



The GOME-type Total Ozone Essential Climate Variable (GTO-ECV) data record from the ESA Climate Change Initiative

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Abstract

We present the new GOME-type Total Ozone Essential Climate Variable (GTO-ECV) data record which has been created within the framework of the European Space Agency's Climate Change Initiative (ESA-CCI). Total ozone column observations – based on the GOME-type Direct Fitting version 3 algorithm – from GOME (Global Ozone Monitoring Experiment), SCIAMACHY (SCanning Imaging Absorption Spec-

troMeter for Atmospheric CHartographY), and GOME-2 have been combined into one homogeneous time series, thereby taking advantage of the high inter-sensor consistency. The data record spans the 15-year period from March 1996 to June 2011 and it contains global monthly mean total ozone columns on a $1^\circ \times 1^\circ$ grid. Geophysical ground-based validation using Brewer, Dobson, and UV-visible instruments has shown that the GTO-ECV level 3 data record is of the same high quality as the equivalent individual level 2 data products that constitute it. Both absolute agreement and long-term stability are excellent with respect to the ground-based data, for almost all latitudes apart from a few outliers which are mostly due to sampling differences between the level 2 and level 3 data. We conclude that the GTO-ECV data record is valuable for a variety of climate applications such as the long-term monitoring of the past evolution of the ozone layer, trend analysis and the evaluation of Chemistry–Climate Model simulations.

1 Introduction

In 2010 the European Space Agency (ESA) set up the Climate Change Initiative (CCI) program, which aims to realize the full potential of long-term Earth Observation data records for a number of Essential Climate Variables (ECVs) from the atmospheric, oceanic and terrestrial domains (Hollmann et al., 2013). These data records are essential to assess the state and future evolution of climate, as observations from space provide unique information and global coverage. However they are often limited by

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a lack of homogeneity and continuity. Therefore the aim of the ESA-CCI program is to provide stable and long-term Climate Data Records (CDRs) derived from multiple satellite data sets which are then suitable for both monitoring and modelling of climate and which meet the target requirements defined within the Global Climate Observing System (GCOS, 2011).

In this paper we focus on measurements of the ozone layer which protects life on Earth from harmful ultraviolet solar radiation and which plays an important role on the radiation budget of the atmosphere. As a consequence of the 1987 Montreal Protocol (UNEP, 1986) and subsequent phasing-out of the emissions of the Ozone Depleting Substances (ODSs) the stratospheric ozone layer is expected to recover within the next decades (WMO, 2011). However, significant uncertainty remains as to the timing of this recovery, because of complex interaction with climate change and continuously increasing emissions of greenhouse gases.

Within the phase I of the ESA's Ozone CCI (Ozone_cci) project, total ozone and ozone profile data records from nadir ultra-violet (UV) backscatter sensors, as well as ozone profiles from limb and occultation sensors (Sofieva et al., 2013), have been created. In this paper we introduce the multi-sensor total ozone data record which covers the period 1996–2011. The record is based on observations from three European instruments – all mounted on sun-synchronous low earth orbit platforms – namely the Global Ozone Monitoring Experiment (GOME) onboard the second European Remote Sensing satellite (ERS-2), the SCanning Imaging Absorption SpectroMeter for Atmospheric CHartography (SCIAMACHY) onboard the ENVironmental SATellite (ENVISAT), and GOME-2 onboard the first of a series of three Meteorological Operational satellites (MetOp-A). Detailed descriptions of the instruments are given in Burrows et al. (1999), Bovensmann et al. (1999), and Callies et al. (2000), respectively. A brief overview of the main platform and sensor characteristics is presented in Table 1.

As part of the Ozone_cci project, the total ozone data sets have been recently reprocessed with the retrieval algorithm GOME-type Direct FITting version 3 (GODFIT_V3) for the entire time series of the GOME, SCIAMACHY, and GOME-2 observations (Lerot

et al., 2014). The GODFIT_V3 algorithm leads to high quality retrievals in all conditions, including high solar zenith angles and large optical depths. Since the deployment of the GODFIT version used in the GOME Data Processor (GDP) operational ground segment version 5 (van Roozendaal et al., 2012), a number of new developments in GODFIT have made the algorithm even more robust. These improvements are related to the tropospheric ozone content, a semi-empirical Ring correction and a correction for atmospheric polarization, as well as enhanced computational performance.

Although common retrieval settings are used for all three sensors, significant differences may appear when individual data sets are compared. These differences are largely due to calibration issues in the level 1 data. To improve inter-sensor consistency, a soft-calibration scheme for measured reflectances has been developed by Lerot et al. (2014), which relies on a statistical comparison of the level 1 sun-normalized radiances with simulated spectra at a few reference sites (viz., European stations equipped with Brewer spectrophotometers). The identification and correction of any artificial offset or spectral structures in the measured reflectances greatly improves the agreement between individual level 2 total ozone data sets. On the other hand, this procedure introduces a dependency of the satellite data on the Brewer observations themselves, and this has to be kept in mind for the assessment of the geophysical validation results.

Together, these level 2 data sets based on the GODFIT_V3 retrieval algorithm span the time period 1996–2012. They have been recently validated using as reference ground-based measurements with Brewer and Dobson spectrophotometers as well as UV-visible DOAS/SAOZ (Differential Optical Absorption Spectroscopy/Système d'Analyse par Observation Zenithale) instruments (Koukouli et al., 2015). The main findings were that the three sensors are characterized by similar patterns (such as seasonality and solar zenith angle dependence) against the reference data sets. No trends or unexplained jumps were detected. Furthermore, a marked improvement with respect to the operational products and an enhanced intersensor consistency was identified.

This paper is the third article on the ESA-CCI total ozone ECV, and it describes the construction and validation of a cohesive merged level 3 data product. The aim is to

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show that the combination of the three individual homogenized total ozone data sets forms a consistent long-term time series, which meets the GCOS requirements and is therefore suitable for climate applications.

The paper is organized as follows: Sect. 2 contains a detailed description of the generation of the GTO-ECV CCI total ozone data record. Section 3 is dedicated to the validation of the level 3 merged product using ground-based measurements systems, and Sect. 4 shows the results of comparisons with two comparable satellite-based data records. Section 5 contains the summary and outlook.

2 Construction of GTO-ECV data record

In this section we describe the construction of the level 3 data set and the inter-satellite calibration approach, which has been developed and applied to combine the individual observations into an homogeneous long-term product. An analysis of issues related to spatial and temporal sampling is presented in Sect. 2.2. Section 2.3 contains a short description of the final output NetCDF (Network Common Data Format) files.

2.1 Level 3 algorithm description and merging approach

The level 3 algorithm is designed to map the level 2 measurements, processed with the GODFIT_V3 retrieval algorithm, onto a daily fixed global grid of $1^\circ \times 1^\circ$ in longitude and latitude. Each grid cell contains an average of all level 2 data from the same GMT (Greenwich Mean Time) day, that overlap with the level 3 cell. Cell values are computed as weighted averages in which the fractional area of overlap of the satellite ground pixel with the given grid cell is used as weight. Level 2 data can be mapped onto more than one grid cell. The gridding algorithm is applied separately to GOME, SCIAMACHY, and GOME-2 measurements.

The next step is to merge the individual level 3 data sets from the three sensors into one homogeneous record using an inter-instrument calibration approach. Predeces-

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sors of this algorithm are described in Loyola et al. (2009a) and Loyola and Coldewey-Egbers (2012). In order to account for inter-sensor differences, which possibly remain from the GODFIT_V3 level 2 algorithm, we apply an external adjustment to SCIAMACHY and GOME-2 results. The GOME record serves as the reference data base.

The calculation of the correction factors is based on a comparison of 1° zonal monthly means, which are computed at first for GOME and SCIAMACHY. These zonal monthly means are based on common daily gridded data only in order to minimize the differences in spatial and temporal sampling. In particular this becomes important after June 2003, when GOME lost its global coverage. We did not consider diurnal changes of ozone in the merging approach, since all three instruments provide measurements within one hour of each other (see Table 1). However, the peak-to-peak difference in total ozone may reach 1 % over the course of a day (Sakazaki et al., 2013).

The correction factors for SCIAMACHY with respect to GOME are derived using the ratios of these zonal monthly means. The correction factors comprise two parts: (1) a “basic” correction for each month of the year (averaged over all years from 2002 to 2011) in terms of third order polynomials as a function of latitude, and (2) an offset for each individual month, which is added to the “basic” correction. This offset does not depend on latitude, but it accounts for the time-dependence in the differences between SCIAMACHY and GOME from 2002 to 2011. The correction factors are then applied to the SCIAMACHY daily gridded data by linear interpolation in time. They are shown in the top panel of Fig. 1 as a function of latitude and time. The correction is well below 2 % without obvious trends. It is between −0.5 and 1.0 % in the tropical region and increases slightly toward higher latitudes.

