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1 Purpose and scope

1.1 Purpose

An End-to-End ECV Uncertainty Budget (E3UB) describes all steps of uncertainty assessment from comprehensive uncertainty estimates of individual measurements to the full error budget of higher level data products. Error budget studies in the O3 CCI+ project (<https://climate.esa.int/en/projects/ozone>) are based on both error propagation and geophysical validation of ozone measurements and their uncertainties. Instrumental drift issues are investigated as well. The purpose of this document is to collect in one place the characterization and geophysical validation of uncertainty estimates of all individual Level 2 datasets participating in the project and provide characterizations of errors of the Level 3 and Level 4 Climate Data Records (CDR) generated within the project.

In this document the focus is on algorithm activities during Phase III of the O3 CCI+ project (2025-2026). For datasets developed in O3 CCI Phase II (2014-2017) and earlier phases of O3 CCI+ (2019-2024), we refer to, respectively, the Comprehensive Error Characterization Report (CERC) [RD3] and End to End ECV Uncertainty Budget document (E3UB) [RD4].

1.2 Reference documents

[RD1] CCI Data Standards v2.3, online at

https://climate.esa.int/media/documents/CCI_DataStandards_v2-3.pdf

[RD2] CCI+ Phase 2 Product Validation and Intercomparison Report (PVIR) v5.2, online at

<https://climate.esa.int/en/projects/ozone/key-documents>

[RD3] CCI Comprehensive Error Characterization Report (CERC) v2, online at

<https://climate.esa.int/en/projects/ozone/key-documents>

[RD4] CCI+ Phase 1 End to End ECV Uncertainty Budget (E3UB) v5.0, online at

<https://climate.esa.int/en/projects/ozone/key-documents>

[RD5] CCI+ Phase 2 Algorithm Theoretical Basis Document (ATBD) v3.2, online at

<https://climate.esa.int/en/projects/ozone/key-documents>

1.3 Summary and terminology

The "**precision**" of an instrument/retrieval is its random (in the time domain) error. It is the debiased root mean square deviation of the measured values from the true values. The precision can also be seen as scatter of multiple measurements of the same quantity. The



difference between the measured and the true state can still be large, because there still can be a large systematic error component unaccounted by the precision.

The "**bias**" of an instrument/retrieval characterizes its systematic (in the time domain) error. It is the mean difference of the measured values from the true values.

The "**total error**" of an instrument/retrieval characterizes the estimated total difference between the measured and the true value. In parts of the literature the expected total error is called "accuracy" but we suggest not using this particular term because its use in the literature is ambiguous.

1.4 Acronyms

ACE-FTS	Atmospheric Chemistry Experiment – Fourier Transform Spectrometer
CCI	Climate Change Initiative
CDR	Climate Data Record
ECMWF	European Centre for Medium-range Weather Forecast
ECV	Essential Climate Variable
ENVISAT	Environmental Satellite (ESA)
ESA	European Space Agency
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FMI	Finnish Meteorological Institute
FORLI	Fast Optimal Retrievals on Layers for IASI
GODFIT	GOME-type Direct-FITting
GOME	Global Ozone Monitoring Experiment
GOMOS	Global Ozone Monitoring by Occultation of Stars
IASI	Infrared Atmospheric Sounding Interferometer
ISS	International Space Station
KNMI	Royal Netherlands Meteorological Institute
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
NASA	National Aeronautics and Space Administration
NDACC	Network for the Detection of Atmospheric Composition Change
OMI	Ozone Monitoring Instrument (aboard EOS-Aura)
OMPS-LP	Ozone Mapper and Profile Suite - Limb Profiler (aboard Suomi-NPP)
OSIRIS	Optical and Spectroscopic Remote Imaging System (aboard Odin)
POAM	Polar Ozone and Aerosol Measurement (aboard SPOT 4)
RAL	Rutherford Appleton Laboratory
SABER	Sounding of the Atmosphere using Broadband Emission Radiometry
SAGE	Stratospheric Aerosol and Gas Experiment
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric CHartography
UTLS	Upper Troposphere Lower Stratosphere



2 Uncertainty of Level 2 data

The Level 2 data (individual ozone profiles or column data) are the starting point for creating climate data variables. For remote sensing measurements, the uncertainty budget is estimated via propagation of measurement noise (random) and other uncertainties (random or systematic) through the inversion algorithm (e.g., Rodgers, 2000). Von Clarmann et al. (2020) uses the term “**ex-ante**” for the uncertainty estimates by an inversion algorithm, so do we in this document. Some CCI projects prefer the term “prognostic” uncertainty.

Ex-ante uncertainty estimates might be incomplete: this might be due to incomplete/simplified models of the processes that describe the satellite measurements or/and unknown/unresolved atmospheric features. Other contributing factors might be the imperfect estimates of measurement uncertainties, as well as the uncertainties of external auxiliary data. Therefore, validation of theoretical (ex-ante) uncertainty estimates is desired for remote-sensing measurements. For atmospheric measurements specifically, a distinction shall be made between a baseline validation, which consists in checking biases and comparing dispersions with the requirements, and a proper validation of ex-ante uncertainty estimates, which is not a trivial task because the measurements are performed in a continuously changing atmosphere. The experimental estimates of uncertainty estimates are called “**ex-post**” estimates in von Clarmann et al. (2020), and we follow this terminology. Other CCI projects refer to such estimates as “diagnostic” uncertainty.

This section presents the characterization of Level 2 uncertainties (ex-ante) and the results of the uncertainty validation. The overview of the methods for uncertainty validation is collected in Section 4 of E3UB Ozone_cci Phase 1 [RD 4], together with a summary of publications on error budget evaluation and uncertainties validation of Level 2 ECV's generated within Ozone_cci.

2.1 Total ozone columns

2.1.1 GODFIT

Within the O3 CCI+ project, the baseline algorithm for total ozone retrieval from backscatter UV sensors is the GOME-type direct-fitting (GODFIT) algorithm. Dominant error sources are

- Ozone absorption cross-section uncertainties,
- Level-1 calibration limitations,
- Interferences with other species, including aerosols,
- Cloud contamination
- A priori ozone profile shape, especially at large solar zenith angles (SZA).

Figure 1 shows that the mean total ozone error due to the profile shape is less than 0.5% at low SZA, and is as large as 4% at extreme SZA for clear sky pixels. The error increases in the case of cloud contamination, especially at low SZA.

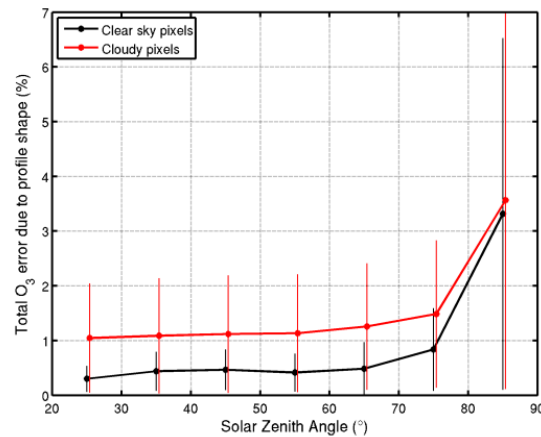


Figure 1: Mean total ozone error due to a priori ozone profile shape, as a function of the SZA for clear sky and cloudy pixels. Error bars represent the standard deviation of the errors.

