



Ozone_cci+ Phase 3



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WP Manager: R. Siddans

WP Manager Organization: STFC Rutherford Appleton Laboratory

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LEAD AUTHOR	Project partner	Richard Siddans	05/03/2026	
CONTRIBUTING AUTHORS	Project partner	M. Coldewey-Egbers, V. Sofieva, C. Wespes, C. Arioso K.-U. Eichmann	05/03/2026	
REVIEWED BY	Science leader	Daan Hubert	18/04/2026	
APPROVED BY	ESA	Michael Eisinger	23/06/2026	
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1	0	7/5/2020	First issued version	
1	1	8/3/2021	Modifications in response to ESA comments on version 1.0: Fig 3 (now 2.3) update (and now shows to TROPOMI - GOME2C, consistent with fig 2.2) p23: Reference to the chlorine activation term added. Ch 3.2.7: Averaging kernel quality check clarified. p32: Clarified text reference to x vs r. p33: Clarification has been added regarding use of x and x-hat. Ch 4.2.3 New section added. Editorial: Table of contents alignment fixed MLS acronym added Some minor typos fixed Rationalised numbering of equations figures and tables throughout.	
2	0	5/11/2021	Updates to Sects. 2.1, 3.2, 4.2, 4.4.	
2	1	24/1/2023	Inclusion of GOP-ECV algorithm (Sect. 3.1)	
3	0	30/1/2023	First version produced in CCI+ phase 2. Only contains sections relevant to algorithms developed in this phase. Sections related to GOP-ECV, IASI FORLI, Limb profile ECV merging are updated. Section on tropospheric ozone is added.	



Issue	Revision	Date	Modified items	Observations
3	1	23/12/2024	S3.1 Updates (mainly the figures) related to GOP-ECV; S3.3 Updates to IASI algorithm description S4.1 Updates to OMPS-LP S5.1 CCD scheme: More detailed description of the harmonisation scheme	
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4	0	24/04/2025	Inclusion of GODFIT section, update to OMI Collection 4 (total ozone column)	
4	1	15/05/2025	Updated references to total ozone ATBD	
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4	3	23/12/2025	Updated for new Contract	
4	4	18/4/2026	Updated following comments from ESA on Sects. 2.1 and 4.1	



Executive Summary

The Algorithm Theoretical Basis Document (ATBD, deliverable D2.1) describes the algorithms developed in CCI+ phase 3 for total ozone columns, nadir-based ozone profiles, limb-based ozone profiles and tropospheric ozone columns.

A series of new algorithms will be developed with a focus on both level-2 and level-3 data products, as follows.

- Total Ozone
 - GTO-ECV clear-sky (DLR)
- Nadir profiles
 - Nadir uv profile algorithm for polar orbiting sensors (RAL)
 - Nadir uv profile algorithm for geostationary sensors (RAL)
 - IASI merging algorithm (ULB)
 - GOP-ECV merging algorithm (DLR)
- Limb profiles
 - OMPS-LP (IUP-UB)
 - SAGE-CCI-OMPS+ merging algorithm (FMI)
 - MEGRIDOP merging algorithm (FMI)
 - LIMB-HIRES merging algorithm (FMI)
 - LIMB-UTLS merging algorithm (FMI)
- Tropospheric column:
 - CHORA single sensor algorithm (IUP-UB)
 - CHORA merging algorithm (IUP-UB)
 - GTO-LIMB algorithm (FMI)



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1 Purpose and scope

1.1 Purpose

This document describes the algorithms used in the Ozone_cci+ Phase 3, addressing total ozone, nadir-based ozone profiles, limb-based ozone profiles, tropospheric ozone columns and related merging algorithms.

1.2 Scope

The scope of the ATBD is to document algorithms used in phase 3 of the CCI+ project, with particular emphasis on algorithm features which are new in this phase. Where algorithms are already described by existing ATBDs or similar documents, references are made to these documents and only a brief overview of the algorithmic basis is given.

1.3 Applicable documents

- [AD-1] 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
- [AD-2] CCI Data Policy v1.1. Available online at: https://earth.esa.int/documents/10174/1754357/RD-7_CCI_Data_Policy_v1.1.pdf

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- [RD-11] Siddans, R., CCI+ Algorithm Theoretical Basis Document: Nadir uv ozone profile scheme, Issue 1.1, Date of issue: 31/10/2025, Reference: Ozone_cci+_D2p1_ATBD-O3P_1.1
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1.5 Acronyms

ACE-FTS	Atmospheric Chemistry Experiment – Fourier Transform Spectrometer
ATBD	Algorithm Theoretical Basis Document
BIRA-IASB	Belgian Institute for Space Aeronomy
CCI	Climate Change Initiative
CHORA	Cloud Height and Ozone Reference Algorithm
C3S	Copernicus Climate Change Service
DLR	German Aerospace Centre
ECV	Essential Climate Variable
ENVISAT	Environmental Satellite (ESA)
EO	Earth Observation
ESA	European Space Agency
EU	European Union
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FMI	Finnish Meteorological Institute
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
GOP	GOME-type Ozone Profile
GTO	GOME-type Total Ozone
IASI	Infrared Atmospheric Sounding Interferometer
MEGRIDOP	MERged GRIdded Dataset of Ozone Profiles
MetOp	Meteorological Operational Platform (EUMETSAT)
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
MLS	Microwave Limb Sounder
NASA	National Aeronautics and Space Administration
OMI	Ozone Monitoring Instrument (aboard EOS-Aura)
OMPS	Ozone Mapping and Profiler Suite
OSIRIS	Optical and Spectroscopic Remote Imaging System (aboard Odin)
RAL	Rutherford Appleton Laboratory
SAGE	Stratospheric Aerosol and Gas Experiment
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric CHartography



TOMS	Total Ozone Mapping Spectrometer
UTLS	Upper troposphere / Lower Stratosphere
UV	Ultraviolet



2 Total Ozone algorithms

2.1 GTO-ECV (DLR)

Work within CCI+ Phase-III related to the merged total ozone column product GTO-ECV focuses on the development of a supplementary daily clear-sky product, which will then serve as input to the tropospheric ozone product GTO-LIMB (see Sec. 5.3). Note that the clear-sky GTO-ECV product can be perceived as intermediate product, and it will not be available to the public as a stand-alone product.

For the daily clear-sky GTO-ECV product, we combine the measurements from the same nadir UV-VIS-NIR satellite sensors as for GTO-ECV (see [RD-2] for details): GOME/ERS-2, SCIAMACHY/ENVISAT, OMI/Aura, GOME-2/MetOp-A, GOME-2/MetOp-B, GOME-2/MetOp-C, and TROPOMI/Sentinel-5p. We use Level-2 total ozone data provided by BIRA and processed with the GODFIT V4 algorithm for GOME, SCIAMACHY, GOME-2, and OMI. For OMI, we use the Level-2 data that are based on the new Level-1 collection 4 data. For TROPOMI the Level-2 processing is performed by DLR.

At first, we generate daily clear-sky Level-3 data for each individual sensor from the Level-2 data. Only those pixels with cloud fraction less than 10% are used for the Level-3 daily averages. The cloud information is provided in the Level-2 products. The spatial resolution is $1^\circ \times 1^\circ$. In a next step, we apply the existing correction factors from the GTO-ECV merging algorithm [RD-2] to each sensor. These correction factors were calculated in order to remove biases and drifts between the reference sensor OMI and the other satellite sensors, and they depend on latitude and time. The final step is to merge the (adjusted) daily Level-3 data into a single daily Level-3 product. Table 2-1: provides an overview of the time period for each individual instrument in GTO-ECV.

Sensor / Platform	Time period in GTO-ECV
GOME / ERS-2	07/1995 – 12/2004
SCIAMACHY / ENVISAT	08/2002 – 12/2004
OMI / Aura	10/2004 – present
GOME-2 / MetOp-A	01/2007 – 12/2017
GOME-2 / MetOp-B	01/2013 – present
TROPOMI / Sentinel-5p	05/2018 – present
GOME-2 / MetOp-C	07/2019 - present

Table 2-1: Overview of satellite sensors incorporated in the daily clear-sky GTO-ECV product and their respective time periods.



3 Nadir Profile ECV Retrieval Algorithms

3.1 *GOME-type Ozone Profile - Essential Climate Variable (GOP-ECV) (DLR)*

Work within CCI+ Phase-II focused on the development of a merged ozone profile climate data record based on the same satellite sensors as the well-established total column product GTO-ECV (see Phase I ATBD). The approach, that is applied to the ozone profiles, consists of two main steps: (1) merging the time series of the individual sensors into a combined product (see Sec. 3.1.1) and (2) harmonization of the combined record with respect to the GTO-ECV total columns in order to achieve broad consistency between both data sets, i.e. with regard to the total ozone amount (see Sec. 3.1.2). A detailed description can also be found in [RD-3].

