Ozone_cci+

End to End ECV Uncertainty Budget (E3UB)

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1. Purpose and scope

1.1. Purpose

The 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

Level 3 data. Error budget studies in this project will be based on both error propagation and geophysical validation of ozone measurements and their uncertainties. Instrumental drift issues will be investigated as well.

Required information for Level 2 data:

- Which error sources are accounted for in the uncertainty estimation?
- Are systematic and random components of the uncertainty or total errors provided?
- Is the information about the vertical resolution of the measurement provided? (e.g. averaging kernel)
- Description of the quality flags reported in Level 2 data and indications on how to use them
- Main factors affecting the data quality and known issues or drifts.

Required information for Level 3 data:

- Which error sources are accounted for in the uncertainty estimation?
- What is the methodology/principle for the error estimation?
- Provide typical uncertainty values.
- Are sampling errors important?
- Relevant issues to be taken into account and possible drifts.

1.2. Reference documents

Data Standards Requirements for CCI Data Producers. Latest version at time of writing is v1.2: ref. CCI-PRGM-EOPS-TN-13-0009, 9 March 2015, available online at:
http://cci.esa.int/sites/default/files/CCI_Data_Requirements_Iss1.2_Mar2015.pdf

CCI Data Policy v1.1. Available online at: https://earth.esa.int/documents/10174/1754357/RD-7_CCI_Data_Policy_v1.1.pdf

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.

Some teams use “smoothing error” concept, despite the fact that smoothing error does not follow Gaussian error propagation. Pros and cons of smoothing error are discussed in details in (von Clarmann 2014).

1.4. Acronyms

ACE-FTS	Atmospheric Chemistry Experiment – Fourier Transform Spectrometer
ATBD	Algorithm Theoretical Basis Document
CCI	Climate Change Initiative
CDR	Climate Data Record
C3S	Copernicus Climate Change Service
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 (aboard ERS-2)
GOME-2	Global Ozone Monitoring Experiment – 2 (aboard MetOp-A)
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 Cartography (aboard Envisat)

2. Uncertainty of level 2 data

2.1. Total ozone

Table 1 summarizes the status of publications on error budget evaluation and uncertainties validation of Level 2 total ozone measurements generated within Ozone_CCI+.

Sensor	Algorithm	Error budget publications
GOME, GOME-2, SCIAMACHY, OMI	GODFIT_V3	Lerot et al. 2014, Coldewey-Egbers et al. 2015

Table 1: Summary of error budget characterization and precision validation publications for total ozone column measurements

Within the Ozone_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 cross-sections uncertainties,
- Level-1 calibration limitations,
- Interferences with other species, including aerosols,
- Cloud contamination,
- A priori O3 profile shape, especially at large solar zenith angles.

Table 2 summarizes the current assessment of the main contributions to the global error budget on total ozone retrieval by GODFIT. Total errors are computed assuming all contributions are mutually uncorrelated.

Error source	**Per cent error**	
	SZA < 80°	**SZA > 80°**
Instrument signal-to-noise	< 0.5	< 2
Soft calibration: Absolute recalibration + structures removal	< 1.5	< 1.5
O_3 absorption cross-sections and its 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	**< 3.6**	**< 5.3**

Table 2: Estimation of the error sources of the direct-fitting total ozone retrieval (single pixel retrieval). Blue fields indicate random errors (precision) associated with instrument signal-to-noise and which can be derived easily 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

Table 3 summarizes the status of publications on error budget evaluation and uncertainties validation of Level 2 ozone profiles from nadir sensors generated within Ozone_CCI+.

Sensor	Algorithm	Error budget publications
GOME GOME-2 SCIAMACHY OMI	RAL	Kerridge et al. 2002, Miles et al. 2015
IASI	FORLI	Hurtmans et al. 2012, Wespes et al. 2016, Boynard et al. 2018, Keppens et al. 2018.

Table 3: Summary of error budget characterization and precision validation publications for nadir sensors.

2.2.1 RAL

Analysis of error budget of RAL scheme is based on retrieval simulations for a set of basic geophysical scenarios which had been defined for the GOME-2 Error Study (Kerridge et al. 2002). Miles et al. (2015) assessed the performance of the RAL ozone profile retrieval scheme for the 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.