Figure 2 illustrates the total ozone errors due to the neglect of aerosols in the forward model for different types of atmospheric aerosols content. These errors are generally within 1%. In particular, it is shown that the fit of the surface albedo leads to a minimization of the errors, which would be much larger without that procedure (up to 4%) in heavily polluted conditions. For a scenario with a strong injection of stratospheric aerosols due to a major volcanic eruption such as Pinatubo, the total errors may reach 10% (right panel).

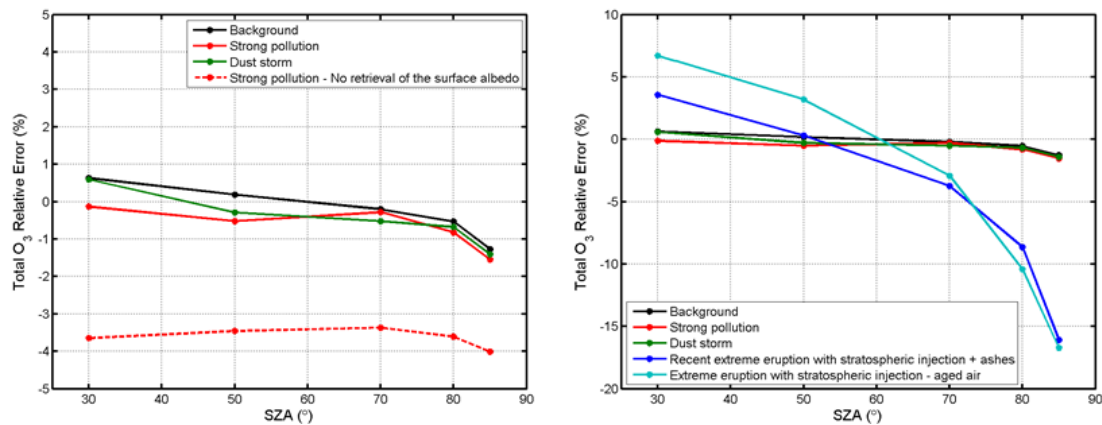


Figure 2: Left: total ozone error (%) due to neglect of aerosols in the retrieval scheme, polluted and dust storm scenarios; Right: same for strong volcanic eruption scenarios.

Table 1 summarizes current assessment of the main contributions to the global error budget on total ozone retrievals by GODFIT. Total errors are computed assuming all contributions are mutually uncorrelated.



Error source	Percent error	
	SZA < 80°	SZA > 80°
Instrument signal-to-noise	< 0.5	< 2
O ₃ absorption cross-sections and atmospheric temperature	< 2.5	< 2.5
Interferences with other species (except in case of volcanic eruption)	< 1.5	< 1
Aerosols (except in case of volcanic eruption)	< 1	< 1.5
Instrument spectral stability (wavelength registration)	< 0.5	< 0.5
Solar I_0 -effect	< 0.2	< 0.2
Ring effect (rotational Raman scattering)	< 0.1	< 0.5
O ₃ profile shape	< 1	< 4
Cloud fraction	< 0.5	< 0.5
Cloud top height	< 1.5	< 1.5
Total random error (including cloud fields)	< 1.7	< 2.6
Total systematic error	< 3.3	< 5.2

Table 1: Estimation of the error sources of the direct fitting total ozone retrievals (single pixel retrieval). Blue fields indicate random errors (precision) associated with instrument signal-to-noise, which can be easily derived by the propagation of radiance and irradiance statistical errors provided in the Level 1 products through the inversion algorithm, and red fields systematic errors. The errors due to the cloud parameters (orange) are random or systematic depending on the time scale.

2.2 Ozone profiles from nadir sensors

2.2.1 RAL processor

This section is unchanged from the CCI Phase 1 document [RD4] and remains relevant for the current publicly released products. In CCI phase 2 a re-engineered and updated version of the profile scheme has been developed, but products are not yet released. Uncertainties on that product are described in the ATBD covering the re-engineered scheme [RD5].

Analysis of error budget of RAL scheme, reported in (Siddans, 2003), is based on performing retrieval simulations for a set of basic geophysical scenarios, which had been defined for the GOME-2 Error Study (Kerridge et al., 2002). Figure 3 shows retrieval precision and base-line



mapped errors for GOME-1 and the April 55°N scenario from Siddans (2003). Dashed and solid lines refer to the 80% and 5% surface albedo cases respectively. Colours distinguish results for the 3 across-track ground pixels in Band 1 (the legend shows the pixel mean off-nadir angle in degrees; positive angle are East of nadir). Dotted lines in each panel other than the top left show (for comparison) the precision where the scale permits. The black dash-dot curve is the a priori error input to the B1 retrieval. Retrieval precision and a priori are also plotted as negative values for comparison with negative mapped errors.

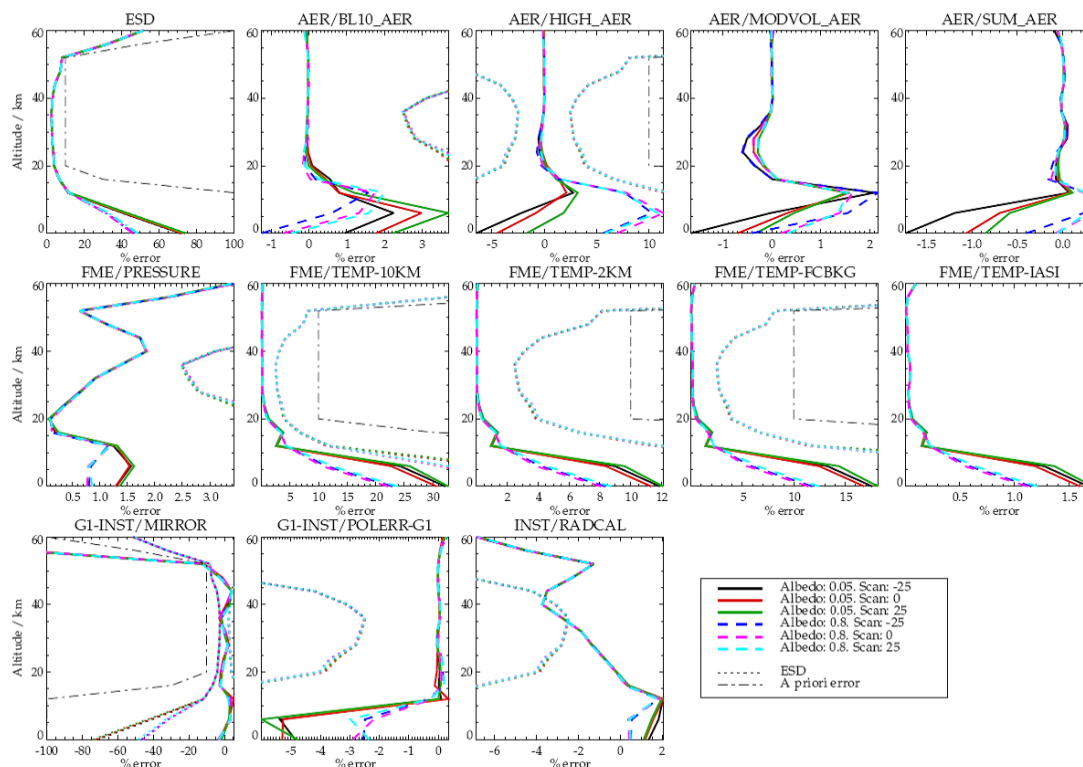


Figure 3: Retrieval precision and base-line mapped errors for GOME-1 and the April 55°N scenario.