3.1.1 Ozone profile merging algorithm

At first, the individual gridded monthly level-3 ozone profile data are merged into a combined record. The spatial resolution is $5^\circ \times 5^\circ$ in latitude and longitude. The level-3 partial column data are based on the level-2 data retrieved with the RAL nadir profile retrieval scheme as described in the next section (Sect. 3.2). Data from five sensors are included: GOME (1995-2011), SCIAMACHY (2002-2012), OMI (2004-present), GOME-2A (2007-2021), and GOME-2B (2013-present). The values given in parenthesis denote the time periods which are covered by the sensors. These sensors are also used to create the GTO-ECV record. Note that within CCI+ Phase-III data from TROPOMI and GOME-2C will be included in the next version of GOP-ECV. The merging is based on deseasonalized anomalies and similar to the method proposed by Sofieva et al. (2021) [RD-16]. Deseasonalized anomalies $\Delta O_{3,i}(\varphi, \lambda, z, t)$ at latitude φ , longitude λ , altitude z , and month t are computed for the time series of all individual instruments i following:

$$\Delta O_{3,i}(\varphi, \lambda, z, t) = O_{3,i}(\varphi, \lambda, z, t) - O_{3,i,c}(\varphi, \lambda, z, m),$$

Equation 3-1

where $O_{3,i}(\varphi, \lambda, z, t)$ is the monthly mean ozone profile. $O_{3,i,c}(\varphi, \lambda, z, m)$ is the corresponding climatological mean value for the month m with m =January, ..., December. Since the individual sensors cover only partially the same periods, the corresponding seasonal cycles have to be computed for different reference periods as follows: GOME (1996-2002), SCIAMACHY (2005-2010), OMI (2005-2020), GOME-2A (2007-2016), GOME-2B (2015-2020). Before merging the anomalies, additive offsets w.r.t. OMI anomalies have to be computed and applied in order to account for biases due to different reference periods. These offsets are obtained from the overlap periods and depend on latitude, longitude, and altitude. One exception is the GOME sensor, which lost its global coverage in June 2003. That means for the overlap period with OMI (2004-2011) additive offsets cannot be derived globally, i.e. for each latitude-longitude grid cell. Instead, mean offsets representative for 5 broadband latitude belts (90°N - 60°N , 60°N - 30°N , 30°N - 30°S , 30°S - 60°S , and 60°S - 90°S) are computed for each calendar month and added to the GOME anomalies.



After the application of the offsets to each sensor, the merged ozone profile for each spatio-temporal bin is obtained from the median of all available instruments as:

$$\Delta O_{3,mer}(\varphi, \lambda, z, t) = \text{median}(\Delta O_{3,i}(\varphi, \lambda, z, t))$$

Equation 3-2

Corresponding uncertainties of the merged data are estimated using the same approach as used for the merged ozone profiles based on limb satellite sensors (MEGRIDOP) as described in Sofieva et al. (2021). Figure 3-1 shows the anomalies 1995-2022 for all sensors for the latitude/longitude bin 12.5°N/0.5°E and for altitude 20km. In addition, the adjusted anomalies for GOME, GOME-2A, and GOME-2B are shown. Finally, in order to reconstruct absolute ozone values, the seasonal cycle obtained from OMI measurements is used and added back to the anomalies:

$$O_{3,mer}(\varphi, \lambda, z, t) = \Delta O_{3,mer}(\varphi, \lambda, z, t) + O_{3,omi,c}(\varphi, \lambda, z, m).$$

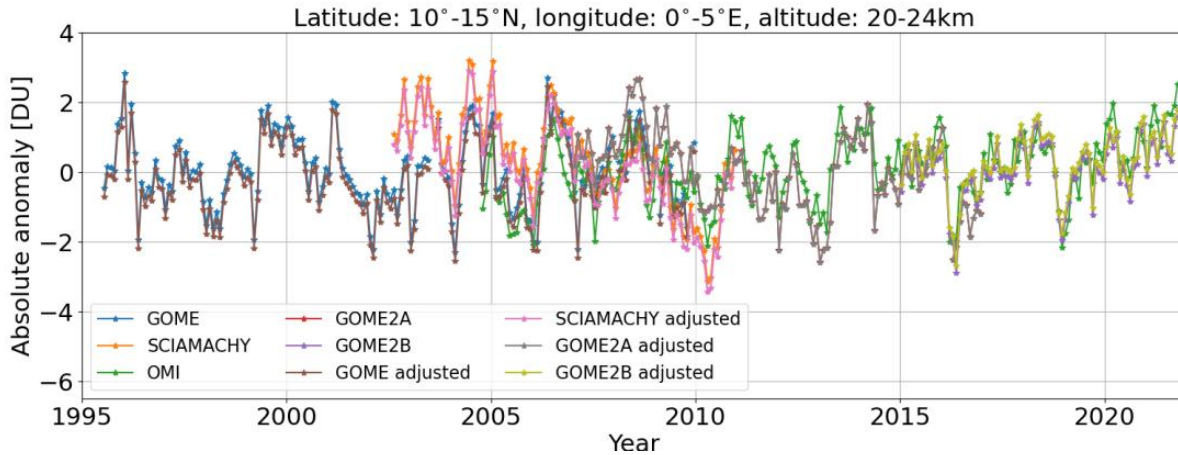
Equation 3-3

Figure 3-1 Deseasonalized anomalies [DU] 1995-2022 for all satellite sensors for the latitude/longitude bin 12.5°N/0.5°E and for the altitude of 20km. In addition, for GOME, SCIAMACHY, GOME-2A, and GOME-2B the adjusted anomalies w.r.t. OMI anomalies are shown.

3.1.2 Harmonization of merged profiles w.r.t. GTO-ECV total columns

The aim of the harmonization of the merged ozone profiles, generated as described in the previous section, is to achieve consistency between the GTO-ECV total column product and the new GOP-ECV ozone profile record with respect to the total column. The harmonization consists of the following steps:



1. A clustering algorithm is applied to a subset of 80,000 profiles randomly selected from the entire merged data record. We use the same k -means clustering procedure as described in Xu et al. (2017) and applied to a set of ozone profiles. From this study we also adopt the optimal number of clusters: $K=11$. Figure 3-2 shows the output of the clustering: the ozone profiles in each class. Colors denote the total column of each profile. Profiles of similar shapes are grouped into the same class. Class 11 contains mainly profiles from the Northern Hemisphere middle latitudes in boreal spring (maximum total ozone columns $>400\text{DU}$) and class 01 contains mostly profiles from high latitudes in the Southern Hemisphere from September to November (ozone hole season).
2. For each class of ozone profiles, a separate Neural Network is trained using as input the total ozone column and as output the corresponding ozone profile shape. The NNs comprise two hidden layers. From the NN training we extract the Jacobians for each class, which provide the information about the altitude-dependent change of the profile, when the total column changes. Figure 3-3 exemplarily shows the derivatives for class 03. The shape of the derivatives depends on the total column, and derivatives can be negative.
3. In order to assign one of the 11 classes to each of the remaining profiles, which were not used for the clustering procedure (step (1)), a k -nearest neighbors classifier method is applied. The training data set for the classifier contains the profiles of the 11 clusters and the class label (1, ..., 11). The fitted classifier is then applied to the remaining profiles in order to predict the corresponding class label, which is needed to select the correct set of derivatives for the altitude-dependent scaling.
4. The last step is the application of the scaling procedure to all merged profiles. The difference ΔTOZ between the total column from the integrated profile and the corresponding total column from the GTO-ECV data record is computed for each spatiotemporal bin and the adjusted profile is computed as follows:

$$O_{3,\text{new}}(\varphi, \lambda, z, t) = O_{3,\text{mer}}(\varphi, \lambda, z, t) + \Delta\text{TOZ}(\varphi, \lambda, t) * d/d\text{TOZ}(z),$$

Equation 3-4

$O_{3,\text{mer}}(\varphi, \lambda, z, t)$ denotes the merged profile from Sect. 3.1.1, $O_{3,\text{new}}(\varphi, \lambda, z, t)$ is the adjusted profile which is consistent with GTO-ECV in terms of the total amount, and $d/d\text{TOZ}(z)$ is the derivative derived from the NN in step (2).

The final monthly mean ozone profiles ($O_{3,\text{new}}$) and corresponding errors are delivered in NetCDF format.