2.2.2 IASI FORLI

In the routine processing of the error matrix, the error introduced by uncertainties on the fixed parameters is not taken into account. For ozone, the error is larger in the tropics (above 30%) due to the increase in humidity and also above cold surfaces, possibly due to a misrepresentation of the emissivity in the polar regions (Hurtmans et al. 2012, Wespes et al. 2016).
There is no bias due to instrument aging: when comparing IASI/MetOpA vs IASI/MetOpB vs IASI/MetOpC, the radiance signals are similar (Chinaud et al. 2019).
The IASI/Metop-A FORLI-O_3 dataset has been extensively validated in Boynard et al. (2018) and Keppens et al. (2018). Typical uncertainty values are reported in the table below.

Random errors: Measurement error Smoothing error	10% over all the profile; 10-35% troposphere, 5-30% middle-lower stratosphere, <10% upper stratosphere.
Systematic errors: Uncertainty in cross-sections Temperature uncertainty	~4% <10% over all the profile

Table 4: Typical uncertainty values for IASI FORLI-O3 dataset

2.3. Ozone profiles from limb sensors

Table 5 summarizes the status of publications on error budget evaluation and uncertainties validation of Level 2 ozone profiles from limb sensors generated within Ozone_CCI+.

Sensor	Algorithm, L2 version	Error budget publications
GOMOS	IPF, V.6; FMI ALGOM2s V1	Tamminen et al. 2010 Sofieva et al. 2017a
MIPAS	IMK Scientific	Steck et al. 2007
SCIAMACHY	IUP Sciatran, v3.5	Rahpoe et al. 2013
ACE-FTS	v3.6/4.0	Dupuy et al. 2009, Boone et al. 2005
OSIRIS	Usask Sasktran, v5.10	Bourassa et al. 2012
OMPS-LP	Usask Sasktran, v1.1.0	Zawada et al. 2018
MLS	v4.2	Froidevaux et al. 2008, Livesey et al. 2008
POAM III	v4	Lumpe et al. 2002
SAGE III M3M	v4	Rault et al. 2005

SAGE III ISS	AO3, v5.1	McCormick et al. 2020
SABER	v2.0	Rong et al. 2009

Table 5: Summary of error budget characterization and precision validation publications for limb sensors

In the following table the links to the data sets are listed:

Sensor L2 data	**Link to L2 data**
GOMOS ALGOM2s	https://earth.esa.int/web/sppa/activities/instrument-characterization-studies/algom/data-resources
MIPAS IMK	https://www.imk-asf.kit.edu/english/308.php#org0f1a3a1
SCIAMACHY IUP	https://www.iup.uni-bremen.de/scia-arc/
ACE-FTS	https://databace.scisat.ca/level2/
OSIRIS	https://research-groups.usask.ca/osiris/data-products.php
OMPS-LP Usask	https://arg.usask.ca/projects/omps-lp/
MLS	https://mls.jpl.nasa.gov/data/datadocs.php
POAM III	https://search.earthdata.nasa.gov/search?q=POAM%20III
SAGE III M3M	https://asdc.larc.nasa.gov/project/SAGE%20III-M3M/g3assp_4
SAGE III ISS	https://asdc.larc.nasa.gov/project/SAGE%20III-ISS/g3bssp_51
SABER	http://saber.gats-inc.com/data.php

Table 6: Links to the limb L2 data sets listed in Tab 5.

2.3.1 GOMOS ALGOM2s

In the CCI project, the new GOMOS data processed with ALGOM2s v.1 Scientific Processor are used (Sofieva et al., 2017a). The error propagation scheme is similar to that used in GOMOS IPF v.6 processor, as the ALGOM 2S ozone profiles are identical to those of IPF v.6 in the stratosphere, and differ in UTLS. The error estimates (square roots of the diagonal elements of the covariance matrix) are provided in the Level 2 files and the part of the covariance matrix (7 off - diagonal elements). The covariance matrix of retrieved profiles uncertainties is obtained via Gaussian error propagation through the GOMOS inversion, see Tamminen et al. (2010) for details. As indicated above, both noise and the dominating random modelling error (due to scintillations) are taken into account on GOMOS inversion. Thus, error estimates provided in Level 2 files represent the total precision estimates. The precision of GOMOS ozone profiles depends on stellar brightness, spectral class and obliquity of occultation.
Other sources of systematic errors are imperfect modelling of the aerosol extinction, uncertainties in the absorption cross sections and temperature. Uncertainties of air density profile, ray tracing and potentially missing constituents have a negligible impact on ozone retrieval.