(Miles et al., 2015) assessed the performance of the RAL ozone profile retrieval scheme for GOME-2 with a focus on tropospheric ozone. The retrieval precision, as given by the square roots of diagonals of the solution error covariance matrix, is generally in the few percent range in the stratosphere increasing to a few tens of percent in the lowest retrieval levels. An example is presented in Figure 4 for a mid-latitude profile in Northern Hemisphere summer. In this case, the retrieval precision on retrieval levels is typically much smaller than a priori error throughout the profile. The retrieval noise error is around a factor of 2 smaller than the retrieval precision.

Figure 5 shows an example of how the retrieval precision varies for a typical orbit cross-section; the uncertainty values are higher at lower altitudes in tropical and polar conditions.

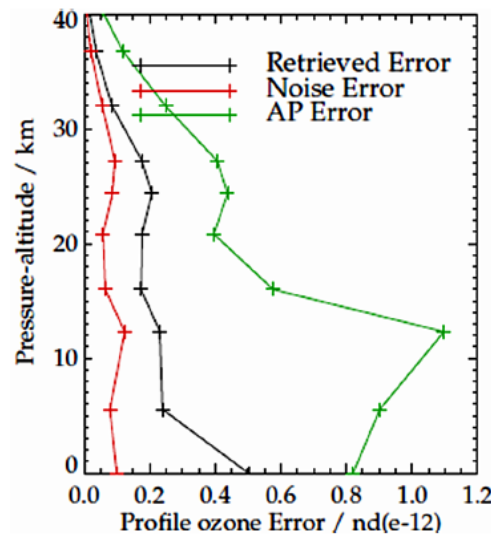


Figure 4: Error assessment for ozone profile for a GOME-2 nadir pixel at 45°N on 25 August 2008.

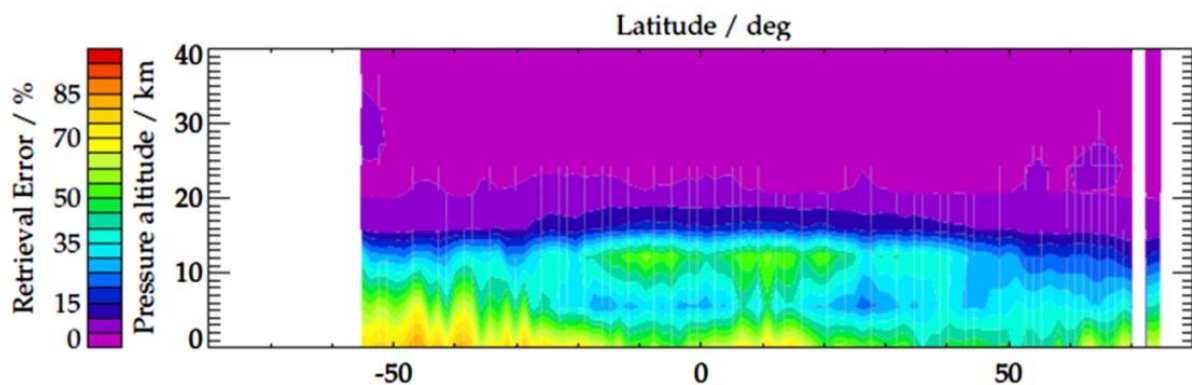


Figure 5: Relative retrieval error of ozone product from GOME-2 retrieved with RAL scheme.

Keppens et al. (2018) reported a relative random error for RAL v2.14 of about:

- 5 % at the altitude of the ozone maximum;
- up to about 10 % at higher altitudes;
- up to 40 % in the lower troposphere.

By comparing nadir ozone profiles and ground-based ozonesonde and lidar measurements, the authors conclude that “the total satellite measurement and retrieval uncertainty is typically underestimated in the RAL v2.14 nadir ozone profile products, because the ex-ante uncertainty under consideration only includes random noise errors.”



Regarding satellite drifts, Keppens et al. (2018) reported:

- negative and insignificant decadal drift on the order of 5 % per decade for GOME;
- insignificant (except for the tropics) drift on the order of –15 and 10 % per decade for OMI's L2 stratospheric and tropospheric observations, respectively;
- a significant positive drift of ~40 % per decade for SCIAMACHY and GOME-2A below the tropopause.
- a significant 30 % per decade negative drift in the UTLS at all latitudes for GOME-2A.

2.3 Ozone profiles from limb sensors

2.3.1 OMPS-LP / NOAA-21

The current version of ozone profiles retrieved from the central slit of the OMPS-LP instrument on board NOAA-21 (N21) is obtained using the same retrieval approach based on spectral fitting as for observations from OMPS-LP on board Suomi-NPP (SNPP). Retrieval settings are also similar, as described in (Arosio et al., 2018).

A study was performed to estimate the error budget for the retrieved profiles from SNPP (Arosio et al., 2022). Results from that study are briefly summarized in the next paragraph and are expected to be valid for the ozone retrievals from N21 observations.

Synthetic simulations with SCIATRAN were used to estimate the error budget. The main source of parameter uncertainties is the pointing accuracy of the instrument, especially in the upper stratosphere. The precision of the retrieved aerosol extinction profiles and surface albedo plays a significant role below 25 km with parameter uncertainty up to 5 %. The cloud filtering is also relevant below 20 km. This contribution is rather systematic and was added to the retrieval bias. Another relevant source of uncertainty was found to be related to the used ozone cross-section. The cross-section error propagated into Level 2 profiles is estimated to be on the order of 2 % in the lower stratosphere and decreasing with altitude. In addition, the analysis of the error from model approximations revealed that the radiative transfer solver and polarisation effect may add to the total ozone error a contribution up to 1-2 %. Errors were classified in random and systematic components, providing a total estimation of the two as a function of latitude.

2.4 Ozone profiles from geostationary sensors

2.4.1 GEMS and TEMPO

The datasets are under development.



3 Uncertainty of level 3 data

3.1 Tropospheric ozone column

3.1.1 CHORA

The convective cloud differential (CCD) method, here CHORA (Cloud Height and Ozone Referencing Algorithm), to retrieve tropospheric ozone columns is applied to level 2 GOME-type data, i.e., ozone total columns and cloud data. This study is performed in O3 CCI Phase 3. The CHORA algorithm is currently applied to GODFIT level 2 data of the following instruments: SCIAMACHY, OMI, GOME-2 (A, B, C), and TROPOMI.

The retrieval data are calculated on $1^\circ \times 3^\circ$ grid with a monthly resolution, therefore within one grid cell several individual observations are averaged. Depending on the instrument the maximum number of averaged observations per grid cell goes up to roughly 4000 for S5P. For SCIAMACHY, GOME-2 and OMI the numbers vary around 50-100. Thus, the influence off the individual measurement and the propagated error is limited and variation between the individual observations dominates the uncertainty.

Uncertainties of daily tropospheric ozone values are estimated as:

$$\sigma_{TrOC}^2 = \sigma_{TOC}^2 + \sigma_{SOC}^2, \quad (3.1.1.1)$$

where σ_{TOC}^2 is the uncertainty of the total ozone column and σ_{SOC}^2 is the uncertainty of the stratospheric ozone column. σ_{SOC}^2 is calculated from the 95% confidence interval of the Theil-Sen regression of the stratospheric column up to 270 hPa for each latitude band. σ_{TOC}^2 is calculated for each grid cell as the 95% confidence interval of total ozone column variation

The 1-day uncertainty $\sigma_{trOC,d}$ is hence propagated to the monthly $\sigma_{trOC,m}$:

$$\sigma_{trOC,m}^2 = \frac{\sum_{month} \sigma_{trOC,d}^2}{month} \quad (3.1.1.2)$$

We found CHORA uncertainties between 4 and 7 DU on a monthly basis for TROPOMI and GOME2. An example is shown for TROPOMI in Fig. 6. The uncertainty depends on stratospheric dynamics and cloud pressure difference changing over the year because of e.g. the ITCZ.