Ozone Profile Clusters

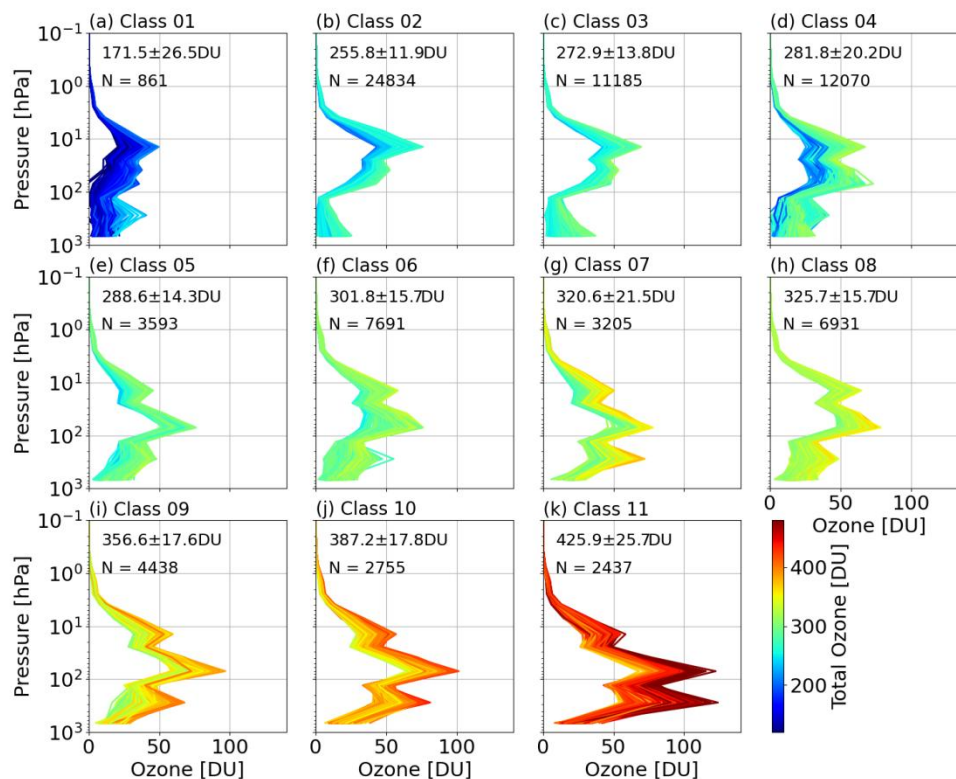


Figure 3-2 Merged ozone profiles grouped in 11 classes using a *k*-means clustering procedure. The total number of profiles is 80,000 randomly selected from the entire data record. Colors denote the total column of each profile.

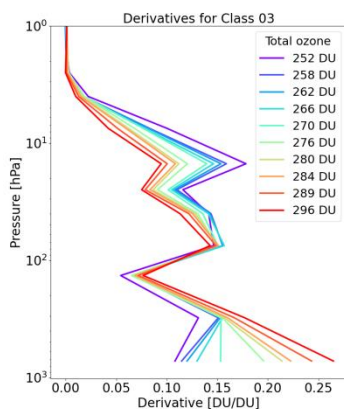


Figure 3-3 Derivatives extracted from the NN training for class 03 (see Figure 3-2). Colors denote the total column.



3.2 Nadir UV profile retrieval algorithms for polar orbiting sensors (RAL)

The RAL profile scheme applied to GOME, GOME-2, SCIAMACHY and OMI within the CCI and C3S was previously described in earlier CCI ATBDs [RD-14], [RD-13], as well as [RD-6], [RD-8] and [RD-5]. The scheme has more recently been developed for application to Sentinel 4 and 5 via ESA contracts and documented via related ATBDs [RD-10] and [RD-9]. The Sentinel 4&5 development has led to implementation of a re-engineered version of the nadir profile scheme which has now been applied to re-process GOME, GOME-2 (Metop A,B and C), OMI and S5P. The S5P algorithm developments are within the remit of CCI+ Phase 3. Reprocessed data from all sensors (except SCIAMACHY) is provided to be validated within Phase 3 and used to generate a new version of GOP-ECV.

In general, the scheme applies the optimal estimation approach to retrieve the ozone profile in two main steps:

1. “B1 fit”: Fit ozone profile to the sun-normalised radiance in the Harley band (in GOME Band 1) from 265-307nm. This provides information mainly on the stratospheric profile and requires good absolute calibration of the sun-normalised radiance spectra.
2. “B2 fit”: Add information on tropospheric ozone from the Huggins bands (320-340nm) using the result from step 1) as prior constraint. This requires fitting of differential structure to precision better than 0.1% (close to the noise level) to allow the ozone absorption cross-section temperature dependence to be exploited for tropospheric information (though the requirements on absolute radiometric calibration are less stringent). Extremely good knowledge of the instrument spectral response function is critical for this step.

A key part of the algorithm development is the development of radiometric calibration corrections to deal with instrument specific issues.

Details are described in the nadir-uv profile supplement to this ATBD [RD-11].

3.3 Nadir UV profile retrieval algorithms for geostationary sensors (RAL)

Within CCI+ Phase 3, the Sentinel 4 operational tropospheric ozone processor (originally developed by RAL under ESA contract) will be adapted and applied to process sub-sets of data from GEMS and TEMPO. The scheme is described in the S4 ATBD [RD-10]. Adaptations to the scheme for GEMS and TEMPO are in development and will be described in a later version of this ATBD.



3.4 Merged IASI-A, -B and -C Level 3 ozone profile dataset (FORLI v20191122)

The Level-3 merged IASI ozone profile data product (IASI L3 MG-FORLI) is based on the Level-2 IASI-A, -B & -C ozone profile datasets (IASI L2 FORLI-v2019) retrieved by the last release of the FORLI (Fast Optimal/Operational Retrieval on Layers for IASI) algorithm (FORLI-O₃ v20191122) that is described in Section 3.3 of the Phase 2 Ozone_cci+_D2p1_ATBD_3.1.

The merging relies on previous investigation performed during Phase 1 of CCI+ that showed excellent inter-platform consistency with no significant bias between the three Level-2 ozone profile products due to instruments aging, in line with the good stability of the three IASI instruments. During Phase 2, a scheme to merge the three IASI ozone profile data records was developed and a first IASI L3 MG-FORLI ozone profile dataset was produced. In this Phase, we improve the merging scheme, in particular, we provide additional parameters to better evaluate the random errors associated with the merged values.

The updated IASI L3 MG-FORLI dataset consists of daily 1° x 1° 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 values assigned to that grid cell and for each retrieved layers in the pressure range from the surface to 40 km with one extra layer from 40 to 60 km.

A series of processing flags (cfr Section 3.3 of the Phase 2 ATBD) were a priori applied to the IASI L2 FORLI-v2019 profile datasets to exclude bad quality data before merging.

3.4.1 Daily means and Error Estimates

The weighted average ozone value and its associated error estimate in a specific level and in a level-3 grid cell are calculated according to equations provided in Sect. 3.1 of the CCI+ Phase 1 End to End ECV Uncertainty Budget (E3UB). 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 its associated total retrieval random errors (σ_i , i.e. measurement and smoothing errors), reported by the FORLI-O₃ (20191122) retrieval algorithm, at that level.

$$Weighted_Mean = \frac{\sum_i \frac{x_i}{\sigma_i^2}}{\sum_i \frac{1}{\sigma_i^2}}$$

Equation 3-5

The uncertainty on the weighted mean is calculated as the reciprocal square root of the sum of all the individual weights assigned to a cell.

$$Associated_Error = \sqrt{\frac{1}{\sum_i \frac{1}{\sigma_i^2}}}$$

**Equation 3-6**

That error estimates corresponds to error propagation. Although that term should be dominant in case of daily 1° x 1° averaged data, the “geophysical” standard error of the weighted mean in the grid cell should also be considered to better evaluate the random uncertainty associated with the weighted mean:

$$Random_Uncertainty = \sqrt{\frac{1}{\sum_i \frac{1}{\sigma_i^2}} + \frac{S^2}{N}}$$

Where S^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.

In the updated IASI L3 MG-FORLI dataset, the error propagation associated with the weighted mean, as well as the geophysical variance and the number of level-2 IASI observations assigned to the cell are provided separately.

3.4.2 Output product description

Formats

The Level-3 IASI ozone profile dataset processed with the merging scheme described above is delivered in NetCDF (v4) format.

Ozone profile and characterization

The daily merged ozone product from IASI-A, -B and -C using the FORLI-v20191122 retrievals is a profile provided on 40 layers between surface and 40 km, with an extra layer from 40 km to the top of the atmosphere (TOA) considered at 60 km. The dataset includes daily merged O₃ total columns along with vertical profiles. It also includes other information such as the random error and the sample variance associated with merged values, the a priori profile and the total column averaging kernel (AK) matrix on the same vertical grid.