In preparation for the GOME-2 adjustment, an intermediate product of averaged GOME and corrected SCIAMACHY daily gridded data is generated for the overlap period with GOME-2 from January 2007 to June 2011. This is referred to as GS_MERGED in the following. 1° zonal monthly means are computed for GS_MERGED and GOME-2 based on common daily gridded data only. The correction factors for GOME-2 with respect to GS_MERGED are derived similarly to those

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for SCIAMACHY: fourth-order polynomials as a function of latitude and month plus a time-dependent offset. They are applied to GOME-2 daily gridded data by linear interpolation in time. The bottom panel of Fig. 1 shows the GOME-2 correction, which is also well below 2 %, as for SCIAMACHY, and without trends. It is between 0.0 and 1.0 % in the Tropics and decreases towards higher latitudes. In September 2009 the behaviour of the GOME-2 instrument changed owing to the second throughput test (Lacan and Lang, 2011). The soft-calibration scheme applied within the GODFIT_V3 retrieval algorithm mitigates the long-term impact of this test, so that only an insignificant increase in the correction factors can be identified. Furthermore, no unexpected jumps with respect to ground-based data were found during the geophysical validation exercise of the level 2 data (Koukouli et al., 2015). Only a small increase in the correction factors for a limited period in time is visible, which is caused by the low time resolution of the soft-calibration scheme.

Once SCIAMACHY and GOME-2 data have been adjusted, $1^\circ \times 1^\circ$ monthly mean gridded data are computed for each instrument. In order to provide representative monthly means that contain a sufficient number of measurements equally distributed over time, cut-off values for latitude as a function of the month have been defined (see Table 2). Thereby we avoid calculating monthly averages based on a small number of measurements at the beginning or end of a month which appear close to the polar night. Nonetheless, differences in monthly means among the instruments may occur due to regular differences in spatial and temporal sampling (see Table 1). This will be discussed in the next subsection.

Subsequently, the three data sets are combined into one single record as follows: only one instrument is used at a time, i.e. the merged GTO-ECV total ozone time series contains GOME measurements from April 1996 to March 2003, adjusted SCIAMACHY measurements from April 2003 to March 2007, and adjusted GOME-2 measurements from April 2007 to June 2011. The whole procedure is summarized in Fig. 2. Red-shaded boxes denote data records which are part of the official ESA Ozone CCI Climate Research Data Package (CRDP). Blue-shaded boxes denote intermediate data

sets needed to create the merged final product and green shading denotes the three steps of the merging approach.

The complete data record with typical total ozone features is shown in Fig. 3. Highest ozone values occur in northern hemispheric springtime, whereas monthly mean values are below 200 DU from September to November south of 70° S. Extreme events such as the anomalous Antarctic ozone hole in 2002 and the severe ozone loss in 1997 and 2011 in the Arctic are visible. Instrument switches from GOME to SCIAMACHY in March 2003 and from SCIAMACHY to GOME-2 in March 2007 are indicated with the black vertical bars.

2.2 Illustration of sampling issues

As already noted in the previous section, inhomogeneous or incomplete sampling – intrinsic to these types of satellite sensors – may have systematic effects and may therefore lead to erroneous average estimates (e.g. Sofieva et al., 2014). Since the platforms are in polar orbits, for each day there are coverage gaps in the tropics (even for GOME-2, which has the largest swath width) as well as repeated views of the summertime poles, leading to nonuniform under- or over-sampling of ozone. This can result in inaccurate monthly average estimates, in particular when natural variability is strongest, i.e. in spring months in the Northern Hemisphere or under ozone hole conditions. The problem is exacerbated when the satellites sample only a few days at the beginning or end of the month owing to the beginning or end of the polar night.

Figure 4 exemplifies the diverse sampling patterns of GOME (left column), SCIAMACHY (middle column), and GOME-2 (right column) for April 1997, 2005, and 2008, respectively. The total number of measurements per month and grid cell, i.e. mapped level 2 data according to the level 3 algorithm described above, are shown in the top row, the number of days for which measurements are available is indicated in the middle row, and the effective mean day d_{eff} representing the monthly mean is found in the

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bottom row. The latter has been calculated using

$$d_{\text{eff}} = \sum_{d=1}^D d \cdot n_d / \sum_{d=1}^D n_d. \quad (1)$$

D is the maximum number of days in the month, i.e. 31 in January, 30 in April, etc., and n_d is the number of measurements per day and grid cell.

GOME-2 has the densest and most uniform sampling, i.e. the highest number of measurements (top right panel). The effective day is close to the middle of the month (between day 14 and 16, bottom right panel), although some longitudinal structures are visible in particular in the tropics. The GOME sampling is less dense and the effective mean day shows a larger spread around the middle of the month as well as pronounced longitudinal structures in low and middle latitudes (bottom left panel). The sampling pattern of SCIAMACHY strongly reflects the alternation of the nadir and limb measurement modes for this instrument, leading to extreme longitudinal as well as latitudinal structures (middle panels).

Toward the north polar regions (in April) the number of measurements increases due to overlapping orbits and hence multiple views per day. Toward the south polar regions the number of measurements increases up to about 65° S and then rapidly decreases due to the beginning polar night. The effective mean day (bottom row) indicates that only the first half of April is sampled. We decided to exclude these regions close to the polar night from the level 3 data record. Therefore, we defined cut-off latitudes (see Table 2) for each month in order to avoid using data covering only a limited part of the month.

Figure 5 illustrates the impact of the diverse sampling patterns on the monthly averages. It shows the percentage differences between SCIAMACHY (sparse sampling) and GOME-2 (dense and most uniform sampling) monthly mean total ozone for April 2008. Biases of $\pm 5\%$ reflect the differences in the sampling patterns, in particular in the middle latitudes, where natural variability is strong in this month. It is less pronounced in the tropics, where variability is low, and in the north polar region, where the

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SCIAMACHY sampling is enhanced due to overlapping orbits and, thus, multiple views per day. These sampling issues will be addressed in more detail in the second phase of the Ozone_cci project.

2.3 GTO-ECV data files

5 The final GTO-ECV CCI total ozone monthly mean output data are stored in NetCDF files (one file per month), which are publicly available via www.esa-ozone-cci.org. All files follow the NetCDF Climate and Forecast (CF) metadata convention version 1.5. Table 3 gives an overview of the content of the individual files. The reported grid of the data record is $1^\circ \times 1^\circ$ in longitude and latitude, i.e. the dimensions are 360×180 and the

10 center of the first grid cell is located at latitude 89.5° N and longitude 0.5° E. Besides the mean total ozone column, the corresponding SD, the standard error, and the number of measurements per month are provided. The sample SD characterizes the scatter of the measured data encompassing the natural variability, the measurement error as well as the sampling uncertainty. The SD of the GTO-ECV product are compared with those

15 from another satellite-based data record in Sect. 4.2. The standard error, however, quantifies the spatial–temporal sampling errors inherent to the satellite measurements. These errors have been estimated using an Observing System Simulation Experiment (OSSE). High-resolution ECMWF (European Centre for Medium-Range Weather Forecasts) data were taken as the reference data set. Then, three sets of daily observations

20 were simulated from the reference using the sampling patterns appropriate to GOME, SCIAMACHY, and GOME-2, respectively. Finally, the average monthly simulations are compared with the corresponding monthly reference in order to estimate the sampling errors corresponding to the total ozone monthly averages. The standard error is shown in Fig. 6 for April 1997 (GOME, left panel), 2005 (SCIAMACHY, middle panel), and

25 2008 (GOME-2, right panel). The errors increase from the Tropics to higher latitudes following the increasing ozone variability. GOME errors are larger than those for SCIAMACHY and GOME-2 due to the much larger ground-pixel size (see Table 1). The SCIAMACHY errors reflect the sampling pattern seen in Fig. 4, middle column, with

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latitudinal and longitudinal variance. GOME-2 errors are quite small and without noticeable structures.

3 Ground-based validation

The validation of level 2 satellite total ozone columns using independent ground-based observations has been a substantial part of retrieval algorithm development for many decades. A well-established procedure exists in assessing the level 2 total ozone products using global ground-based Brewer, Dobson, and UV-visible SAOZ spectrophotometer measurements (e.g. Balis et al., 2007b; Loyola et al., 2011; Koukouli et al., 2012; Labow et al., 2013, and references therein). Taking into account that the long-term climate study of the total ozone atmospheric content is based on using level 3 gridded products, one must ensure that the transition from level 2 to level 3 does not introduce artifacts. These might be induced by the level 3 algorithm itself, mainly through sampling issues which could lead to inaccurate average estimates, or by the merging approach through improper inter-sensor calibration. The aim of the following section is to compare the current level 2 validation of the individual satellite GOME, SCIAMACHY, and GOME-2 GODFIT_V3 products with the new level 3 GTO-ECV CCI integrated long-term record of total ozone on a global scale.

3.1 Representativeness of the ground-based network

The representativeness of the ground-based reference network used to validate a product with global coverage determines both the validation approach, and the representativeness of the validation results. While validation results (and the level 3 data themselves) are often shown and used as zonal averages, e.g. plotted against time and latitude as in Fig. 3, Fig. 7 illustrates the significant representativeness error when comparing zonal means of global gridded data with zonal means of the ground-based reference measurements.