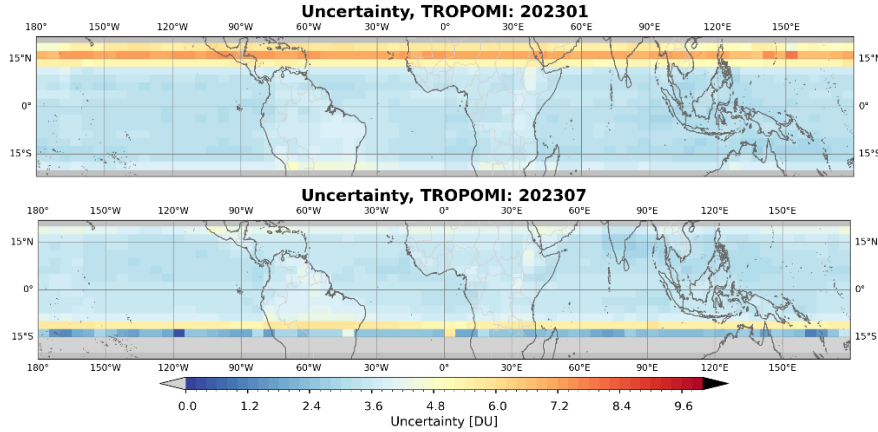


Figure 6. CHORA/TROPOMI tropospheric ozone uncertainties (DU) for January 2023 (top) and July 2023 (bottom). Grey areas show no data.

3.1.2 GTO-LIMB

The random uncertainty of the resulting tropospheric ozone column is estimated via error propagation through all steps of the retrieval algorithm.

For daily total ozone column, the uncertainty is computed as:

$$\sigma^2 = \frac{1}{N} \sum_i \sigma_i^2 + \frac{1}{N} \text{var}(\rho_i) \quad (3.1.2.1)$$

where σ_i are uncertainties reported by the retrieval algorithm and $\text{var}(\rho_i)$ is the variance of N individual ozone values in the bin. The typical daily gridded clear-sky total ozone column and the corresponding random uncertainties are in the range of 0.5 - 5 DU (typically 1-2 DU).

The uncertainty estimation of daily gridded and interpolated ozone profiles is described in Sect. 3.3.3. Uncertainties of the stratospheric ozone column are then estimated using error propagation, it is mostly 5-8 DU (< 2%).

Uncertainties of daily tropospheric ozone values are estimated as:

$$\sigma_{TrOC}^2 = \sigma_{TOC}^2 + \sigma_{SOC}^2, \quad (3.1.2.2)$$

where σ_{TOC}^2 is the uncertainty of the total ozone column and σ_{SOC}^2 is the uncertainty of the stratospheric ozone column.

The uncertainties of monthly average data are estimated similarly to uncertainties of the gridded data, i.e., by Eq. (3.1.2.1). In this case, all parameters are related to tropospheric ozone column. In the majority of tropical locations, the estimated uncertainty of the tropospheric ozone column is 5-7 DU. Over Indonesia, where the tropospheric ozone column has the smallest values, the relative uncertainty increases to 100%. In the mid-latitudes, the



estimated uncertainties are mostly within the range of 15-40%. The largest uncertainty is close to the polar vortex boundary, as expected. The illustrations of the uncertainties are shown in Figure 7 and in Sofieva et al. (2022).

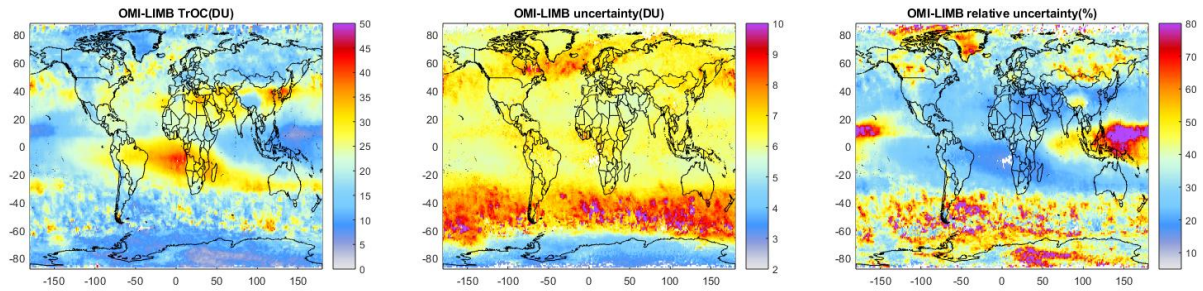


Figure 7. Adapted from Sofieva et al. (2022): OMI-LIMB tropospheric ozone distributions (DU, color) for September 2018 (left). The stratospheric ozone column is estimated from 3 km below the tropopause. The corresponding estimated uncertainties are shown in absolute values (DU) on the central panel and in relative values (%) on the right panel.

3.2 Merged data sets

3.2.1 GOP-ECV

The merged ozone profile data record GOP-ECV (GOME-type Ozone Profile Essential Climate Variable) from the nadir ultraviolet-visible satellite sensors consists of monthly mean ozone partial columns for 19 atmospheric layers covering 0-80 km and 5°x5° latitude-longitude grid cells. Data from five sensors (GOME, SCIAMACHY, OMI, GOME-2A, and GOME-2B) are merged into a homogeneous record spanning the period 1995-2021. The merged profiles are finally adjusted with respect to the GTO-ECV total column data record (Coldewey-Egbers et al., 2015, 2022).

The uncertainties are approximated analogously as described in detail in Sofieva et al. (2021). At first, monthly mean profiles $\rho_{k,i}$ from each individual sensor k are computed for each spatio-temporal bin i , and the uncertainties of the averages are evaluated by the standard error $\sigma_{k,i}$ of the mean

$$\sigma_{k,i} = \frac{s_{k,i}}{\sqrt{n}} \quad (3.2.1.1)$$

$s_{k,i}$ is the standard deviation and n is the number of measurements in that spatio-temporal bin. Since the merging is based on de-seasonalized anomalies, the climatological means $\rho_{k,m}$ and their corresponding uncertainties $\sigma_{k,m}$ for each sensor k and each month m from January to December are computed as well. The uncertainty of the seasonal cycle is estimated via

$$\sigma_{k,m}^2 = \frac{1}{N_m} \sum_{j=1}^{N_m} \sigma_{k,j}^2 \quad (3.2.1.2)$$



where N_m is the number of monthly mean values for month m for all available years. The uncertainty $\sigma_{k,i}$ of the monthly mean profile and the uncertainty $\sigma_{k,m}$ of the climatological mean are used to obtain an estimate of the uncertainty of the de-seasonalized anomaly $\sigma_{\Delta_{k,i}}$:

$$\sigma_{\Delta_{k,i}} = \Delta_{k,i} \sqrt{\frac{\sigma_{k,i}^2}{\rho_{k,i}^2} + \frac{\sigma_{k,m}^2}{\rho_{k,m}^2}} \quad (3.2.1.3)$$