4 Limb profile ECV Retrieval / Merging Algorithms

4.1 OMPS-LP retrieval algorithm (IUP-UB)

We provide here an overview of the updated version of the UBR-IUP retrieval for observations from OMPS-LP on board NOAA-21 (N21). This retrieval version shares the same approach based on spectral fitting and similar settings with the ozone retrieval implemented for OMPS-LP onboard Suomi NPP [RD-15]. It implements a first-order Tikhonov regularization within the SCIATRAN radiative transfer model. As described in [RD-15], five spectral segments are selected: three in the Hartley and Huggins bands, and two in the visible spectral range. An adjustment of the spectral range in the visible was needed, restricting it to 508-630 nm. We have to take into account the presence of water vapor and O₂ absorption features in the Chappuis band used for the lowest altitude range (*) so that wavelengths in the 585-600 nm interval are rejected. The treatment of these absorption features requires line-by-line calculations, which are computationally expensive to be implemented for the whole time series.

Considering the decreasing sensitivity above 55 km and the saturation of limb signal in the lower stratosphere, the retrieval of ozone profiles is performed over the altitude range between 8.5 and 60.5 km, with the lower boundary that can be higher in the presence of a cloud. An evenly spaced vertical grid spans this vertical range with steps every 1 km.

The measurement vector consists of the logarithms of the normalized limb reflectance (sun-normalized radiance). In detail, OMPS-LP spectrum in the five spectral segments at each altitude is normalized by a limb measurement at an upper tangent height (TH). This provides a self-calibration of the instrument and reduces the effects of surface/cloud reflectance uncertainties. Table 4-2 lists the details about spectral segments and the used normalization altitudes.

For each TH a polynomial is subtracted from the logarithm of the normalized radiance to remove slowly variable spectral features, for example, related to Rayleigh or aerosol scattering. The last column of Table 4-2 provides information about the order of the polynomial subtracted: zeroth order or no polynomial in the UV region and first order for the Chappuis band.

Tangent height [km]	Spectral segment [nm]	Normalization TH [km]	Poly. order
48-60	290-302	63.5	-
34-49	305-312	53.5	-
28-39	321-330	51.5	0
16-31	508-630	42.5	1
8-16 (*)	508-630	42.5	1



Table 4-2: List of the spectral segments considered for the ozone retrieval with corresponding TH ranges, altitudes used for the normalization and order of the subtracted polynomial.

As O₃, NO₂ and O₄ have relevant spectral signatures in the selected spectral ranges, the radiation field in the forward model is calculated, taking into account these three gases. The respective cross-sections are taken from [RD-7], [RD-1] and [RD-4] and are beforehand convolved to the OMPS-LP spectral resolution.

Surface albedo is retrieved simultaneously, by assuming a Lambertian surface and using the sun-normalized radiance. For the aerosol retrieval, we adapted the NPP algorithm to obtain an extinction product for N21. With respect to the approximation used in the previous version (zonally averaged NPP extinction profiles), the largest changes are in the lowermost stratosphere, with an average discrepancy of about 2-5 % below 18 km.

So far, only the central slit of the instrument has been processed, however an attempt to retrieve observations from the right slit is ongoing. Due to calibration issues for the side slits of the instrument, we are using the UV measurements from the central slit and the visible only spectra from the side slit.

4.2 SAGE-CCI-OMPS+ merging algorithm

The original version of the merged SAGE-CCI-OMPS dataset (Sofieva et al., 2017 [RD-12]) was created using ozone profiles from seven limb and occultation instruments: SAGE II, OSIRIS, GOMOS, SCIAMACHY, MIPAS, ACE-FTS and OMPS-LP (processed at University of Saskatchewan, USask). The extended version - SAGE -CCI-OMPS+ (Sofieva et al., 2023 [RD-18]), includes the data from two more instruments, POAM III and SAGE III/ISS, and the OMPS-LP data from both University of Saskatchewan and University of Bremen processors.

In this phase of Ozone_cci+ project, we explore the possibility of inclusion of OMPS-LP data from the NASA processor in the merged dataset. The latest version of the SAGE-CCI-OMPS+ merging algorithm is presented below. The details on uncertainty estimation are provided in the E3UB document.

The information about the ozone data from different limb instruments is presented in Table 4.2.1

Instrument/ satellite	Processor, references	Time period	Local time	Vertical resolution	Estimated precision	Profiles per day
SAGE II/ ERBS	NASA v7.0	Oct 1984 – Aug 2005	sunrise, sunset	~1 km	0.5–5%	14–30
OSIRIS/ Odin	USask v7.4	Nov 2011 – present	6 a.m., 6 p.m.	2–3 km	2-10%	~250
GOMOS/ Envisat	ALGOM2s v1.0	Aug 2002 – Aug 2011	10 p.m.	2–3 km	0.5–5 %	~110



Instrument/ satellite	Processor, references	Time period	Local time	Vertical resolution	Estimated precision	Profiles per day
MIPAS/ Envisat	KIT/IAA V8	Jan 2005 – Apr 2012	10 p.m., 10 a.m.	3–5 km	1–4%	~1000
SCIAMACHY/ Envisat	UBr v3.5	Aug 2003- Apr 2012	10 a.m.	3–3.5 km	1–7%	~1300
ACE-FTS/ SCISAT	V5	Feb 2004 – present	sunrise, sunset	~3 km	1–4%	~30
OMPS-LP/ Suomi NPP	USask 2D v1.3.0 UBr v4.1 NASA v.2.6	Apr 2012–present	1:30 p.m.	~2 km ~2-3 km	2–10%	~1600
SAGE III /ISS	NASA, AO3 v5.3	2017 – present	sunrise, sunset	~1 km	2–4%	~30
POAM III /SPOT 4	NASA v.4	1998–2005	sunrise, sunset	~ 1 km stratosphere, 2-3 km upper troposphere	3–5 %	~30

Table 4-3: Information about the datasets used in the latest version of the SAGE-CCI-OMPS + dataset.

For the merged dataset, first the monthly zonal mean ozone profiles in 10° latitude bands from individual instruments are computed. Then, for each instrument, the deseasonalized anomalies are computed as

$$\Delta(t_i) = \frac{\rho(t_i) - \rho_m}{\rho_m},$$

Equation 4-7

where $\rho(t_i)$ is the monthly zonal mean number density value at a certain altitude and latitude band corresponding to time t_i and ρ_m is the mean over the whole considered time period, for the corresponding month m for this altitude and latitude. For GOMOS, MIPAS, SCIAMACHY, ACE-FTS and OSIRIS, the seasonal cycle is evaluated using the overlapping period 2005–2011. The seasonal cycle for SAGE II is computed using years 1985–2004 and for OMPS using the years 2012–2020. Relative representation of deseasonalized anomalies is chosen for visualization convenience.



The merging is performed as follows. In the first step, the median of GOMOS, MIPAS, SCIAMACHY, ACE-FTS and OSIRIS deseasonalized anomalies is computed (pre-merging). In the second step, SAGE II deseasonalized anomalies are offset to the pre-merged anomalies in the years 2002–2005.

For OMPS, we use the median of deseasonalized anomalies from 3 processors. Then the OMPS deseasonalized anomalies are offset to pre-merged anomalies (which are based on OSIRIS and ACE-FTS measurements in this period) in the years 2012–2020. After offsetting, all deseasonalized anomalies are aligned and the median of deseasonalized anomalies from all instruments is computed. In the merging, we also applied a method for detection of outliers: we filtered out individual anomaly values (locally for each latitude band and altitude level), which differ from the median anomaly more than 10% at latitudes 40°S–40°N and more than 20% in other latitude bands. These thresholds are rather loose and do not affect the merged ozone in the overwhelming majority of cases; it removes only a few exceptional anomalies, which appear in rare cases for the instruments with rather coarse sampling (such as GOMOS and ACE-FTS).

The merged deseasonalized anomalies can be used directly to estimate ozone trends. For other applications, the merged ozone number density profiles are also provided. The computation of number density profiles from the merged deseasonalized anomalies is performed via restoring the seasonal cycle according to Eq.(1). For the SAGE-CCI-OMPS, the amplitude of the seasonal cycle is estimated using MIPAS measurements because they provide all season pole-to-pole measurements with dense sampling. The absolute values of the seasonal cycle are estimated from SAGE II and OSIRIS in the overlapping period (which are very close to each other and to GOMOS measurements), thus preserving the consistency in the dataset through the whole observation period.

The detailed description of the SAGE-CCI-OMPS+ processing is presented in (Sofieva et al., 2023 [RD-18]). The new part is computation of the median of OMPS-LP anomalies as a contribution of OMPS_LP into the merged dataset. Using 3 OMPS-LP datasets allows us to use the median estimate and thus remove outliers efficiently. During comparison, we found that all 3 OMPS-LP datasets agree well with each other and with other datasets. In merging, USask data are ignored in one zone 70–80 N at altitudes only below 14 km due to their large deviations, otherwise data used as they are.