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For this figure, IFS-MOZART modelled fields (Inness et al., 2013) were averaged to zonal monthly means, either using all data or using only data coincident (in space and time) with actual ground-based measurements. The relative difference between these two simulated zonal means yields estimated representativeness errors. As these errors exceed the expected performance of the level 3 product, the validation work presented here is based solely on level 3 grid-cells co-located with actual ground-based measurements, and on zonal statistics derived from those co-locations. Besides avoiding the representativeness error, this approach allows for a straightforward comparison with the validation results of the level 2 datasets. However, it must be kept in mind that this validation strategy is blind to the product quality outside of the ground network. This issue is tackled by comparing the product with other satellite data sets in Sect. 4.

3.2 Comparison with Dobson and Brewer measurements

The Brewer and Dobson spectrophotometer measurements, as extracted from the World Ozone and UV radiation Data Center (WOUDC, <http://www.woudc.org>) have already been used numerous times in the last two decades for the validation of various satellite-based global total ozone records (e.g. Loyola et al., 2011; Koukouli et al., 2012; Labow et al., 2013, and references therein). A comprehensive description of the individual station selection criteria has been presented in Balis et al. (2007a, b). Station selection updates may be found in more recent papers listed above. The measurements involved in this current study are the same as those used and discussed in the companion level 2 validation paper by Koukouli et al. (2015). Any level 2 comparisons shown in the following are discussed by Koukouli et al. (2015).

For comparison consistency, the Dobson/Brewer WOUDC ground-based data set was transformed into a monthly level 3 field in order to match the $1^\circ \times 1^\circ$ grid of the GTO-ECV CCI data. Measurements from all stations were gridded in the same latitude–longitude boxes with some specific considerations. First, only the Direct Sun observations have been used. Even though in some cases, as is shown in the subsequent figures, this severely decreases the number of measurements, after rigorous

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testing it was found that the usage of Direct Sun ground-based observations ensures an optimal level 3 ground-based product. Secondly the threshold on the number of measurements available before the computation of the associated monthly mean was investigated. As a compromise between obtaining the highest global coverage possible and the most representative monthly means, especially at high latitudes, a lower limit of ten measurements per month and grid box was imposed. The monthly mean total ozone columns obtained by using the effective mean day as a limit (see Sect. 2.2) was also examined; however, this choice was rejected for optimization reasons.

The validation of the GTO-ECV CCI level 3 product against the Dobson and Brewer network is presented here as a series of comparative figures: in each plot, four lines are presented, namely the level 3 comparison (in dark blue) and three level 2 comparisons for GOME (in light blue), SCIAMACHY (in green), and GOME-2 (in red), respectively. In order to compare as closely as possible the same validation results for level 3 and level 2, a time constraint was imposed on the level 2 comparisons according to the time periods for each instrument in the merged data record (see Sect. 2.1). Furthermore, the same latitudinal constraints for the monthly means were imposed (see Table 2).

Figure 8 shows the latitudinal dependency of the percentage differences for both Brewer (left) and Dobson (right) instrument types. The three satellite instruments reveal a remarkable inter-sensor consistency for all latitudes and an excellent agreement with the ground data. The level 3 comparison (blue) closely follows that for level 2. The slight positive deviation of about 0.5 % of level 3 data (compared to level 2) for the 40–60° N belt (right panel) will be discussed in the next section.

3.2.1 Northern Hemisphere statistics

The Northern Hemisphere time series comparisons are shown separately for the Brewer and Dobson instrument types in Fig. 9. The Brewer comparisons (left panel) show a very good agreement between level 3 and individual level 2 lines; well within the ± 1 % difference level for most of the 15-year data record. The two outliers during the GOME period and the two during the SCIAMACHY period are discussed below. The

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Dobson analysis (right panel) shows equally good comparisons, falling within the 1.5 % difference level with a bias of ~ 1.25 %, due to the known differences in the treatment of the stratospheric temperature dependence of the ozone absorption cross-sections and how this issue is dealt with by the ground-based algorithm (van Roozendaal et al., 1998; Scarnato et al., 2009, and references therein).

Figure 10 shows the percentage differences as a function of time for six zonal belts 0–10, 30–40, 40–50, 50–60, 60–70, and 70–90° N (from top to bottom) and for the Brewer comparisons (left) and the Dobsons (right). The patterns of the level 3 comparison are nearly identical to those from the individual level 2 comparisons. The agreement for both types of instruments is excellent up to high latitudes, except for a small number of outliers in the 60–70° N belt for the Brewer and in the 50–60° N belt for the Dobson comparisons. For this latter belt, some strong disagreement up to 5–10 % between level 3 and level 2 coincidences is shown for the SCIAMACHY period. These outliers, during years 2004 and 2005, were basically due to sampling issues. A different set of days was considered for creating the monthly mean differences for the level 2 dataset and the level 3 dataset, due to the 6 day SCIAMACHY global coverage and the scarcity of ground-based stations in those latitudes. We have to keep in mind that the level 2 comparisons are based on coincident measurements with respect to geolocation (150 km radius) and time (same day), whereas the level 3 comparisons are based on coincident measurements with respect to geolocation (same $1^\circ \times 1^\circ$ grid box) only. Therefore, a different set of days might form the basis for the level 3 monthly averages from ground-based and satellite-based data, respectively. Consequently, these larger differences do not necessarily indicate poorer quality of the level 3 data record. A similar reason explains the outliers noted in the 60–70° N belt for the Brewer comparisons. Furthermore, for the high latitude belts it is possible that we include comparisons with one ground-based station alone. Overall, considering the excellent agreement for the remainder of the belts, the consistency between the level 2 and level 3 validation results is very satisfactory.

3.2.2 Southern Hemisphere statistics

In the Southern Hemisphere, the validation is restricted to Dobson measurements. Figure 11 shows the percentage differences between satellite and ground-based data as function of time for seven 10° belts from 0–70° S and one belt from 70–90° S (top to bottom). As for the Northern Hemisphere the level 3 comparisons show a near-perfect agreement with the level 2 comparisons up to 50° S. The outliers in higher latitudes are mostly due to differences in sampling.

3.2.3 Seasonal variability statistics

The seasonal variability of the GTO-ECV CCI data compared to the Dobson network is shown in Fig. 12 as a contour plot of latitude vs. month of year. Very small seasonal features are observed with a slight oscillation of ± 1 %. For the very high Southern latitudes some underestimations are seen for the summer months (around -2 to -2.5 %) and overestimations for the winter months (around $+3$ to $+4$ %). This seasonality probably originates from the Dobson sensitivity to atmospheric effective temperature, which leads to positive differences between Dobson and satellite observations for high effective temperatures in local summer (negative differences in winter). For the Brewer stations no seasonal features are observed in the contour comparison.

3.2.4 Summary of the Brewer/Dobson comparisons

In conclusion, the GTO-ECV CCI level 3 validation results were found to be very consistent with the separate GOME, SCIAMACHY, and GOME-2 level 2 validation comparisons. In particular, on a monthly mean basis, for the Dobson comparisons, both the Northern and Southern Hemisphere time series are in very close agreement. Similarly, for the Brewer comparisons (Northern Hemisphere), an excellent agreement is found apart from a handful of outliers. On a seasonal basis, both the Brewer and the Dobson level 3 comparisons show close agreement to the level 2 comparisons.

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According to Table 5 of the Ozone_cci User Requirement Document (van der A, 2011) it was stated that the decadal stability of the total ozone column provided by the three instruments must fall within 1–3 %, the long-term accuracy of each product at 2 % and short term accuracy at 3 %. The seasonal cycle and inter-annual variability must also fall within the 3 % level. In Table 4, the statistics extracted from the Dobson (left) and Brewer (right) comparisons, respectively, are presented. Under the header “mean bias” we refer to the mean bias and SD ($1-\sigma$) of the Northern Hemisphere time series; the header “monthly mean variability” refers to the variance of the standard deviation of the monthly mean values in the Northern Hemisphere time series. The header “drift per decade” refers to the decadal drift and drift error calculated from the Northern Hemisphere time series; the header “seasonality” indicates the mean difference from the seasonal plots and the amplitude of the seasonal variability on a global scale. The header “latitude” refers to the mean bias and SD as calculated by the latitudinal variability plots on a global scale.

It is evident that the product meets easily the User requirement levels listed above. Hence, we can conclude that the current GTO-ECV CCI level 3 total ozone product is of the same high quality as the constituent level 2 total ozone products.

3.3 Comparison with SAOZ UV-visible instruments

The NDACC (Network for the Detection of Atmospheric Composition Change, <http://www.ndacc.org>) UV-visible working group operates about 35 certified SAOZ zenith-sky UV-visible absorption spectrometers (Pommereau and Goutail, 1988) distributed from the Arctic to the Antarctic. Most of the instruments perform twice-daily measurements of the total ozone column during twilight between 86–91° solar zenith angle at all latitudes and seasons. The retrieval is based on the DOAS approach in the visible Chappuis band of ozone between 470 and 540 nm.

Figure 13 shows time series of monthly mean differences between GTO-ECV CCI level 3 data and the UV-visible network grouped by latitude zones of 30°. Red dots correspond to comparisons for single stations and the white-faced red circles represent

the mean of those differences over all stations within a given latitude zone. For belts 0–30° N (bottom left panel) and 30–60° S (middle panel on the right) only one station contributes for the better part of the time series, and the zonal mean therefore coincides with the station's difference.