$\Delta_{k,i}$ is the de-seasonalized relative anomaly for sensor k and spatio-temporal bin i and computed as

$$\Delta_{k,i} = \frac{\rho_{k,i} - \rho_{k,m}}{\rho_{k,m}} \quad (3.2.1.4)$$

The merged de-seasonalized anomaly $\Delta_{\text{merged},i}$ then corresponds to the median of the individual sensors

$$\Delta_{\text{merged},i} = \text{median}(\Delta_{k,i}) \quad (3.2.1.5)$$

Following Sofieva et al. (2021), the uncertainty $\sigma_{\Delta_{\text{merged},i}}$ of the merged de-seasonalized anomaly $\Delta_{\text{merged},i}$ is finally estimated as

$$\sigma_{\Delta_{\text{merged},i}} = \min \left(\sigma_{\Delta_{k_{\text{median}}}}, \sqrt{\frac{1}{N} \sum_{k=1}^N \sigma_{\Delta_{k,i}}^2 + \frac{1}{N^2} \sum_{k=1}^N (\Delta_{k,i} - \Delta_{\text{merged},i})^2} \right) \quad (3.2.1.6)$$

In that equation the first term $\sigma_{\Delta_{k_{\text{median}}}}$ is the uncertainty of the anomaly of the sensor corresponding to the median value. For more details we refer to Sofieva et al. (2021).

Figure 8 illustrates the estimated uncertainties provided with the GOP-ECV product for two layers (surface-450hPa (top row) and 100-50hPa (bottom row)) for two months: April (left) and October (right).

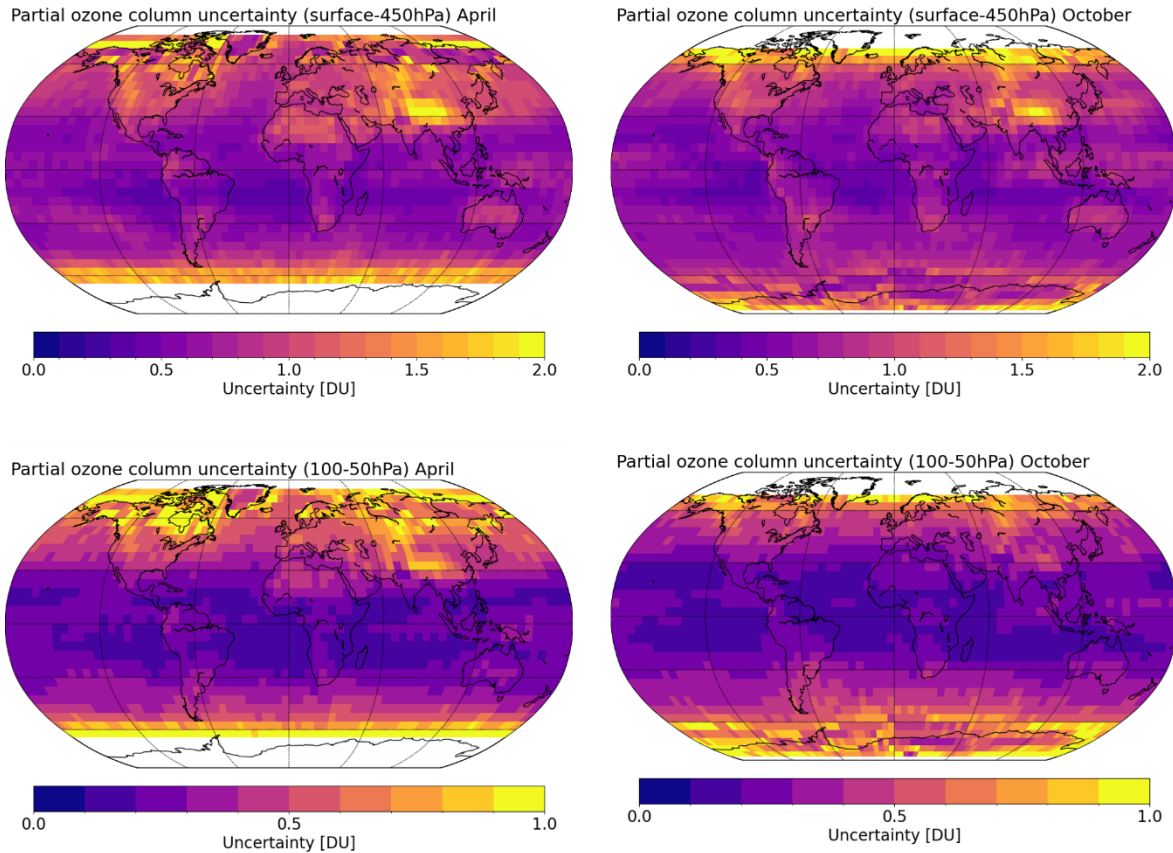


Figure 8. Illustration of uncertainty provided with the GOP-ECV product. Top left: partial column uncertainty for lowermost tropospheric ozone (surface-450hPa) in April and top right: partial column (surface-450hPa) uncertainty for October. Bottom row: partial ozone column uncertainty in 100-50hPa layer for April (left) and October (right).

3.2.2 IASI MG-FORLI

The IASI L3 MG-FORLI dataset consists of daily $1^\circ \times 1^\circ$ gridded clear-sky weighted average of all IASI-A (from 20080101 to 20190919), -B (from 20130308 to now) and -C (from 20190920 to now) O3 profiles assigned to that grid cell in the pressure range from the surface to 40 km with one extra layer from 40 to 60 km.

The weighted average ozone value ($\bar{x}_w$) and its associated error estimate (σ) in a specific level and in a level-3 grid cell are calculated.. The weighted mean is computed over all IASI-A, -B and -C values (x_i) assigned to that bin; the weight of each measurement i is the reciprocal square of the associated total retrieval random errors (σ_i , i.e. measurement and smoothing errors), reported by the FORLI-O3 (v20191122) retrieval algorithm, at that level (the details are provided in Sect. 3.1 of [RD4]).



$$\bar{x}_w = \frac{\sum_i \frac{x_i}{\sigma_i^2}}{\sum_i \frac{1}{\sigma_i^2}}$$

The random uncertainty σ on the weighted mean is calculated from the sum of two terms:

$$\sigma^2 = \frac{1}{\sum_i \frac{1}{\sigma_i^2}} + \frac{S_w^2}{N}$$

The first term, the reciprocal sum of all the individual weights assigned to a cell, corresponds to error propagation and the second term corresponds to the “geophysical” standard error of the weighted mean in the grid cell, where S_w^2 is the sample weighted variance (variance around the weighted mean in the cell) and N , the total number of IASI observations assigned to the grid cell. Although the sample variance does not properly characterize the data variability in case of small data sample (such as, in our case, in daily $1^\circ \times 1^\circ$ averaged data), it is still preferable to consider both error terms to provide a conservative estimate of random uncertainty σ associated with the mean (Sofieva et al., 2022). In the previous version of IASI L3 MG-FORLI ozone profile dataset (V1.0 provided in Phase 2), only the error propagation was reported. In this version (V2.0), error propagation, weighted variance and number of IASI observations assigned to the grid are all provided in order to derive a better estimate of the random uncertainty.

Figure 9 shows an example of daily distribution (20190616; merged IASI-A and -B) of (a) weighted mean total ozone columns, $\bar{x}_w$, and of its random uncertainty estimate, σ , calculated (b) without and (c) with including the standard error of the weighted mean. The uncertainty estimates in the updated IASI L3 MG-FORLI dataset (V2.0) are around twice larger than in the previous V1.0 dataset. The high values around the areas without measurements usually reflect grids with poor representativeness, i.e. with high weighted variance and low number of IASI observations.