We analyzed also the influence of OMPS-LP NASA datasets inclusion on estimated ozone trends. Figure 4-1 shows ozone trends with the standard SAGE-CCI-OMPS+ dataset and with included OMPS-NASA dataset. Trends are evaluated using multiple linear regression with solar, QBO and ENSO proxies.

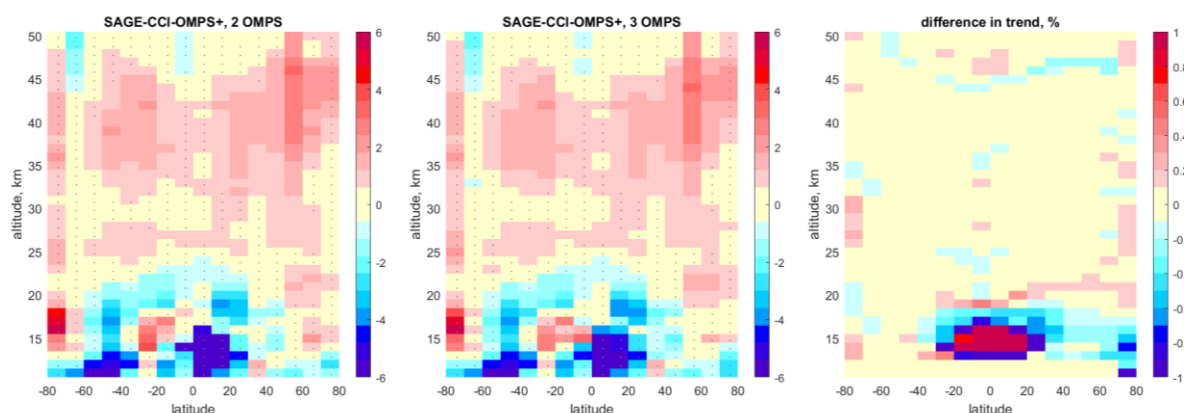


Figure 4-1. The influence of inclusion of OMPS-NASA dataset into the merged SAGE-CCI-OMPS+ dataset on estimated ozone trends in the stratosphere. Left: post-1997 ozone trends in % decade⁻¹ when 2 OMPS-LP datasets from USask and UBr are used. Center: ozone trends when 3 OMPS-LP datasets are included. Right: the differences in trend estimates (% decade⁻¹)

The updated SAGE-CCI-OMPS+ dataset contains profiles of deseasonalized anomalies and ozone concentrations from 1984 to present (latest version is until December 2024), in 10° latitude bins from 90°S to 90°N, and in the altitude range from 10 km to 50 km.

4.3 MEGRIDOP merging algorithm (FMI)

The MErged GRIdded Dataset of Ozone Profiles (MEGRIDOP) is derived from data by six limb and occultation satellite instruments: GOMOS, SCIAMACHY and MIPAS on Envisat, OSIRIS on Odin, OMPS on Suomi-NPP, and MLS on Aura (Sofieva et al., 2021 [RD-16]). The monthly mean gridded ozone profile dataset is provided in the altitude range from 10 to 50 km in bins of 10° latitude x 20° longitude provides the monthly zonal mean gridded ozone profiles in the altitude range from 10 km to 50 km. MEGRIDOP covers the time period from late 2001 until now.

The merging method used for creating MERGRIDOP (Sofieva et al., 2021 [RD-16]) is similar to that used in creating the merged SAGE-CCI-OMPS dataset [RD-12]. The deseasonalized anomalies of all instruments except OMPS are aligned, as the seasonal cycle was estimated using the same period.

The new development in Phase 3 of the Ozone_cci+ project is using 3 OMPS-LP datasets – processed by University of Saskatchewan, University of Bremen and NASA, instead of one OMPS-LP dataset (USask) in the original development. Similarly to the SAGE-CCI-OMPS+ dataset, we use the median of deseasonalized anomalies from 3 OMPS-LP datasets as the contribution from OMPS-LP. The main advantages of using three OMPS-LP datasets are improved spatiotemporal coverage and reduced number of outliers. An example of OMPS-LP deseasonalized anomalies for USask (as used in the previous version of the MEGRIDOP dataset) and the median of 3 OMPS deseasonalized anomalies is shown in Figure 4-2.

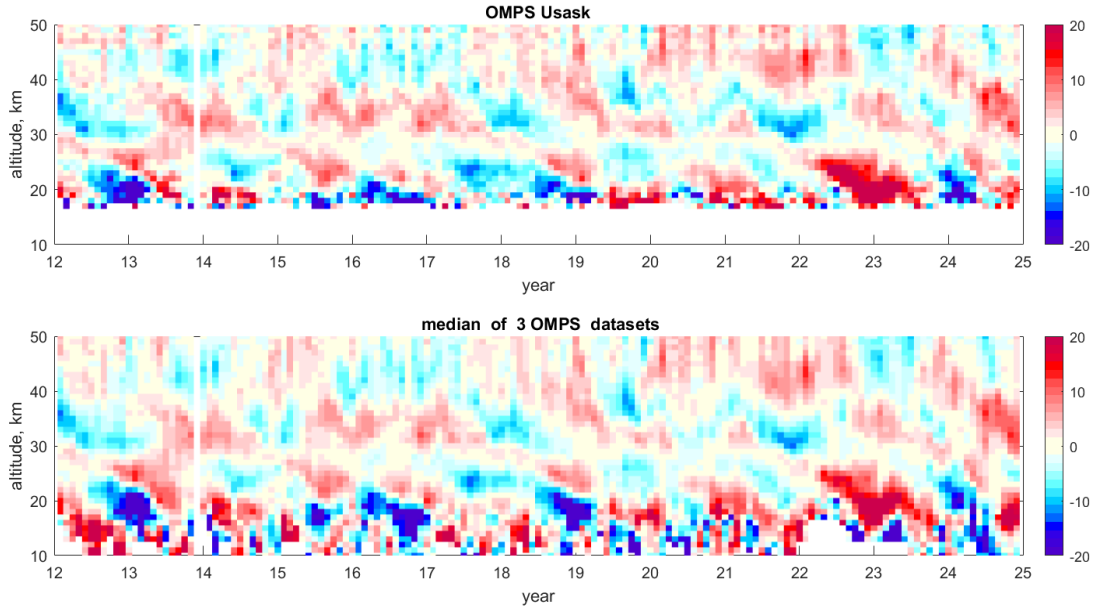


Figure 4-2. The deseasonalized anomalies (in %) of OMPS-LP USask (top) and the median of 3 OMPS-LP datasets (bottom) for the bin 0-10° N, 0-20° E.

After computation of the median of the OMPS anomalies, we offset it to the median of the deseasonalized anomalies from all other instruments. These additive offsets are computed using the data from years 2012-2018.

Then the merged ozone profiles in each spatiotemporal bin and at each altitude level is obtained from the median of the deseasonalized anomalies corresponding to individual instruments:

$$\Delta_{merged}(z, b, t) = median(\Delta_i(z, b, t))$$

Equation 4-8

The advantage of using the median estimate is that the merged anomaly follows the majority of the data, and it is not very sensitive to exclusion/addition of an individual data record, in cases where there are several (and consistent) anomaly datasets available.

The uncertainties of the merged deseasonalized anomalies are computed similarly to those used for the merged SAGE-CCI-OMPS dataset [RD-12]. For each instrument, the uncertainty of the deseasonalized anomalies, σ_{Δ_i} , is estimated via Gaussian error propagation; it is given by

$$\sigma_{\Delta_i} = \Delta_i \sqrt{\frac{\sigma_i^2}{\rho_i^2} + \frac{\sigma_{m,i}^2}{\rho_{m,i}^2}}$$

Equation 4-9



where σ_i is the uncertainty of the gridded ozone profiles and $\sigma_{m,i}$ is the uncertainty of the seasonal cycle $\rho_{m,i}$, which can be estimated via propagation of random uncertainties to the mean value:

$$\sigma_{m,i}^2 = \frac{1}{N_m^2} \sum_{j=1}^{N_m} \sigma_i^2(z, b, t_j)$$

Equation 4-10

Analogously to [RD-12], the uncertainties of the merged deseasonalized anomalies are estimated as:

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

Equation 4-11

where $\sigma_{\Delta, j_{med}}$ is the anomaly uncertainty of the instrument corresponding to the median value. In cases where there are even number of measurements, the mean of two neighbours to the median is used.

Examples of deseasonalized anomalies and their estimated uncertainties are displayed in Figures 6 and 7, respectively.