These comparisons with UV-visible instruments in general confirm the validation results based on the Dobsons and Brewers. Large discrepancies are evident in the southernmost bin, in particular during Antarctic ozone hole conditions. These are in large part due to co-location space–time mismatches and differences in horizontal smoothing of the large gradients occurring at the border of the polar vortex (Verhoelst et al., 2015). Noteworthy is the positive bias observed in the northernmost bin, which is not seen in the comparisons with Brewers. While the GODFIT_V3 retrieval uses more recent ozone cross-sections than those used in the default Brewer data processing, the good agreement between the GTO-ECV CCI total ozone column level 3 product and the Brewers should be interpreted with care as the GODFIT_V3 uses a soft-calibration scheme based on total ozone measurements obtained with Brewer measurements at a set of northern mid-latitude reference sites (Lerot et al., 2014). As such, the accuracy of the GTO-ECV CCI level 3 product somehow depends on that of the Brewer network. On the other hand, as this positive bias between the GTO-ECV product and the SAOZ instruments only appears at high latitudes, errors in the SAOZ AMFs cannot be ruled out either.

4 Comparison with other satellite data

In this section the GTO-ECV CCI level 3 monthly mean total ozone product is compared with two other satellite-based data records: (1) its predecessor product GTO-ECV GDP and (2) the SBUV version 8.6 merged ozone data record.

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4.1 GTO-ECV GDP

The preceding GTO-ECV GDP data record (Loyola et al., 2009a; Loyola and Coldewey-Egbers, 2012) is based on GOME, SCIAMACHY, and GOME-2 total ozone columns obtained with the GDP 4.X retrieval algorithm (van Roozendaal et al., 2006; Lerot et al., 2009; Loyola et al., 2011; Hao et al., 2014). The first version of GTO-ECV GDP covered the period from 1995 to 2008, but this has now been extended to June 2013. In addition to the retrieval algorithm, the level 3 and the merging algorithm differ from the approach used for GTO-ECV CCI. Regarding the level 3 generation, only one measurement per day and grid cell is used. Regarding the merging approach, all available satellites are averaged instead of using only one at a time. GTO-ECV GDP was incorporated in the last WMO scientific assessment of ozone depletion (WMO, 2011). Moreover, it has been used for Chemistry–Climate Model evaluation (Loyola et al., 2009a) as well as the investigation of decadal ozone trends and variability (Loyola et al., 2009b; Coldewey-Egbers et al., 2014). Both data records agree very well regarding the long-term trends emphasizing their excellent decadal stability.

Figure 14 presents the percentage differences between GTO-ECV CCI and GDP $1^\circ \times 1^\circ$ monthly means in terms of a 2-D histogram (blue shading) as a function of latitude. In addition the mean difference and standard deviation per 5° belt are plotted in black. Both data records show a remarkable inter-consistency; the overall mean difference is $0.2 \pm 1.7\%$. The deviations are slightly positive in low and middle latitudes and negative in high latitudes. The jumps in the histogram toward high latitudes (in particular seen between 70 and 90° N) are due to abrupt changes in number of measurements as a consequence of the implementation of the latitudinal and monthly constraints to the CCI data record (see Sect. 2.3).

4.2 SBUV version 8.6 merged ozone data record

Within the framework of the NASA (National Aeronautics and Space Administration) program MEaSUREs (Making Earth System data records for Use in Research En-

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vironments) data from a series of nine BUV, SBUV, and SBUV/2 instruments have been reprocessed using the version 8.6 ozone retrieval algorithm (Labow et al., 2013; McPeters et al., 2013). From these data records a coherent long-term 5° zonal monthly mean ozone time series covering the periods 1970–1972 and 1979–2014 has been created which contains both profile and total ozone column information (Frith et al., 2014). Chiou et al. (2014) compared this merged data set (referred to as SBUV-MOD in the following) with GTO-ECV CCI and ground-based total ozone columns for the 16 year overlap period from March 1996 to June 2011. They found very good agreement in terms of monthly zonal mean total ozone and monthly zonal mean anomalies (their Figs. 6 and 8). The mean difference between both data sets is $0.3 \pm 1.1\%$.

Figure 15 shows the percentage difference between GTO-ECV CCI and SBUV-MOD 5° zonal mean ozone columns as a function of latitude. The black curve denotes the annual mean difference and its SD (grey shaded area), and the blue, red, yellow, and green lines denote the seasonal differences. On average, the differences are positive in middle and low latitudes, and negative in high latitudes, where largest deviations occur in the summer months. Largest scatter is found in the Southern Hemisphere poleward of 50° S. The amplitude of the seasonal cycle in the differences is about 1%. However, a small but significant time dependence in the differences was identified (not shown here). The drift is around 0.2 DU year^{-1} in the southern middle latitudes and in the tropics, whereas it is negligible in the northern middle latitudes. Figure 4a in Chiou et al. (2014) and Fig. 6 in McPeters et al. (2013) indicate that this time dependence is due to larger positive differences in the period 2008–2011 compared to the preceding years.

In addition to total ozone columns we compare the SD of the 5° zonal monthly means. Figure 16 indicates that the latitudinal and temporal structures of the SD agree very well. The absolute differences (shown in the bottom panel) are small in low and middle latitudes, and reveal larger spread in the months and latitudes close to the polar night terminator.



5 Summary and outlook

In this paper, which is the third in a series of three on the ESA Ozone_cci total ozone products, we have described the new GTO-ECV CCI level 3 global monthly mean data record spanning the 15-year time period 1996–2011. The data record is composed of total ozone measurements from three European nadir UV backscatter sensors GOME/ERS-2, SCIAMACHY/ENVISAT, and GOME-2/MetOp-A. It is publicly available at <http://esa-ozone-cci.org>. The companion papers by Lerot et al. (2014) and Koukouli et al. (2015) introduced the ozone retrieval algorithm GODFIT_V3 and presented the validation of the level 2 total ozone products, which form the basis for the GTO-ECV CCI merged level 3 product described herein.

The merging approach relies on an inter-sensor calibration procedure using GOME as the reference. Small corrections have been applied to SCIAMACHY and GOME-2 in order to reduce the differences among the instruments. Special emphasis was placed on the analysis of sampling issues intrinsic to the satellite data and their impact on the final GTO-ECV CCI product.

We presented level 3 product geophysical validation results using as reference ground-based measurements with Brewer, Dobson and UV-visible SAOZ instruments. The validation of the GTO-ECV CCI level 3 data record was found to be very consistent with the equivalent separate GOME, SCIAMACHY, and GOME-2 level 2 validation (Koukouli et al., 2015). In particular, on a monthly mean basis, for the Dobson comparisons, both the Northern and Southern Hemisphere time series are in strong agreement. Similarly, for the Brewer comparisons (Northern Hemisphere), an excellent agreement is found apart from a handful of outliers. On a seasonal basis, both the Brewer and the Dobson level 3 comparisons show close agreement to the level 2 comparisons. We conclude that the current 15-year GTO-ECV CCI level 3 total ozone data product is of the same high quality as the equivalent individual level 2 data products that constitute it. This is due to a very high level of consistency among the level 2 products themselves and a robust merging approach. Both absolute agreement and

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long-term stability are excellent for almost all latitudes apart from a few outliers which are mostly due to sampling differences between the level 2 and level 3 data that cannot be completely eradicated.

This study demonstrates that the current GTO-ECV CCI data record is suitable for a variety of applications. In particular it is useful for the long-term monitoring of the past evolution of the ozone layer. Due to its excellent decadal stability it is valuable for long-term trend analysis on global and regional scales as recently demonstrated by Coldewey-Egbers et al. (2014).

Furthermore, global long-term data records such as GTO-ECV CCI can be compared with Chemistry–Climate Model (CCM) simulations. CCMs are three-dimensional atmospheric circulation models with fully coupled stratospheric chemistry. One of the main purposes of these models is to identify and quantify relevant processes and forcings affecting the ozone layer and to project their future evolution. In particular, the simulations are analyzed to assess the returning of ozone to historical levels and the complete recovery from ODSs as a consequence of the 1987 Montreal Protocol (UNEP, 1986). The satellite-based data records enable us to evaluate these model projections and to calibrate the efficacy of the model system (Loyola et al., 2009a).

Regarding total ozone, the second phase of ESA-CCI is dedicated to an improvement of the sampling errors (see Sects. 2.2 and 2.3) using spatio-temporal statistical tools and an extension of the GTO-ECV CCI data record. The GOME-2 sensor used in this study is the first of a series of three identical instruments. GOME-2 on Metop-B was launched in September 2012 and the data will be included in the new version of GTO-ECV. In addition measurements performed with the Ozone Monitoring Instrument (OMI) onboard the NASA Aura satellite (2004–present) and the Ozone Mapping and Profiler Suite (OMPS) onboard the NASA Suomi National Polar-orbiting Partnership satellite (2011–present) will be included. The GOME-2 on Metop-C is planned to be launched in 2018, and together with the Sentinel-5 precursor (to be launched in 2016) and the Sentinel-4 and Sentinel-5 sensors (to be launched by the end of this decade), these future instruments will contribute to the extension of this reference data set.