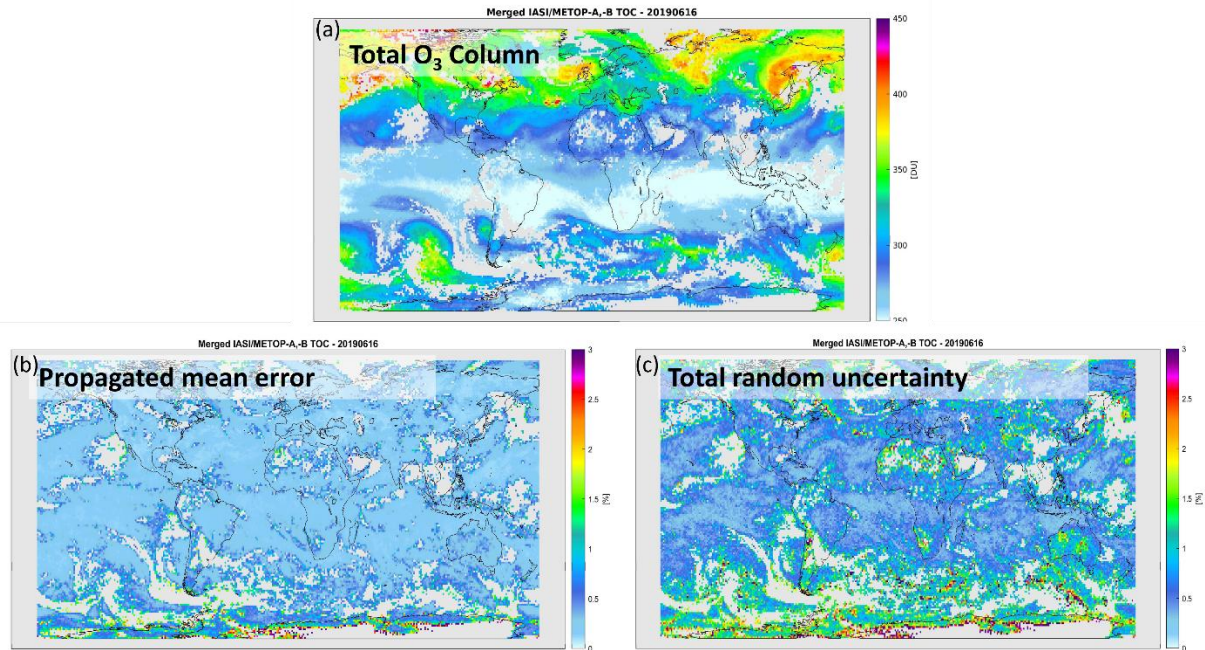


Figure 9. (a) Weighted mean total O₃ columns in daily 1° x 1° grids (20190616; merged IASI-A & -B in DU) and associated random uncertainty estimates (in %), (b) without and (c) with including the standard error of the weighted mean

3.2.3 LIMB-HIRES

The high-resolution gap-free dataset of ozone profiles consists of daily gridded profiles in the pressure range from 900 to 0.02 hPa with a horizontal resolution of 1° x 1°. Ozone profiles from satellite limb instruments are debiased to Aura MLS and their random uncertainties are a-posteriori estimated by the method described in Sofieva et al. (2022). These uncertainties are used in the kriging-type interpolation.

The estimation of uncertainties associated with the interpolated dataset of ozone profiles are evaluated as follows. Firstly, we used the error propagation to evaluate the uncertainty after the kriging step. In addition, we estimated the interpolation uncertainty using the SILAM data: we run the same interpolation but on the SILAM fields sub-sampled at the measurements locations, and evaluated the error as the absolute difference of true and interpolated data. The final uncertainty is the root-mean-square of error propagation and model-assessed interpolation errors. The illustration of error estimation can be found in the Supplement of Sofieva et al. (2022). It is presented also in Figure 10.

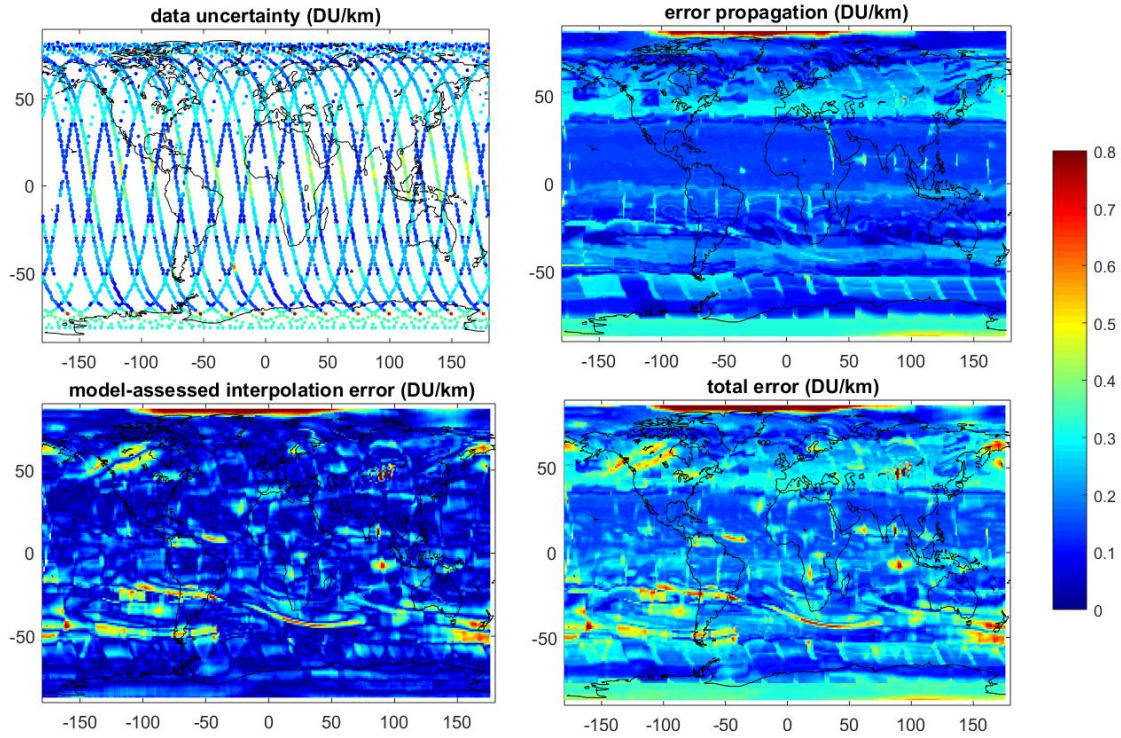


Figure 10. From Sofieva et al. (2022): Illustration of uncertainty estimation of the interpolated ozone data. Data are for 1 Sep 2018, at 10 hPa. Top left: uncertainty of satellite data, top right: error propagation after kriging-type interpolation, bottom left: interpolation error from SILAM data, bottom right: total uncertainty.

3.2.4 SAGE-CCI-OMPS+

The description of the merged SAGE II - CCI - OMPS+ data set can be found in (Sofieva et al., 2017, 2023). The merged SAGE-CCI-OMPS dataset consists of deseasonalized anomalies of ozone in 10° latitude bands from 90S to 90N and from 10 to 50 km in steps of 1 km covering the period from October 1984 to present. In addition, merged monthly zonal mean number density profiles are also included.