2.3.2 MIPAS IMK Scientific

The estimated random error is dominated by the instrumental noise above 14 km (Steck et al. 2007). Below 14 km, the error due to uncertain water vapor concentration becomes dominant because water vapor increases exponentially with decreasing altitude; the strong water vapor lines are slightly interfering with ozone lines leading to a dependence of the retrieved ozone on the pre-retrieved water vapor amount.
The estimated systematic error is dominated by uncertainties in spectroscopic data (Steck et al. 2007). Their altitude-dependence is due to the fact that the micro-windows used in the retrieval are varying with altitude. Errors caused by uncertainties in the instrumental line shape are in the order of 1 to 4% and thus nearly negligible compared to spectroscopic uncertainties.

2.3.3 SCIAMACHY IUP Sciatran

Total systematic ($\pm\sigma_{sys}$) and random ($\pm\sigma_{rnd}$) errors for retrievals of ozone profiles with SCIATRAN processor are calculated, for three latitude bands and different altitudes in Rahpoe et al. (2013). The contribution to total systematic error is coming from the aerosol (up to 15 %), albedo (up to 8 %), tangent height (up to 8 %), temperature (up to 1 %), and pressure (up to 2 %). The maximum random error is in the order of 43 % in the tropics at 10 km.

2.3.4 ACE-FTS

Analysis of the detailed error budget including systematic errors for the ACE-FTS data products is in progress. Main inputs into the uncertainties are expected to be the strength of the signal and the spectroscopic uncertainties. The uncertainties reported in the data files are the statistical fitting errors from the least-squares process and do not include systematic components or parameter correlations (Boone et al. 2005). The mean relative fitting errors are lower than 3% between 12 and 62 km and typically less than 2% around the VMR peak (30–35 km).

The vertical resolution is not reported for each profile and it is dependent on the beta angle and the altitude of the measurement. When the beta angle is zero, the sampling rate can be 6 km. When the beta angle is at a maximum, the sampling can be ~2 km. However, the field of view limits the sampling to 3 km. Below 50 km, refraction affects the sampling and the spacings get closer. There is no simple function to use to calculate the vertical resolution so the data provider estimates a value of 3 km as an average for all measurements.

2.3.5 OSIRIS

To estimate the OSIRIS ozone error budget, a random sampling of scans was chosen and the ozone was repeatedly retrieved with randomly perturbed inputs. The inputs were adjusted by a random factor chosen from a normal distribution of values with a 3σ of 10%. This was performed in turn for the aerosol profile, albedo, neutral density profile, and NO_2 profile. For the altitude registration a 3σ of 300m was used. The precision was calculated using a method described in (Bourassa et al, 2012). The total error is calculated using a sum in quadrature of the error components.

2.3.6 OMPS-LP Usask 2D

The OMPS-LP USask 2D retrieval process uses Gaussian error propagation to estimate the covariance of the retrieved solution. Currently only the random error component of the radiance measurements is accounted for. The reported precision is the square root of the diagonal elements of the converged solution covariance matrix. Smoothing error is not included in the reported error estimate, however representative averaging kernels are available as diagnostic quantities. Refer to Zawada et al. (2018) for details.

2.3.7 MLS

The random component of the uncertainty is reported for every profile in Level 2 data, under the variable ‘Precision’. Typical values of precision and accuracy are reported in the user guide (available at https://mls.jpl.nasa.gov/data/v4-2_data_quality_document.pdf). To assess the accuracy component, estimated systematic errors are propagated, e.g. from calibration and spectroscopy. Details in Froidevaux et al. (2008), Livesey et al. (2008).
A reference averaging kernel matrix is provided as an ASCII file for ozone profile and the average vertical resolution is reported also in the user guide.
Several quantities are provided in the Level 2 data, such as convergence, status and quality; detailed description of their use is provided in the user guide.
Known artefacts: oscillations in the tropical UTLS. Very good long term stability.

2.3.8 POAM III

Detailed description of retrieval, uncertainties and vertical resolution can be found in Lumpe et al. (2002). The total error provided in v4 of Level 2 data is the rms of 3 error sources: a total random error obtained from uncertainty propagation, a component related to sunspots and an aerosol feedback loading error. For a detailed description refer to Lumpe et al. (2002)
The typical values of the vertical resolution are reported in the user guide and in Lumpe et al. (2002) but not in Level 2 data.

A quality flag is provided in Level 2 data related to high aerosol loads or high sunspots errors. For a conservative approach all flagged data points should be removed.

2.3.9 SAGE III M3M (Solar occultations)

SAGE III measurements are provided with uncertainty estimates for random components. Systematic uncertainties are normally secondary and can be assessed through sensitivity analysis. Three are the primary sources of the random component of the uncertainty: the line-of-sight optical depth measurement errors, the Rayleigh optical depth estimate, and the uncertainties resulting from the removal of contributions by interfering species. These uncertainties are propagated into the reported quantities. Retrieval errors are evaluated and presented in Rault (2005), based on the inversion algorithm covariance matrices. The largest sources of uncertainty are the altitude registration, the stray light removal process and the dark current evaluation.
A retrieved profile bit flag is provided in Level 2 data for each observation.
A constant vertical resolution of 0.5 km is currently assumed for all profiles and altitudes.