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Table 1. European total ozone satellite instrument characteristics.

Parameter	GOME	SCIAMACHY	GOME-2
Data availability	Jul 1995–Jun 2011 ^a	Aug 2002–Apr 2012	Jan 2007–today
Organization	ESA	ESA	EUMETSAT ^b
Satellite	ERS-2	ENVISAT	MetOp-A
Spectral coverage	240–790 nm	240–2380 nm	240–790 nm
Spectral resolution	0.2–0.4 nm	0.2–1.5 nm	0.2–0.4 nm
PMD ^c coverage	3 p-PMD 300–800 nm	6 p-PMD 320–2380 nm	15 p-PMD and 15 s-PMD 310–790 nm
Viewing geometries	nadir	nadir, limb, occultation	nadir
Ground pixel size	320 km × 40 km	60 km × 30 km	40 km × 80 km
Swath width	960 km	960 km	1920 km
Altitude	785 km	800 km	817 km
Equator crossing	10:30 LT ^d	10:00 LT	09:30 LT
Global coverage	3 days	6 days	almost daily ^e
Reference	Burrows et al. (1999)	Bovensmann et al. (1999)	Callies et al. (2000)

^a No global coverage since June 2003.^b European Organisation for the Exploitation of METeorological SATellites.^c PMD: Polarization Measurement Device detecting polarised light perpendicular (p-) or parallel (s-) to the optical plane.^d LT: Local Time.^e Until June 2013.

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M. Coldewey-Egbers
et al.**Table 2.** Latitudinal and monthly constraints imposed on the GTO-ECV CCI monthly mean calculation.

Month	Latitude Range
Jan	60.0° N–90.0° S
Feb	70.0° N–90.0° S
Mar	80.0° N–80.0° S
Apr	90.0° N–65.0° S
May	90.0° N–60.0° S
Jun	90.0° N–57.5° S
Jul	90.0° N–57.5° S
Aug	90.0° N–62.5° S
Sep	82.5° N–72.5° S
Oct	72.5° N–85.0° S
Nov	65.0° N–90.0° S
Dec	60.0° N–90.0° S

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Table 3. Description and dimensions of all variables contained in the level 3 monthly mean total ozone NetCDF files. $N_{\text{lat}} = 180$ and $N_{\text{lon}} = 360$.

Description of variable	Unit	Dimension
Latitude of grid center	degree	N_{lat}
Longitude of grid center	degree	N_{lon}
Mean total ozone column	DU	$N_{\text{lat}} \times N_{\text{lon}}$
Standard deviation of mean total ozone column	DU	$N_{\text{lat}} \times N_{\text{lon}}$
Standard error of mean total ozone column	DU	$N_{\text{lat}} \times N_{\text{lon}}$
Number of measurements used to derive the monthly mean total ozone column	–	$N_{\text{lat}} \times N_{\text{lon}}$

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M. Coldewey-Egbers
et al.**Table 4.** The statistics following the figures presented in Sect. 3.2 on a global scale.

GTO-ECV CCI	Dobson	Brewer
Mean bias	$1.00 \pm 0.75 \%$	$0.16 \pm 0.66 \%$
Monthly mean variability	$\pm 2.35 \%$	$\pm 2.20 \%$
Drift per decade	$-0.12 \pm 0.12 \%$	$0.17 \pm 0.11 \%$
Seasonality	$0.80 \pm 0.21 \%$	$0.16 \pm 0.30 \%$
Latitude	$0.72 \pm 0.96 \%$	$0.30 \pm 0.41 \%$

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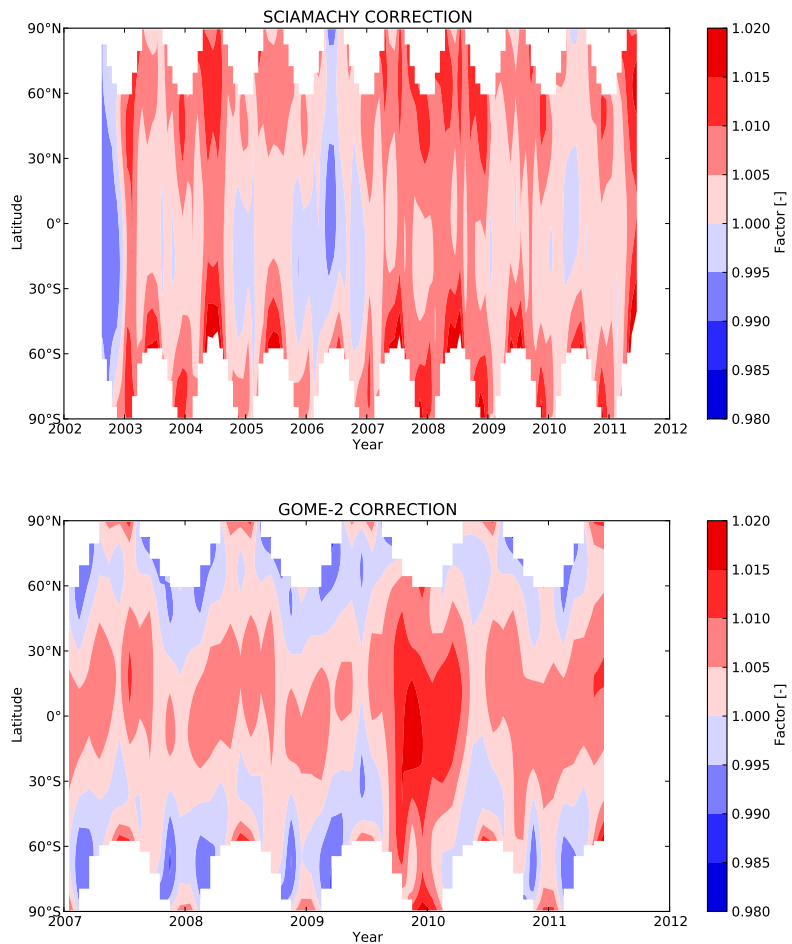


Figure 1. Correction factors for SCIAMACHY 2002–2011 (top panel) and GOME-2 2007–2011 (bottom panel) as a function of latitude.

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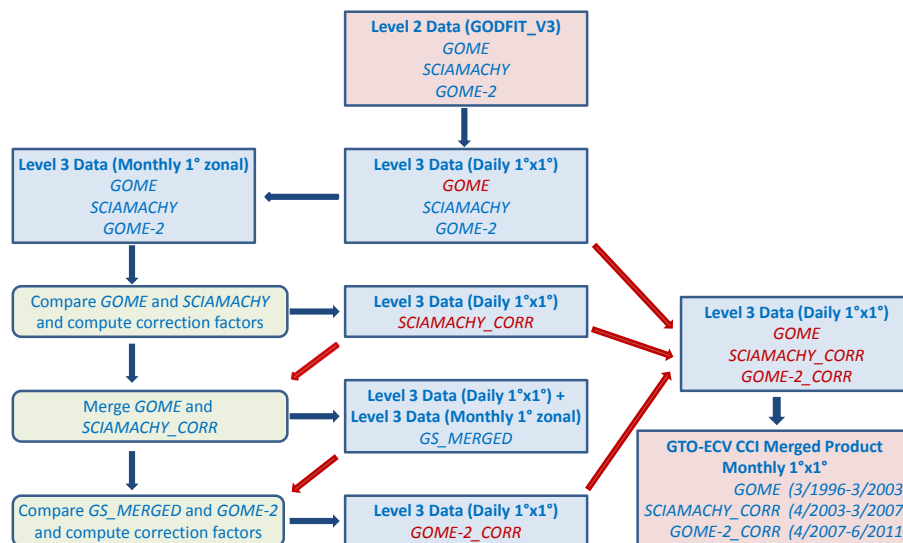
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Figure 2. Flow chart of the GTO-ECV CCI level 3 algorithm and merging approach. Red-shaded boxes denote data records which are part of the official ESA Ozone CCI Climate Research Data Package (CRDP). Blue-shaded boxes denote intermediate data sets needed to create the merged final product and green shading denotes the steps of the merging approach.

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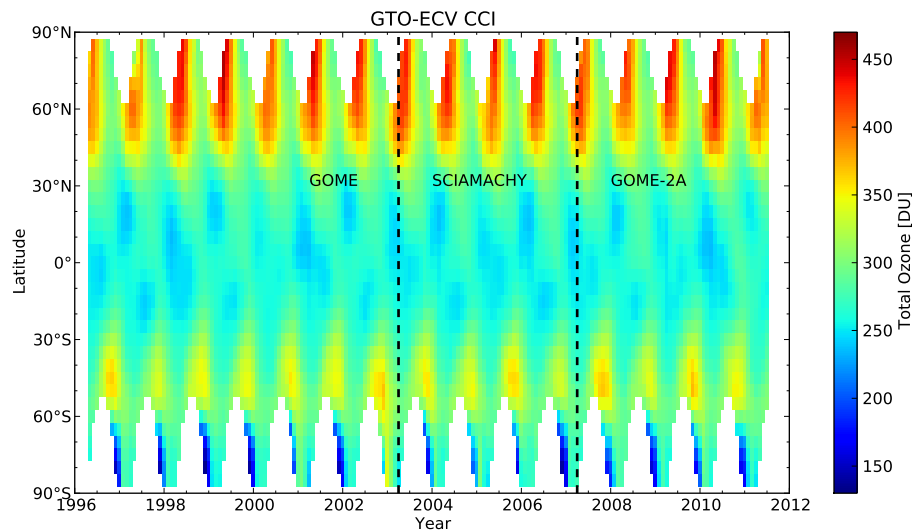
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Figure 3. GTO-ECV CCI total ozone column data record 1996–2011 as a function of latitude. Vertical black dashed lines indicate the change-over from GOME to SCIAMACHY in March 2003 and from SCIAMACHY to GOME-2 in March 2007.