The merging is performed via taking the median of deseasonalized anomalies. Each data in the merged SAGE-CCI-OMPS dataset is provided with estimated uncertainty, which is estimated as follows. First, uncertainties of individual deseasonalized normalized anomalies for each month and each latitude-altitude bin $\sigma_{\Delta i}$ are evaluated as

$$\sigma_{\Delta i} = \frac{1}{\rho_m} \sqrt{\sigma_{\rho,i}^2 + \sigma_m^2}, \quad (3.2.4.1)$$

where $\sigma_{\rho,i}$ is the uncertainty of the monthly zonal mean value from Eq. (2), and σ_m is uncertainty of the seasonal cycle (Sofieva et al., 2017).



The uncertainties of the merged deseasonalized anomalies (which correspond to median value) are estimated as

$$\sigma_{\Delta,merged} = \min \left(\sigma_{\Delta,j_{med}}, \sqrt{\frac{1}{N} \sum_{j=1}^N \sigma_{\Delta,j}^2 + \frac{1}{N^2} \sum_{j=1}^N (\Delta_j - \Delta_{merged})^2} \right), \quad (3.2.4.2)$$

where $\sigma_{\Delta,j_{med}}$ is the uncertainty of the anomaly of the instrument corresponding to the median value. Eq. (5) can be interpreted as follows. If individual anomalies are significantly different, i.e., the corresponding error bars do not intersect, the uncertainty of the merged anomaly is the uncertainty corresponding to the median value. In case several instruments report a similar anomaly (intersecting error bars), this provides more confidence of this anomaly value, and the resulting uncertainty of the merged anomaly is approximated as

$$\sqrt{\frac{1}{N} \sum_{j=1}^N \sigma_{\Delta,j}^2 + \frac{1}{N^2} \sum_{j=1}^N (\Delta_j - \Delta_{merged})^2}.$$

The uncertainty of the merged dataset is illustrated in Figure 11 for several latitude bands. As expected, the uncertainties in the time period when only SAGE II data were available are larger than uncertainties for time periods when several instruments have contributed. The average uncertainty is usually less than 4% before 2001 and below 1% for the years 2002-2017. In the UTLS, uncertainties are larger than in the stratosphere and are in the range of 3-9 %. At mid-latitudes, uncertainties are larger in winter than in summer due to larger ozone variability during winter; this is observed clearly in the period before 2001.

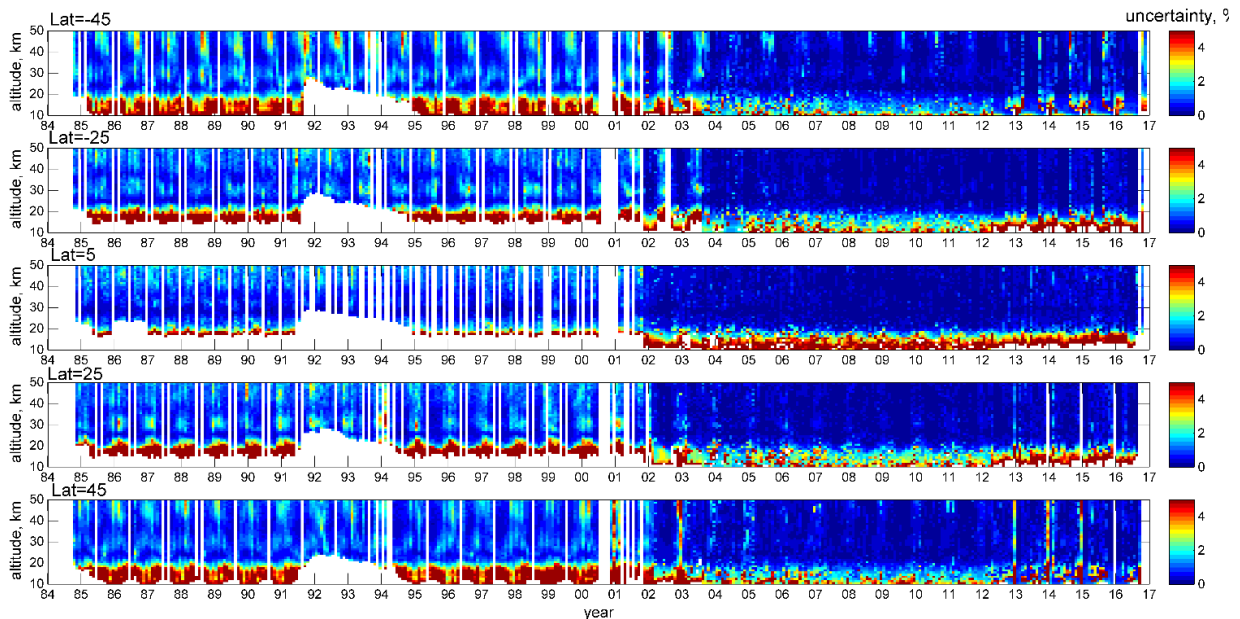


Figure 11: Uncertainties of the merged deseasonalized anomalies in %, Eq. (5), for several 10° latitude bands, centers of which are specified in the legend.

3.2.5 MEGRIDOP

The merging in the MEGRIDOP dataset is performed in the same way as for SAGE-CCI-OMPS+ dataset, thus the uncertainties are evaluated in a similar way. The detailed information about uncertainty estimates, which is analogous to that provided in Section 3.2.4 is provided in (Sofieva et al., 2021).

The average estimated uncertainty of the merged ozone is usually less than 2% before 2012 and below 1% after 2012. In the UTLS, uncertainties are larger than in the stratosphere; they are typically in the range of 2-12 % before 2012 and 2-6 % after 2012.

3.2.6 LIMB-UTLS

The dataset is under development. The principle of uncertainty estimation is the same as for the SAGE-CCI-OMPS+ dataset.

3.2.7 Merged OMPS-LP

Level-2 profile data from the two OMPS-LP instruments, onboard Suomi NPP and NOAA-21 are merged into a L3 gridded data set covering the period 2012-present. The merging was performed on deseasonalized anomalies and the time series reconstructed adding the average seasonal cycle of the two instruments. The gridding is on a monthly basis, with a 5° latitude x 20° longitude binning and a 1.5 km vertical sampling.



Uncertainty estimation will be provided later.

4 References

Arosio, C., Rozanov, A., Malinina, E., Eichmann, K.-U., Clarmann, T. von, and Burrows, J. P.: Retrieval of ozone profiles from OMPS limb scattering observations, *Atmospheric Measurement Techniques*, 11, 2135–2149, <https://doi.org/10.5194/amt-11-2135-2018>, 2018.

Arosio, C., Rozanov, A., Gorshchev, V., Laeng, A., and Burrows, J. P.: Assessment of the error budget for stratospheric ozone profiles retrieved from OMPS limb-scatter measurements, *Atmospheric Measurement Techniques Discussions*, 2022, 1–27, <https://doi.org/10.5194/amt-2022-116>, 2022.

Boynard, A., Clerbaux, C., Coheur, P.-F., Hurtmans, D., Turquety, S., George, M., Hadji-Lazaro, J., Keim, C., and Meyer-Arnek, J.: Measurements of total and tropospheric ozone from IASI: comparison with correlative satellite, ground-based and ozonesonde observations, *Atmos. Chem. Phys.*, 9, 6255–6271, <https://doi.org/10.5194/acp-9-6255-2009>, 2009.