2.3.10 SAGE III ISS (Solar occultation, Least Square Ozone)

Error analysis for SAGE III ISS ozone profiles is ongoing, first validation of the results can be found in McCormick et al. (2020).
A constant vertical resolution of 0.5 km is currently assumed as a preliminary average value for all profiles and altitudes. No other information is available.
Several flags are currently reported in Level 2 data but not tested by the data provider, only the ‘retrieved profile bit flag’ is recommended.

3. Uncertainty of level 3 data

3.1. *Monthly mean single instrument measurements*

3.1.1 Total ozone

Single monthly mean gridded (1°x1°) ozone data products from the nadir-viewing instruments GOME, SCIAMACHY, GOME-2, and OMI are computed as monthly averages from all level 2 measurements allocated to the respective grid cells. The sample standard deviation and the standard error of the mean are provided. The latter takes into account spatial-temporal sampling errors inherent to the satellite data, which were obtained from an Observing System Simulation Experiment (OSSE). See Coldewey-Egbers et al. (2015) for more details.

3.1.2 Ozone profiles from nadir sensors

The average value in a level-3 grid cell is a weighted average of all values assigned to that grid cell (and for that layer). The weights used for the averaging are equal to 1/variance, i.e,: 1/(error^2) on the individual parameter. Nadir and off-nadir pixels are treated in the same way, which means that though the errors on individual profiles may have systematic differences across-track, the mathematical treatment is the same. If the data are uncorrelated, this estimate is optimal in the sense that it gives the smallest possible error. In mathematical notation the mean is calculated as:

$$mean = \frac{\sum \frac{x_i}{{error_i}^2}}{\sum \frac{1}{{error_i}^2}}$$

The error on the averaged values is the standard error of the weighted mean. With variance as weights, this error is calculated as:

$$Std_{Err} = \sqrt{\left(\frac{1}{\sum \frac{1}{error_i^{2}}}\right)}$$

The ozone values x_i and the associated error_i come from the Level 2 profile data and are interpolated in the vertical to the standard Level 3 vertical grid.

3.1.3 Monthly zonal mean ozone profiles from limb instruments

Monthly zonal mean data from the individual limb instruments are computed in 10° latitude bands from 90°S to 90°N. For all sensors, the monthly zonal average is computed as the mean of ozone profiles. The uncertainty of the monthly mean is estimated as the standard error of the mean. In addition, the inhomogeneity measures in latitude and in time (Sofieva et al., 2014b) are provided with the data. The detailed description of uncertainties of monthly zonal mean data (including formulae) can be found in (Sofieva et al., 2017b).

3.2. Merged data sets

3.2.1 Total ozone

The merged Level-3 monthly gridded (1°x1°) mean total ozone product (GTO-ECV) incorporates measurements from five nadir-viewing satellite sensors: GOME/ERS-2, SCIAMACHY/ENVISAT, OMI, GOME-2/MetOp-A, and GOME-2/MetOp-B. Merging is performed on a daily basis. Finally, monthly means are computed. The sample standard deviation and the standard error of the mean are provided. The latter takes into account spatial-temporal sampling errors inherent to the individual satellite data, which were obtained from an Observing System Simulation Experiment (OSSE). See Coldewey-Egbers et al. (2015) for more details.

3.2.2 Ozone profiles from nadir sensors

Product currently not available

3.2.3 Merged SAGE-CCI-OMPS dataset

The description of the merged SAGE II - CCI - OMPS_LP data set can be found in (Sofeva et al., 2017). The merged SAGE-CCI-OMPS dataset consists of deseasonalized anomalies of ozone in 10 deg 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 deasonalizied anomalies. Each data in the merged SAGE-CCI-OMPS dataset is provided with estimated uncertainty, which is estimated as follows. First, uncertainties of individual deaseasonalized anomalies are evaluated. Then the uncertainty of the median value is estimated: it contains the term due to uncertainties of individual values, and due to their spread. The corresponding equations can be found in (Sofieva et al., 2017b).

3.3. Merged LAT-LON limb data set

The merging in LAT-LON merged monthly mean dataset is performed in the same way as for SAGE-CCI-OMPS dataset, thus the uncertainties are evaluated in a similar way.

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