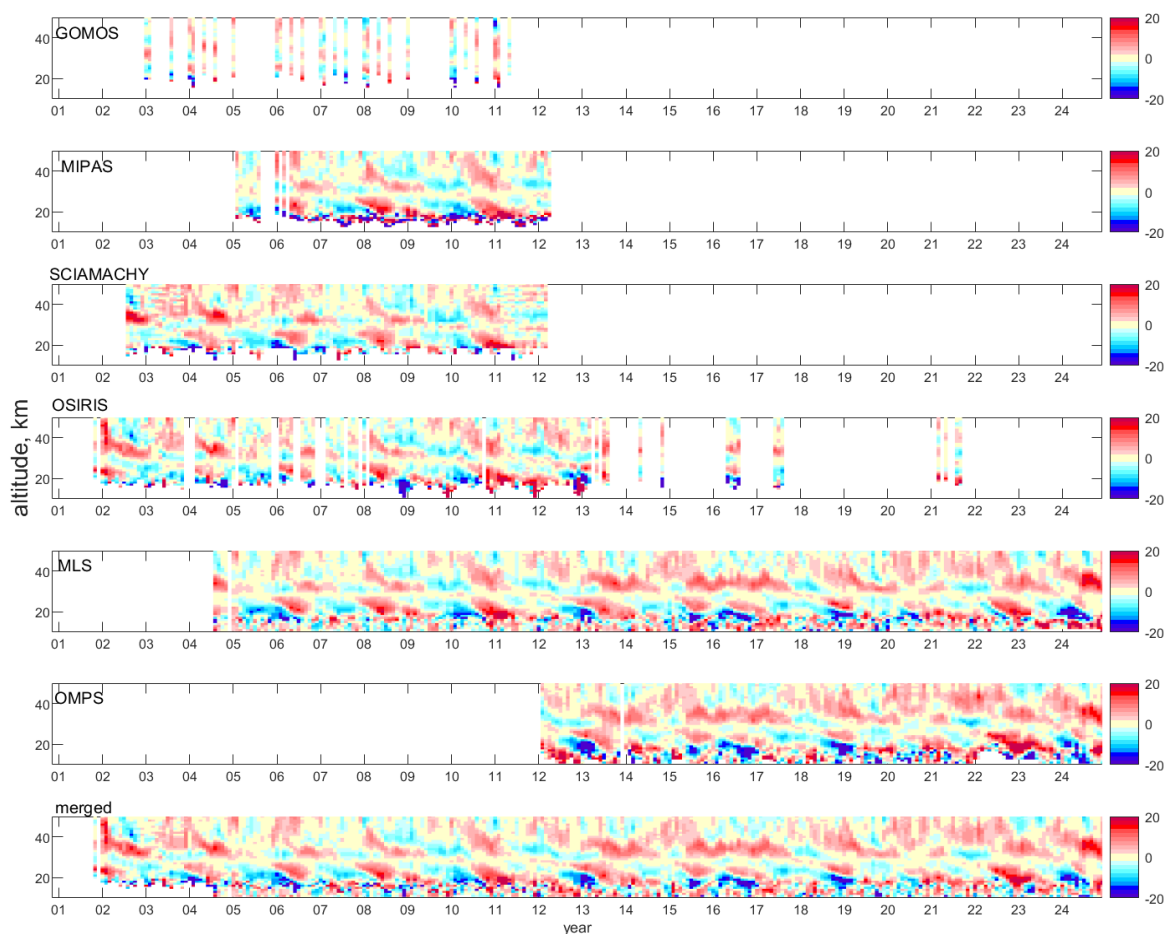


Figure 4-3. An example of deseasonalized anomalies (in %) for individual instruments and the merged dataset in the spatial bin 0-10° N, 0-20° E.

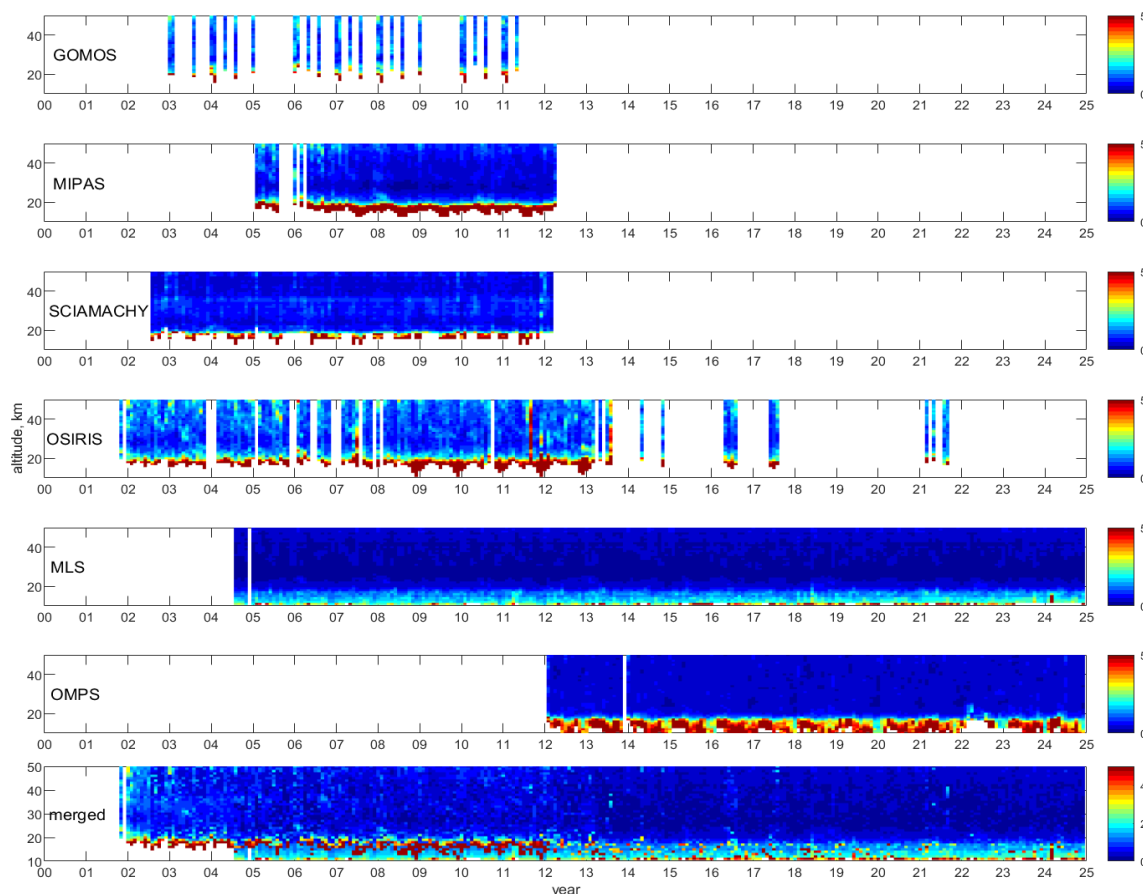


Figure 4-4. An example of uncertainties in deseasonalized anomalies (in %) for individual instruments and the merged dataset in the spatial bin 0-10° N, 0-20° E

The merged deseasonalized anomalies can be used directly for evaluation of ozone trends. For other applications, the MEGRIDOP is also available in the form of ozone number density profiles. The restoration of seasonal cycle is done in a similar way as in the original MEGRIDOP dataset: the amplitude is the mean of the (relative) amplitudes of seasonal cycle of MIPAS and MLS, while the absolute mean number density corresponds to the mean of OSIRIS and MLS.

4.4 LIMB-HIRES merging algorithm (FMI)

The high-resolution gap-free dataset of ozone profiles is daily gridded profiles in the pressure range from 900 to 0.02 hPa with the horizontal resolution of 1°x 1°. It covers year from 2002 to present. The dataset is created using the ozone profiles data from MLS, OSIRIS, GOMOS, MIPAS, SCIAMACHY, OMPS-LP, ACE-FTS, and SAGE III/ISS.



The details of data processing are provided in [RD-17]. In our algorithm, the creation of homogenized interpolated dataset of ozone profiles consists of three main steps:

- (1) Homogenization of ozone profile data from the limb satellites measurements;
- (2) Interpolation of the limb profiles from each day to $1^\circ \times 1^\circ$ horizontal grid;
- (3) A smooth transition to the adjusted model data below the tropopause.

In the first step, the data from different satellite instruments are homogenized. We use MLS as a reference dataset. For all other instruments, the biases with respect to MLS are evaluated for each month and for each latitude (with 1° increment), using 10° overlapping zones and corrected via adding latitude-dependent offset. This procedure removes the biases between the limb datasets. After that, we applied a simple approach for validation / a-posteriori estimation of random uncertainties. For each instrument and each month, we evaluated sample variance s^2 in 10° latitude zones from experimental data and the SILAM-adjusted field, which is sub-sampled at measurements locations. This sample variance s^2 provides the estimates of natural variability σ_{nat}^2 . Then a posteriori (ex-post in von Clarmann et al. (2020) [RD-20] terminology) uncertainties can be estimated as $\sigma_{ex-post}^2 = s^2 - \sigma_{nat}^2$. We computed latitude and altitude dependent offset $\Delta = \sigma_{ex-post} - \sigma_{ex-ante}$ ($\sigma_{ex-ante}$ is the mean error estimate provided with profiles, in the same 10° latitude zones over the month) and applied it to each profile. By construction, the resulting uncertainty estimates are also compatible with the observed ozone variability.