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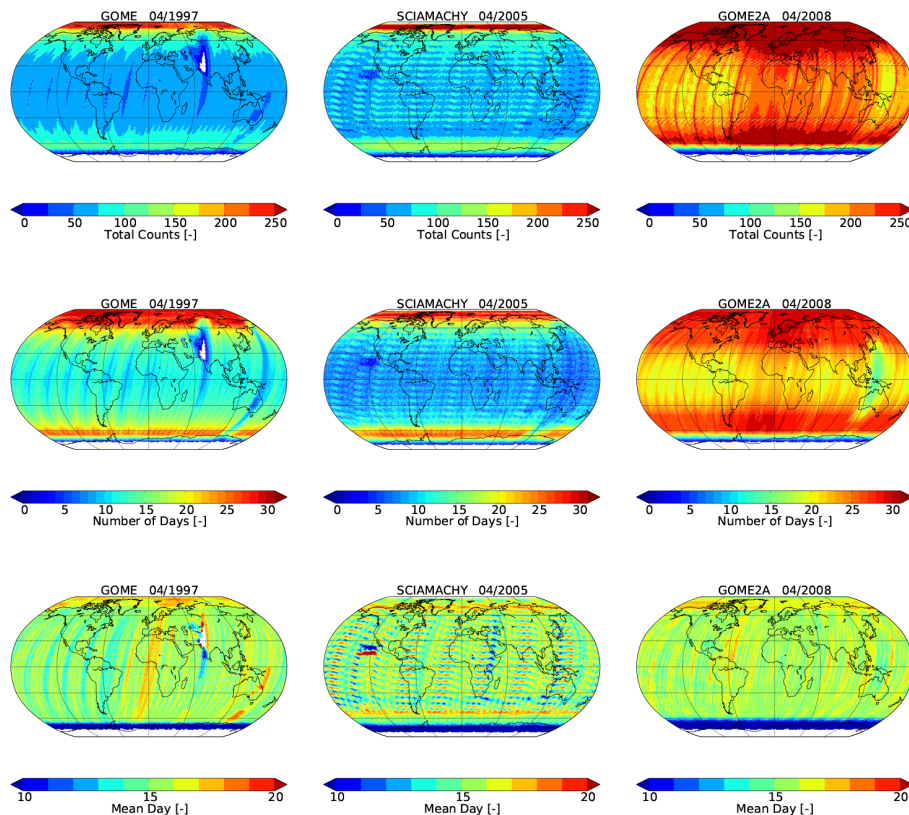


Figure 4. Sampling patterns of GOME (left column), SCIAMACHY (middle column), and GOME-2 (right column) exemplified for April 1997, 2005, and 2008, respectively. Top row: total number of measurements per month and grid cell, middle row: number of days for which measurements are available, and bottom row: effective mean day d_{eff} representing the monthly mean according to Eq. (1).

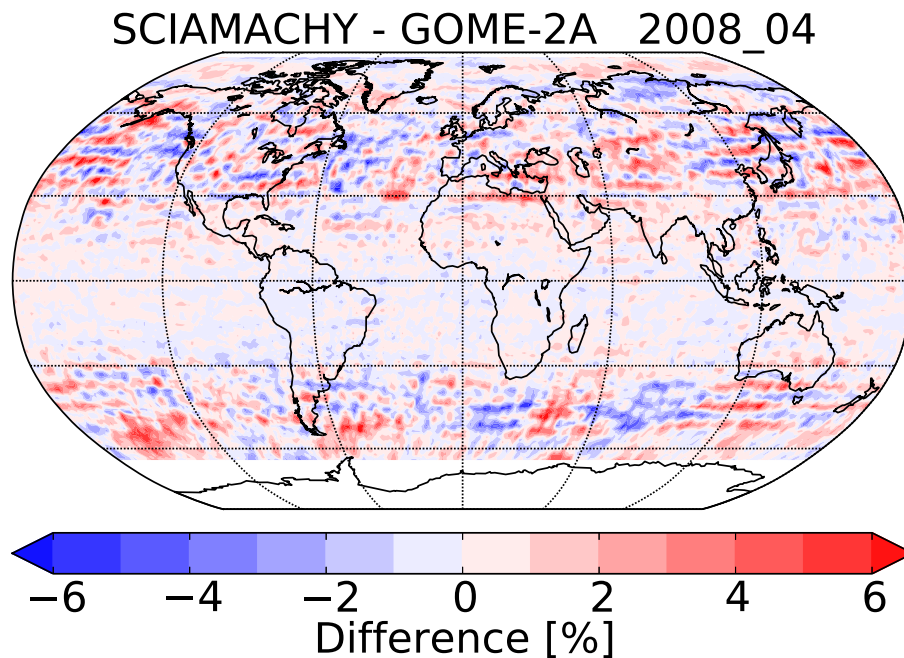


Figure 5. Percentage differences between SCIAMACHY and GOME-2 monthly mean total ozone for April 2008.

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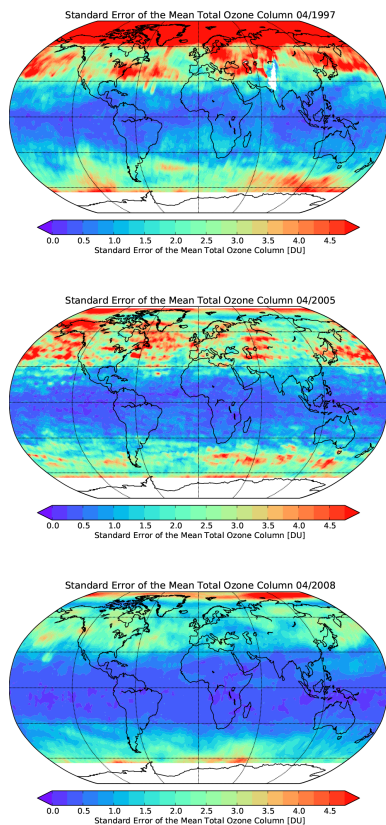


Figure 6. Standard error associated with the product for GOME (top), SCIAMACHY (middle), and GOME-2 (bottom) for April 1997, 2005, and 2008, respectively.

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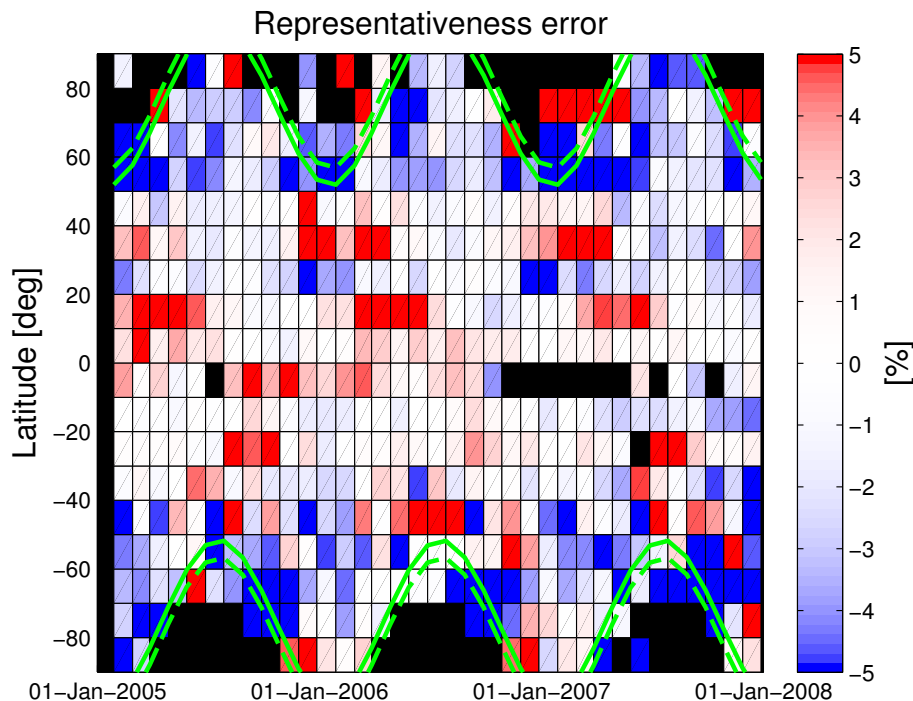


Figure 7. Simulated differences between zonal means based either on data coincident (in space and time) with ground-based reference measurements, or on full global gridded data. These differences constitute the so-called representativeness error. Data used for this graph are 6-hourly modelled fields calculated with IFS-MOZART for MACC (Inness et al., 2013). The green solid and dashed lines correspond to 75° and 80° Solar Zenith Angles at noon, respectively.

