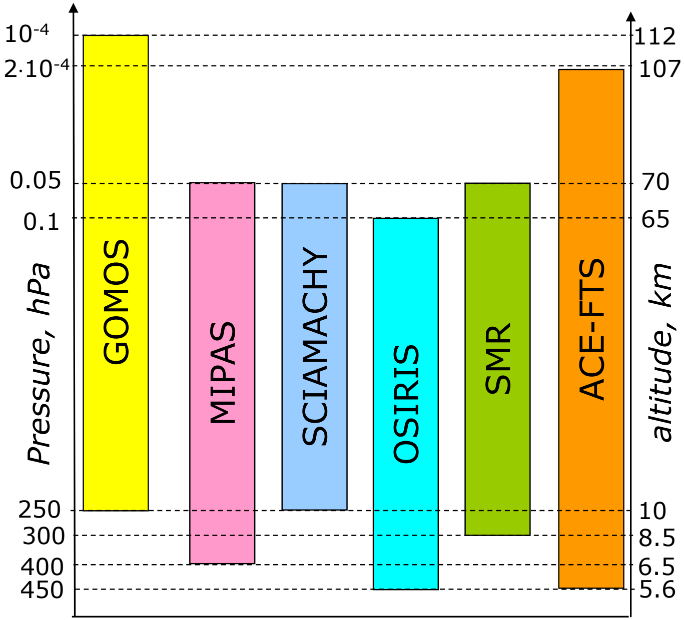

Fig. 3. Illustration of altitude ranges of ozone measurements for the individual instruments in HARMOZ. The vertical axis is not to scale.

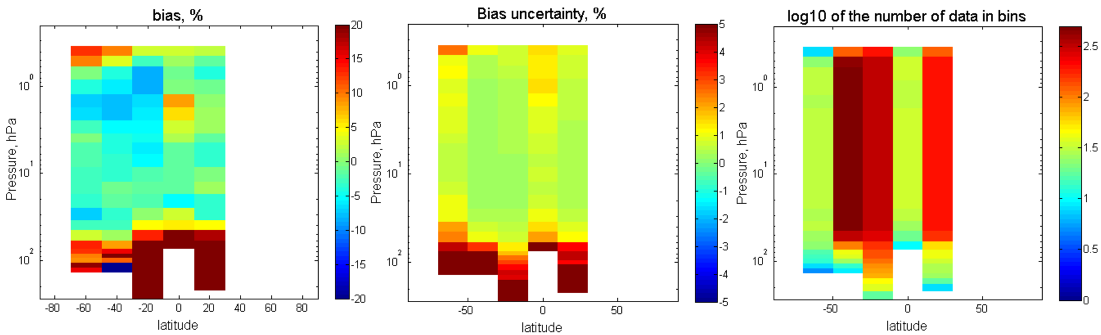

Fig. 4. A visualization example of bias-related parameters from bias tables, for GOMOS versus OSIRIS in January 2008.