Boynard, A., Hurtmans, D., Garane, K., Goutail, F., Hadji-Lazaro, J., Koukouli, M. E., Wespes, C., Vigouroux, C., Keppens, A., Pommereau, J.-P., Pazmino, A., Balis, D., Loyola, D., Valks, P., Sussmann, R., Smale, D., Coheur, P.-F., and Clerbaux, C.: Validation of the IASI FORLI/EUMETSAT ozone products using satellite (GOME-2), ground-based (Brewer–Dobson, SAOZ, FTIR) and ozonesonde measurements, *Atmos. Meas. Tech.*, 11, 5125–5152, <https://doi.org/10.5194/amt-11-5125-2018>, 2018.

Clarmann, T. von, Degenstein, D. A., Livesey, N. J., Bender, S., Braverman, A., Butz, A., Compernelle, S., Damadeo, R., Dueck, S., Eriksson, P., Funke, B., Johnson, M. C., Kasai, Y., Keppens, A., Kleinert, A., Kramarova, N. A., Laeng, A., Langerock, B., Payne, V. H., Rozanov, A., Sato, T. O., Schneider, M., Sheese, P., Sofieva, V., Stiller, G. P., Savigny, C. von, and Zawada, D.: Overview: Estimating and reporting uncertainties in remotely sensed atmospheric composition and temperature, *Atmospheric Measurement Techniques*, 13, 4393–4436, <https://doi.org/10.5194/amt-13-4393-2020>, 2020.

Coldewey-Egbers, M., Loyola, D. G., Koukouli, M., Balis, D., Lambert, J.-C., Verhoelst, T., Granville, J., Roozendael, M. van, Lerot, C., Spurr, R., Frith, S. M., and Zehner, C.: The GOME-type Total Ozone Essential Climate Variable (GTO-ECV) data record from the ESA Climate Change Initiative, *Atmospheric Measurement Techniques*, 8, 3923–3940, <https://doi.org/10.5194/amt-8-3923-2015>, 2015.

Coldewey-Egbers, M., Loyola, D. G., Lerot, C., and Van Roozendael, M.: Global, regional and seasonal analysis of total ozone trends derived from the 1995–2020 GTO-ECV climate data record, *Atmos. Chem. Phys.*, 22, 6861–6878, <https://doi.org/10.5194/acp-22-6861-2022>, 2022.



El Aabaribaoune, M., Emili, E., and Guidard, V.: Estimation of the error covariance matrix for IASI radiances and its impact on the assimilation of ozone in a chemistry transport model, *Atmos. Meas. Tech.*, 14, 2841–2856, <https://doi.org/10.5194/amt-14-2841-2021>, 2021.

Heue, K.-P., Eichmann, K.-U., and Valks, P.: TROPOMI/S5P ATBD of tropospheric ozone data products Issue 2.3, 2021.

Keppens, A., Lambert, J.-C., Granville, J., Hubert, D., Verhoelst, T., Compernelle, S., Latter, B., Kerridge, B., Siddans, R., Boynard, A., Hadji-Lazaro, J., Clerbaux, C., Wespes, C., Hurtmans, D. R., Coheur, P.-F., Van Peet, J. C. A., Van Der A, R. J., Garane, K., Koukouli, M. E., Balis, D. S., Delcloo, A., Kivi, R., Stübi, R., Godin-Beekmann, S., Van Roozendael, M., and Zehner, C.: Quality assessment of the Ozone_cci Climate Research Data Package (release 2017) – Part 2: Ground-based validation of nadir ozone profile data products, *Atmos. Meas. Tech.*, 11, 3769–3800, <https://doi.org/10.5194/amt-11-3769-2018>, 2018.

Kerridge, B. J. K., R. Siddans, Latter, B. L., Burrows, J. P., Weber, M., Beek, R. De, Aben, I., and Hartman, W.: GOME-2 Error Assessment Study. Final Report EUMETSAT Contract No EUM/CO/01/901/DK., 2002.

Miles, G. M., Siddans, R., Kerridge, B. J., Latter, B. G., and Richards, N. A. D.: Tropospheric ozone and ozone profiles retrieved from GOME-2 and their validation, *Atmospheric Measurement Techniques*, 8, 385–398, <https://doi.org/10.5194/amt-8-385-2015>, 2015.

Rodgers, C. D.: *Inverse Methods for Atmospheric sounding: Theory and Practice*, World Scientific, 2000.

Siddans, R.: *Height Resolved Ozone Retrievals from Global Ozone Monitoring Experiment.*, University of Reading, 2003, 2003.

Sofieva, V. F., Kyrölä, E., Laine, M., Tamminen, J., Degenstein, D., Bourassa, A., Roth, C., Zawada, D., Weber, M., Rozanov, A., Rähpö, N., Stiller, G., Laeng, A., Clarmann, T. von, Walker, K. A., Sheese, P., Hubert, D., Roozendael, M. van, Zehner, C., Damadeo, R., Zawodny, J., Kramarova, N., and Bhartia, P. K.: Merged SAGE II, Ozone_cci and OMPS ozone profile dataset and evaluation of ozone trends in the stratosphere, *Atmospheric Chemistry and Physics*, 17, 12533–12552, <https://doi.org/10.5194/acp-17-12533-2017>, 2017.

Sofieva, V. F., Szélag, M., Tamminen, J., Kyrölä, E., Degenstein, D., Roth, C., Zawada, D., Rozanov, A., Arosio, C., Burrows, J. P., Weber, M., Laeng, A., Stiller, G. P., Clarmann, T. von, Froidevaux, L., Livesey, N., Roozendael, M. van, and Retscher, C.: Measurement report: regional trends of stratospheric ozone evaluated using the MERGED GRidded Dataset of Ozone Profiles (MEGRIDOP), *Atmospheric Chemistry and Physics*, 21, 6707–6720, <https://doi.org/10.5194/acp-21-6707-2021>, 2021.

Sofieva, V. F., Hänninen, R., Sofiev, M., Szélag, M., Lee, H. S., Tamminen, J., and Retscher, C.: Synergy of Using Nadir and Limb Instruments for Tropospheric Ozone Monitoring (SUNLIT),



Atmospheric Measurement Techniques, 15, 3193–3212, <https://doi.org/10.5194/amt-15-3193-2022>, 2022.

Sofieva, V. F., Szelag, M., Tamminen, J., Arosio, C., Rozanov, A., Weber, M., Degenstein, D., Bourassa, A., Zawada, D., Kiefer, M., Laeng, A., Walker, K. A., Sheese, P., Hubert, D., van Roozendaal, M., Retscher, C., Damadeo, R., and Lumpe, J. D.: Updated merged SAGE-CCI-OMPS+ dataset for the evaluation of ozone trends in the stratosphere, *Atmos. Meas. Tech.*, 16, 1881–1899, <https://doi.org/10.5194/amt-16-1881-2023>, 2023.

Van Der A, R. J., Allaart, M. A. F., and Eskes, H. J.: Extended and refined multi sensor reanalysis of total ozone for the period 1970–2012, *Atmos. Meas. Tech.*, 8, 3021–3035, <https://doi.org/10.5194/amt-8-3021-2015>, 2015.

Wespes, C., Hurtmans, D., Emmons, L. K., Safieddine, S., Clerbaux, C., Edwards, D. P., and Coheur, P.-F.: Ozone variability in the troposphere and the stratosphere from the first 6 years of IASI observations (2008–2013), *Atmospheric Chemistry and Physics*, 16, 5721–5743, <https://doi.org/10.5194/acp-16-5721-2016>, 2016.