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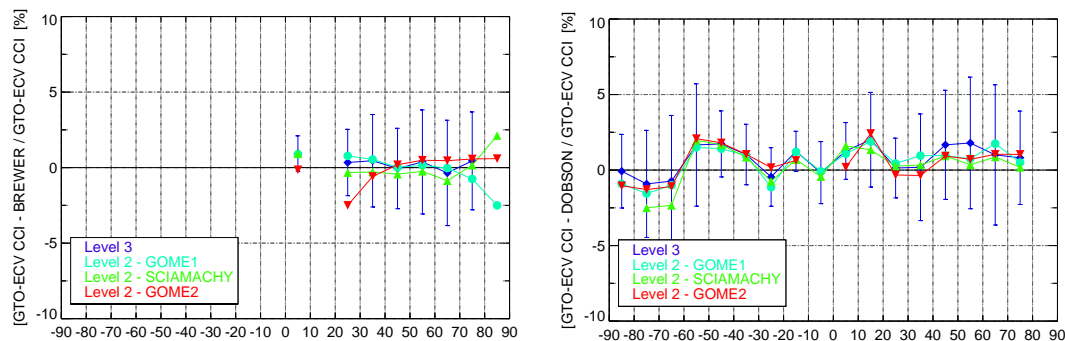
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Figure 8. Percentage difference between satellite data records and ground-based data as a function of latitude. Left: Brewer comparison and right: Dobson comparison. Level 3 comparison in dark blue, GOME level 2 comparison in light blue, SCIAMACHY in green and GOME-2 in red. The $1-\sigma$ SD of the averaging is given only for the level 3 lines.

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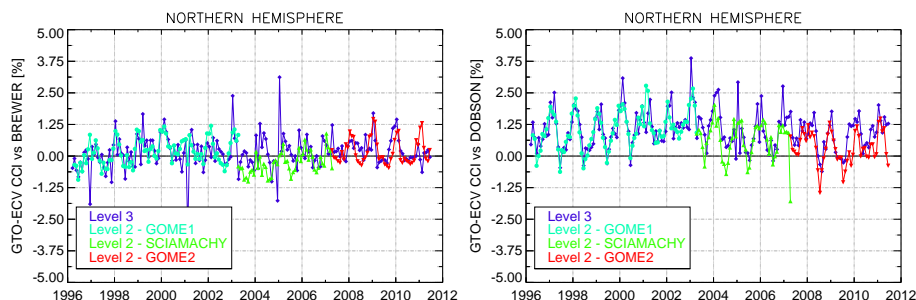
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Figure 9. Percentage difference between satellite data records and ground-based data as a function time for the Northern Hemisphere. Left: Brewer comparison and right: Dobson comparison. Level 3 comparison in dark blue, GOME level 2 comparison in light blue, SCIAMACHY in green and GOME-2 in red.

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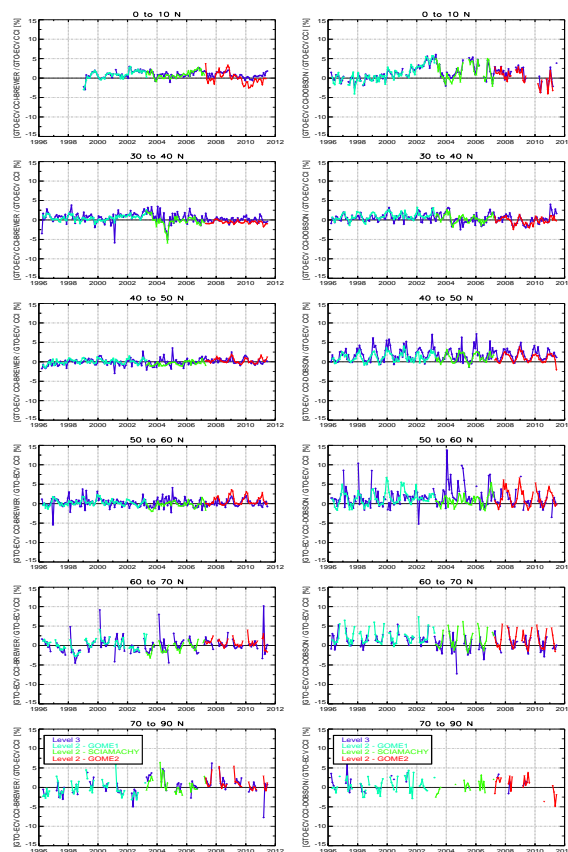


Figure 10. Percentage difference between satellite data records and ground-based data as a function of time for the Northern Hemisphere for six zonal belts 0–10, 30–40, 40–50, 50–60, 60–70, and 70–90° N from top to bottom. Left column: Brewer comparison and right column: Dobson comparison. Level 3 comparison in dark blue, GOME level 2 comparison in light blue, SCIAMACHY in green and GOME-2 in red.

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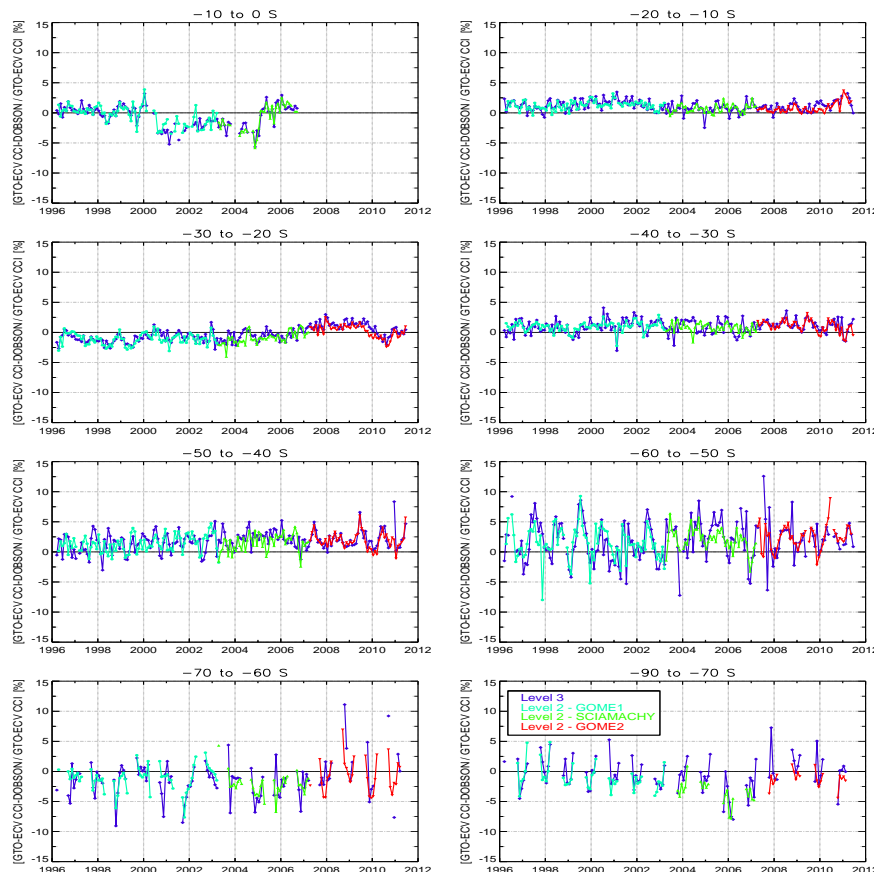


Figure 11. Percentage difference between satellite data records and Dobson ground-based data as a function of time for the Southern Hemisphere for seven 10° zonal belts from 0–70° S and one belt from 70–90° S. Level 3 comparison in dark blue, GOME level 2 comparison in light blue, SCIAMACHY in green and GOME-2 in red.

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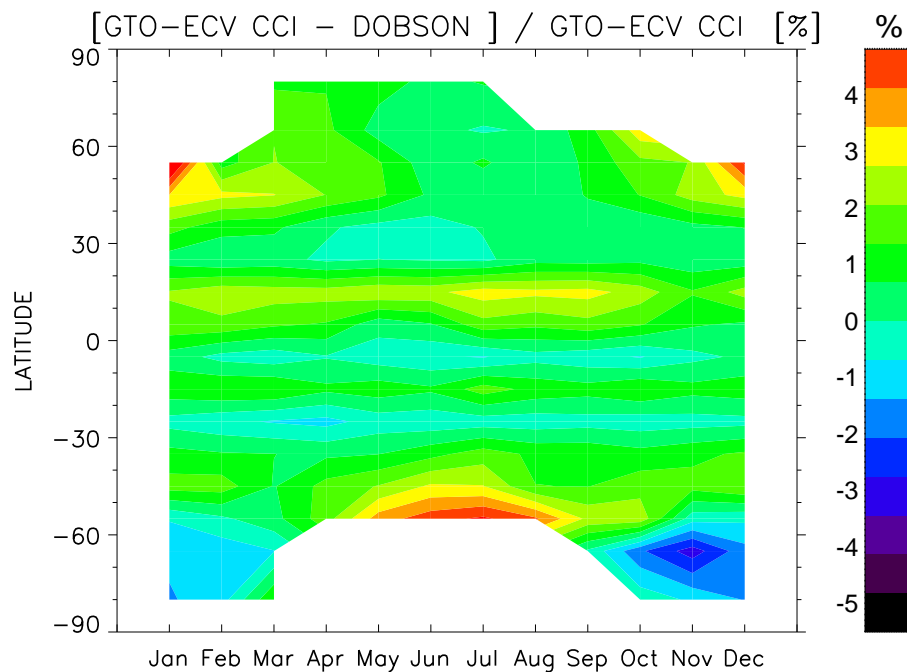
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Figure 12. Seasonal variability of the GTO-ECV CCI data compared to the Dobson network as a contour plot of latitude vs. month of the year.