After homogenization, the limb data are interpolated to form a high-spatial resolution dataset. We apply a kriging-type interpolation, in which both data uncertainty and the structure of the data variability are taken into account. In this approach, the value at the point $\mathbf{r}$ is taken as a weighted mean of data in the neighbourhood:

$$x(\mathbf{r}) = \sum_i w_i x(\mathbf{r}_i), \quad (1)$$

Equation 4-12

with the weights w_i inversely proportional to the total uncertainties:

$$\sigma_{tot,i}^2 = \sigma_{noise,i}^2 + D(\mathbf{r}_i - \mathbf{r}), \quad (2)$$

Equation 4-13

where σ_{noise}^2 is the estimate of the noise in the data, and $D(\mathbf{r}_i - \mathbf{r})$ is the uncertainty due to the spatial mismatch, which is usually estimated via the structure function. In our interpolation method, $D(\mathbf{r}_i - \mathbf{r})$ is taken from the adjusted SILAM field, for each day. The weighted mean is assessed using the $10^\circ \times 20^\circ$ latitude -longitude area around each point [RD-17].

The interpolation of ozone profiles is performed at each pressure level separately. An example of the interpolated field is shown in Figure 4-5.

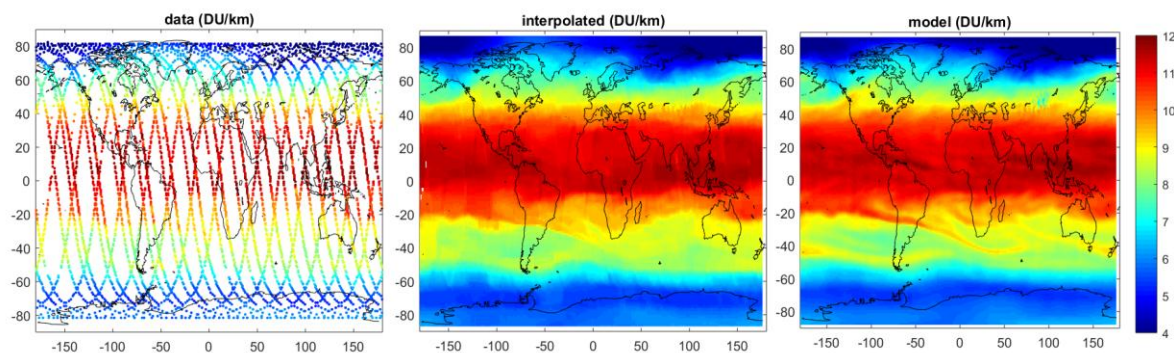


Figure 4-5. Left: ozone at limb satellite measurements at 10 hPa on 1 September 2018. Center: after interpolation. Right: corresponding adjusted SILAM ozone field at the same pressure level.

Since satellite data have limited accuracy, non-homogeneous and rather sparse coverage below the tropopause, we extended the satellite-based ozone profiles to lower altitudes by using the smooth transition to the adjusted SILAM profiles. The linear transition is performed in such a way that above 200 hPa the profile follows fully the experimental data and below 400 hPa - fully the model data. The illustration of the transition to the model data at lower altitudes is shown in Figure 4-6, for tropical and polar atmospheres.

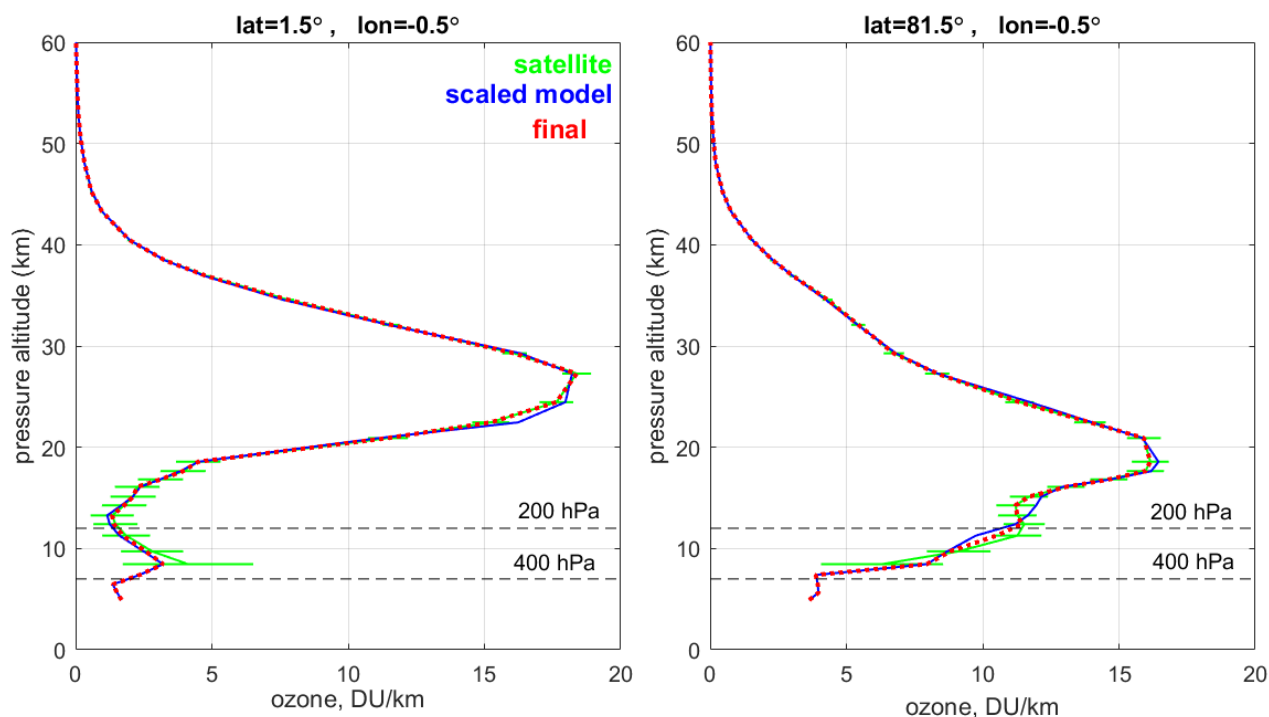


Figure 4-6. Illustration of transition to model-adjusted profiles at lower altitudes for tropical (left) and polar region (right). The vertical coordinate is pressure altitude $z = 16 \log_{10}(P_0/P)$, where $P_0=1013$ hPa is the standard pressure and P is pressure in hPa.

The resulted ozone profiles are included into the high-resolution gap-free dataset of ozone profiles.

4.5 LIMB-UTLS merging algorithm (FMI)

The LIMB -UTLS is the merged dataset of ozone profiles referenced to the tropopause. It is currently under development. The main data processing will consist of the following steps:

- 1 step: Re-gridding of individual ozone profiles to the tropopause-referenced coordinates. The resulting ozone profiles will cover the vertical range from -5 km below to + 10 km above the tropopause.
- 2 step: creating tropopause-references monthly zonal mean ozone profiles for each individual satellite instrument
- 3 step: creating the merged tropopause-referenced dataset of ozone profiles

Data from SAGE II, POAM III, OSIRIS, GOMOS, MIPAS, SCIAMACHY, ACE-FTS, OMPS-LP SNPP(N21), MLS and SAGE III/ISS will be used for the LIMB-UTLS dataset.



5 Tropospheric Ozone Algorithms

5.1 CHORA single sensor algorithm (IUP-UB)

The Cloud Height and Ozone Reference Algorithm (CHORA) is developed from the standard CCD (convective cloud differential) technique (Ziemke, 1998 [RD-19]) with a few additions. It calculates the tropical tropospheric ozone column (TCO) and is based on level 2 nadir total column ozone and cloud products from the different sensors. CHORA is described in [RD-66].

We calculate TCO as the difference between the stratospheric ozone column (SOC) and the total ozone column (TOZ). SOC or ACCO (Above Cloud Column Ozone) is the column above the pressure level of 270 hPa (or 200 hPa) that is computed from cloudy pixels ($CF > 0.85$, $CP < 340$ hPa) in the Pacific sector for latitude bands of 0.5° width. TOC is computed for boxes of 0.5° latitude and 0.5° longitude of TROPOMI on a daily basis. For other lower resolution sensors more days of data and larger longitude widths are needed. For TROPOMI, Total ozone columns extracted from the operational offline/reprocessed total column product are used. The cloud parameters (cloud top height and cloud fraction) are retrieved with the OCRA/ROCINN-CRB algorithm.