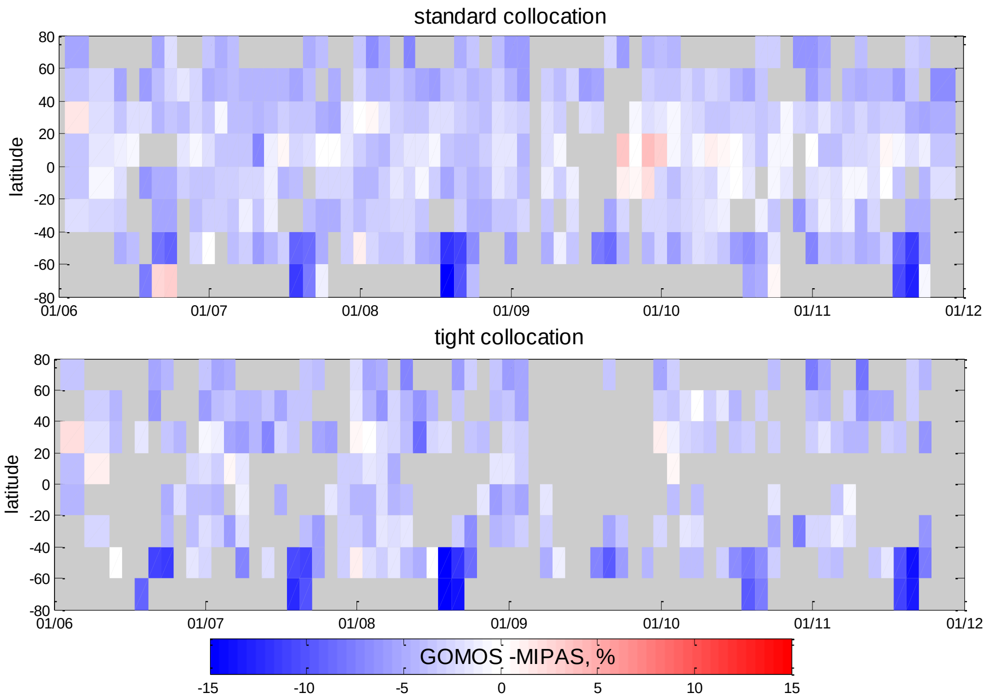

Fig. 5. GOMOS minus MIPAS (in % indicated by color scale) at 30 km, as a function of latitude and time, for standard (top) and tight (bottom) collocation criteria.

ESSDD
6, 189–222, 2013

Harmonized dataset of ozone profiles

V. F. Sofieva et al.

Title Page
Abstract
Instruments
Data Provenance & Structure
Tables
Figures
◀
▶
Back
Close
Full Screen / Esc
Printer-friendly Version
Interactive Discussion

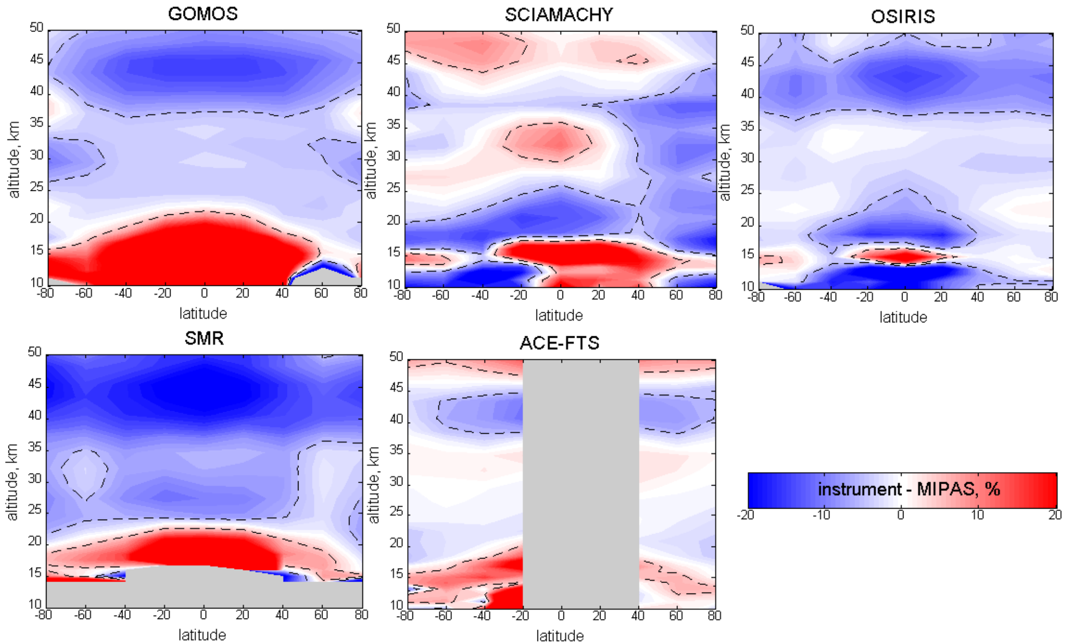

Fig. 6. Latitude-altitude dependence of biases with respect to MIPAS ("instrument minus MIPAS" in % is shown in color scale). Dashed black lines indicate ±5 %.

ESSDD
6, 189–222, 2013

Harmonized dataset of ozone profiles

V. F. Sofieva et al.