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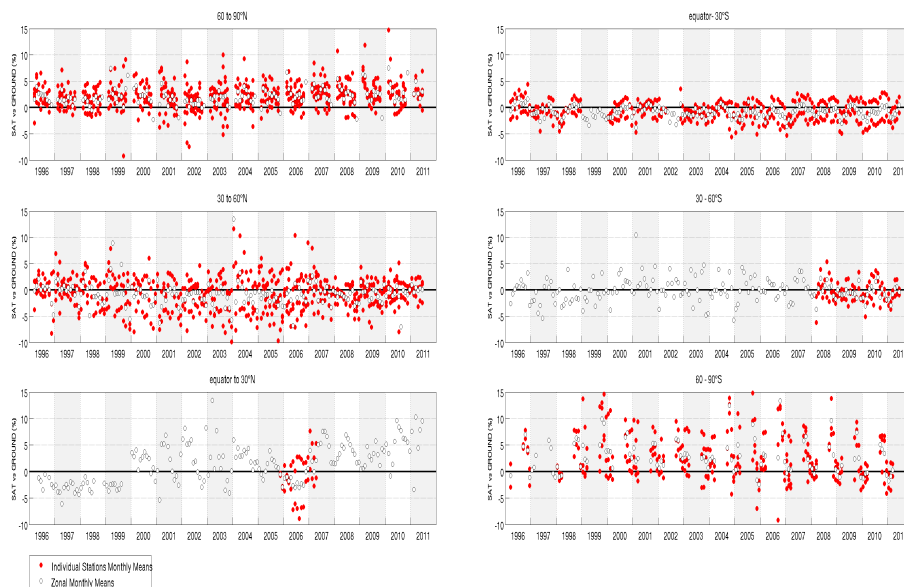


Figure 13. Time series of monthly mean relative differences for NDACC UV-visible instruments for six 30° latitude zones; Northern Hemisphere in the left panels (from top to bottom: high, middle, and low latitudes), Southern Hemisphere in the right panels (from top to bottom: low, middle, and high latitudes). Red dots correspond to individual stations, red open circles correspond to the zonal means. If only one station contributes, the single-station differences are coincident with the zonal mean.

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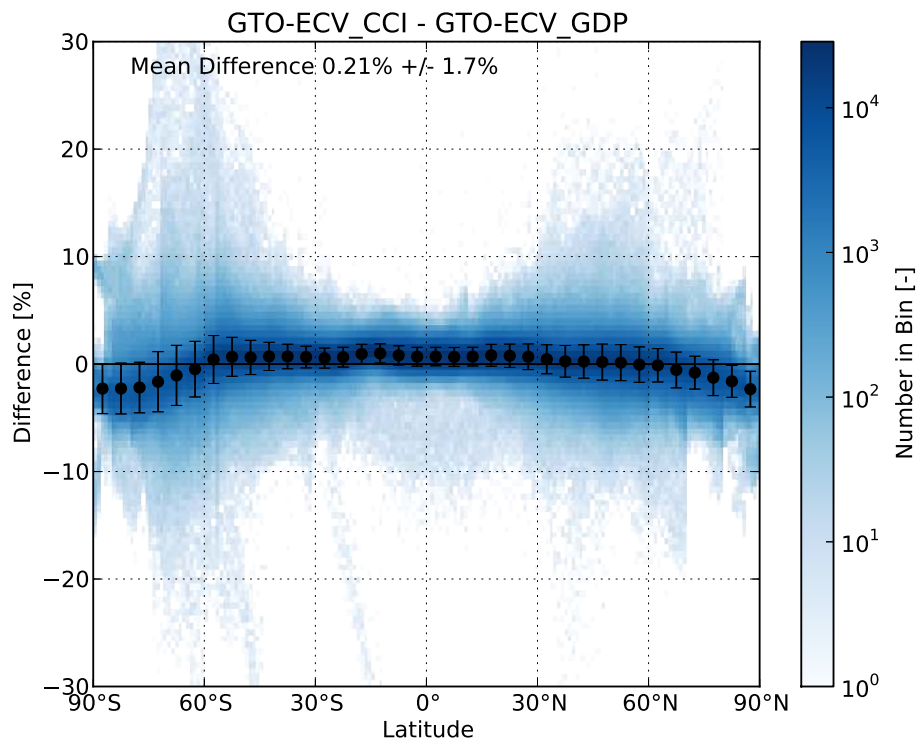


Figure 14. Percentage differences between GTO-ECV CCI and GDP $1^\circ \times 1^\circ$ monthly means 1996–2011 as a function of latitude. The blue shading denotes the number of measurements pairs used to compute the percent difference in each bin. The mean difference and standard deviation per 5° latitude belt are plotted in black.

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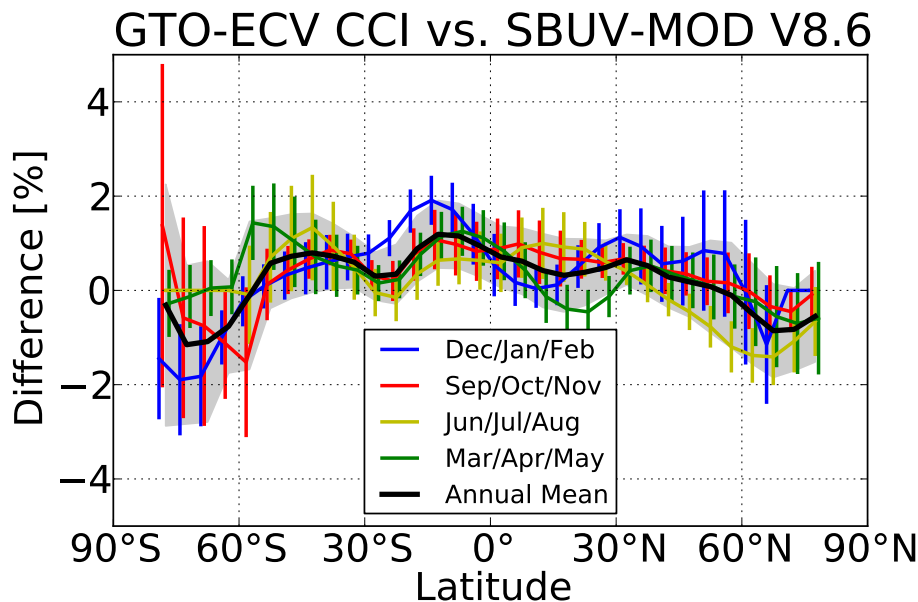
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Figure 15. Percentage differences between GTO-ECV CCI and SBUV-MOD 5° monthly zonal mean ozone columns as a function of latitude. Black: annual mean difference and its SD (grey shaded area). Blue, red, yellow, and green lines denote the differences for northern hemisphere winter, autumn, summer, and spring, respectively.

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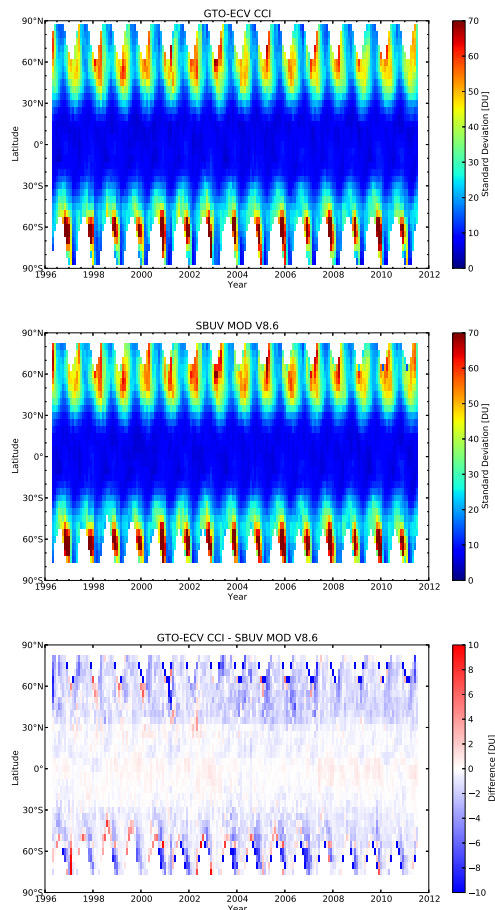


Figure 16. Standard deviation of 5° monthly mean ozone columns as a function of latitude and time: GTO-ECV CCI (top panel) and SBUV-MOD (middle panel). The bottom panel shows the absolute difference between GTO-ECV CCI and SBUV-MOD SD.