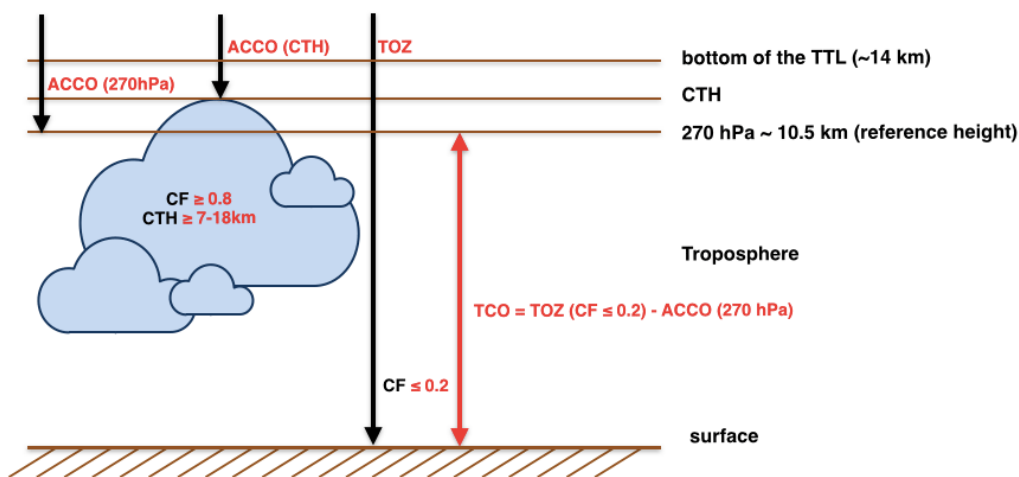


Fig. 5-1: Illustration of the CCD technique [RD-66]. TCO is the tropical tropospheric-column ozone, TOZ is the total ozone under clearsky conditions, ACCO is the above-cloud-column ozone, CF is the cloud fraction, and CTH is the effective cloud top height.

The main **error** source of the CCD method is introduced from retrieving the **ACCO**. We calculate the height correction not using a climatology but directly from the measurements in the Pacific sector by using a Theil-Sen regression of ACCO vs cloud top pressure (CTP). We thus calculate a slope and interpolate the ACCO to 270 hPa (or any other pressure level). For most cases, the CTP spread for one retrieval is high enough to interpolate.

Due to sparsity of measurements of high, optically thick clouds in the latitude band, the ACCO vector retrieved over the Pacific exhibits gaps and outliers. Data gaps can occur due to missing data and seasonal cloud height/fraction changes. High frequency scatter is detected towards the extratropics, mainly in winter. This is addressed in a post-processing step where missing data gaps



are filled using interpolation mainly in time direction and the whole 2d ACCO field (time, latitude) is smoothed as shown in Fig. 5-2.

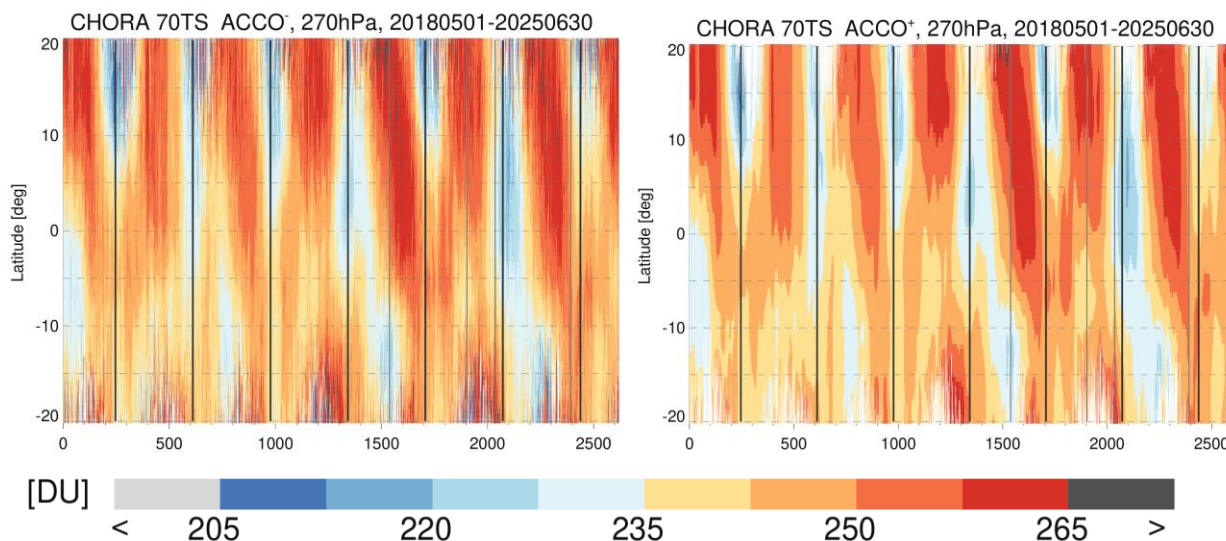


Fig. 5-2: Original ACCO data [DU] (left) for TROPOMI as function of days and latitude and the upgraded ACCO (right).

The TROPOMI TCO and corresponding uncertainty for a four year mean (2019-2022) is shown in Fig. 5-3. A larger uncertainty of up to 8 DU is detected towards the extra-tropics.

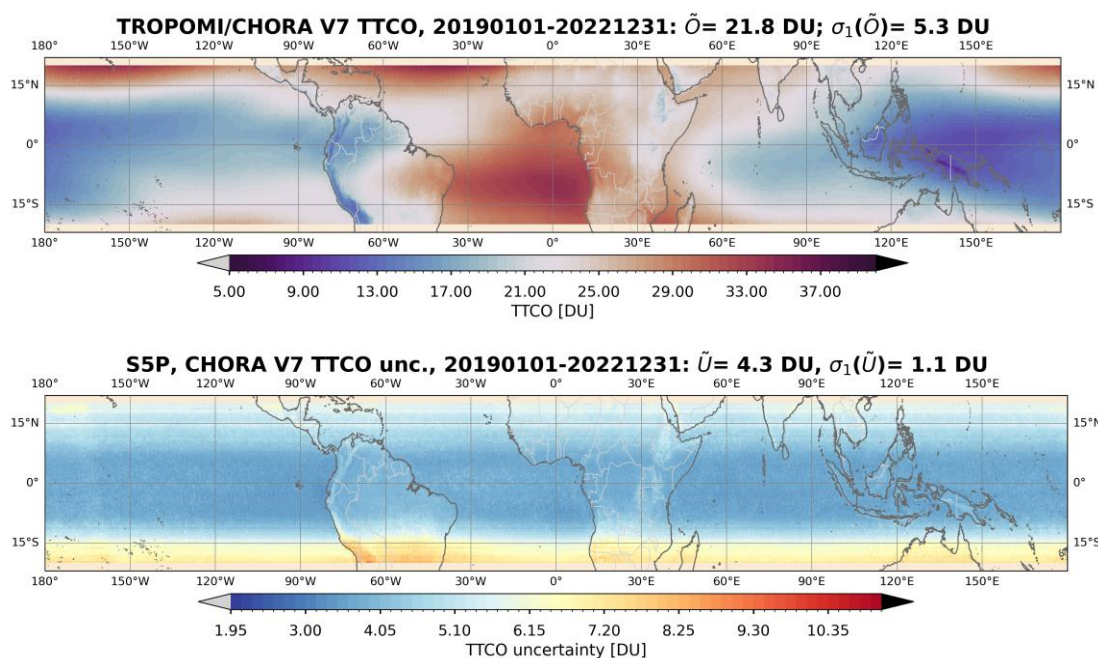


Fig. 5-3: TROPOMI tropospheric column ozone in the tropics and the uncertainty for 2019-2022.



Table 5-4 shows the retrieval parameters used for the different instruments and the total ozone L2 algorithm.

Instrument	Spatial resolution TOC pix, SOC lat	Temporal Res.	Cloud fraction TOC, SOC	Algorithm
TROPOMI	0.5°×0.5°, 1.5°	1 day	<0.8, >0.8	UPAS-3.2.0
GOME2	1° × 3°, 1.5°	5 days	<0.8, 0.85	GODFIT
OMI	1° × 1°, 1.5°	3 days	<0.8, >0.85	GODFIT col 4

Table 5-4: Grid sizes, temporal resolution, cloud fraction level, and algorithm baseline.

5.2 CHORA merging algorithm (IUP-UB)

The merging algorithm is currently under development and is based on the harmonization technique from Sofieva (2017) [RD-12].

5.3 GTO-LIMB algorithm (FMI)

[Algorithm under development, section to be added in later version of ATBD]