Ozone_cci+

Algorithm Development Plan (ADP)

Date : 04/10/2023
Version : 2.1
Reference : Ozone_cci+_D2.3_ADP_v2.1_20231004

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DOCUMENT PROPERTIES

Title	D2.3 Algorithm Development Plan (ADP)
Reference	Ozone_cci+_D2.3_ADP_v2.1_20231004
Issue	2
Revision	1
Status	Final
Date of issue	04/10/2023
Deliverable	D2.3

	FUNCTION	**NAME**	**DATE**	**SIGNATURE**
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ISSUED BY	Science Leader	Daan Hubert	04/10/2023	

DOCUMENT CHANGE RECORD

Issue	Revision	Date	Modified items	Observations
0	0	25/11/2022	Initial template	Creation of document
	1	15/12/2022	Input from algorithm teams	
	2	21/12/2022	First complete draft for revision	
1	0	24/01/2023	Accepted by ESA	
2	0	05/07/2023	Input from algorithm teams	
2	1	04/10/2023	Accepted by ESA	

Executive Summary

This Algorithm Development Plan (ADP, deliverable D2.3 in Ozone_cci+ Phase 2) describes the plans for algorithmic developments addressing total ozone columns, tropospheric ozone columns, nadir- and limb-based ozone profiles.

A series of new algorithms will be developed with a focus on ozone data products at different product levels.

For **total ozone**, the following activities will be undertaken:

- backward extension of MSR to 1960 (level-4).

For ozone **profiles from nadir sensors**:

- updated level-1 and level-2 retrieval schemes for GOME and GOME-2A;
- prototype retrieval and reprocessing of S5P (level-2);
- prototype combined retrieval of GOME-2 and IASI on MetOp-A (level-2);
- extension and update of merged GOME-type profile data record (GOP-ECV, level-3);
- reprocessing of IASI profile data using a climate version of FORLI: FORLI-O3-CDR (level-2);
- prototype merging scheme for IASI profile and column data based on standard FORLI (level-3).

For ozone **profiles from limb sensors**:

- extension and updates to homogenised level-2 from seven sensors;
- extension and updates to high-resolution level-3, combining data from seven sensors;
- prototype retrieval of OMPS-LP onboard JPSS-2 (level-2);
- prototype merging scheme for OMPS-LP onboard SNPP and JPSS-2 (level-3).

For **tropospheric ozone**:

- merging of GOME-type tropospheric column data over the tropics using the GTTO-ECV scheme and using CHORA retrievals (level-3);
- global tropospheric column data from nadir total ozone and homogenised limb profiles, and from SNPP/OMPS (level-3);
- improvements to tropospheric measurements resulting from refined profile retrievals for UV/visible and infrared nadir sounders.

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1 Purpose and scope

1.1 Purpose

This document summarises the plans of the Ozone_cci+ team for algorithmic developments addressing total ozone columns, nadir- and limb-based ozone profiles, and tropospheric ozone. This plan is expected to evolve and shall be updated as the definition of the ozone ECV product consolidates and the understanding of algorithmic issues improves.

1.2 Scope

The scope of the ADP is to establish through analysis of the trade-off between requirements and feasibility, a prioritisation of what R&D on ECV data product generation should be developed to maximise benefits to the users. The document also includes a specification of the ECV products planned for development in the project. The ADP is provided as an annex to the Project Management Plan (PMP).

1.3 Applicable documents

[AD-1] CCI Data Standards v2.3, ref: CCI-PRGM-EOPS-TN-13-0009, 26 July 2021. Available online at: https://climate.esa.int/documents/1284/CCI_DataStandards_v2-3.pdf

[AD-2] CCI Data Policy v1.1, ref: CCI-PRGM-EOPS-TN-13-0019, 12 July 2013. Available online at: http://cci.esa.int/sites/default/files/CCI_Data_Policy_v1.1.pdf

1.4 References documents

[RD-1] GCOS Climate Monitoring Implementation Principles, November 1999. Available online at: https://gcos.wmo.int/en/essential-climate-variables/about/gcos-monitoring-principles

[RD-2] Guideline for the Generation of Satellite-based Datasets and Products meeting GCOS Requirements, GCOS Secretariat, GCOS-143, May 2010 (WMO/TD No. 1530). Available online at: https://library.wmo.int/index.php?lvl=notice_display&id=12884#.Y5nN-XbTVOR

[RD-3] The Space Agency's Response to GCOS Implementation Plan (IP). The Joint CEOS/CGMS Working Group on Climate (WGClimate), 2017. ESA-ECO-EOPS-WGCL-RP-17-0061. Version 1.0. Available online at: https://ceos.org/document_management/Publications/Space-Agency-Response-to-the-GCOS-IP/Space%20Agency%20Response%20to%20GCOS%20IP%20v1.5.pdf

[RD-4] Quality assurance framework for earth observation (QA4EO): http://qa4eo.org

[RD-5] EU Research Programmes on Space and Climate: Horizon 2020 (H2020), (http://ec.europa.eu/programmes/horizon2020/en/h2020-section/space, https://ec.europa.eu/programmes/horizon2020/en/h2020-section/climate-action-environment-resource-efficiency-and-raw-materials) and Copernicus (http://www.copernicus.eu/).

[RD-6] The Global Observing System for Climate: Implementation Needs, GCOS-200, October 2016. Available online at: http://library.wmo.int

[RD-7] Status of the Global Observing System for Climate, GCOS-195, October 2015. Available online at: http://library.wmo.int

[RD-8] The GCOS Status Report 2021, GCOS Secretariat, GCOS-240, September 2021. Available online at: https://gcos.wmo.int/en/gcos-status-report-2021

[RD-9] The 2022 GCOS Implementation Plan, GCOS-244, October 2022. Available at : https://gcos.wmo.int/en/publications/gcos-implementation-plan2022

[RD-10] Hollmann, R., et al., The ESA climate change initiative: Satellite data records for essential climate variables. American Meteorological Society. Bulletin, Vol. 94, No. 10, 2013, p. 1541-1552.

[RD-11] Joint Committee for Guides in Metrology, 2008, Evaluation of measurement data — Guide to the expression of uncertainty in measurement (GUM), JGCM 100: 2008. Available online at http://www.bipm.org/en/publications/guides/gum.html.

[RD-12] Merchant, C. J., Paul, F., Popp, T., Ablain, M., Bontemps, S., Defourny, P., Hollmann, R., Lavergne, T., Laeng, A., de Leeuw, G., Mittaz, J., Poulsen, C., Povey, A. C., Reuter, M., Sathyendranath, S., Sandven, S., Sofieva, V. F., and Wagner, W.: Uncertainty information in climate data records from Earth observation, Earth Syst. Sci. Data, 9, 511–527, https://doi.org/10.5194/essd-9-511-2017, 2017.

[RD-13] Ohring, G., et al. (2007), Achieving satellite instrument calibration for climate change, Eos Trans. AGU, 88(11), 136– 136, doi:10.1029/2007EO110015.

[RD-14] Popp, T., Hegglin, M.I., Hollmann, R., Ardhuin, F., Bartsch, A., Bastos, A., Bennett, V., Boutin, J., Brockmann, C., Buchwitz, M. and Chuvieco, E., 2020. Consistency of satellite climate data records for Earth system monitoring. Bulletin of the American Meteorological Society, 101(11), pp.E1948-E1971, https://doi.org/10.1175/BAMS-D-19-0127.1

[RD-15] Copernicus Space Component: https://www.esa.int/Our_Activities/Observing_the_Earth/Copernicus/Space_Component

[RD-16] User requirements for monitoring the evolution of stratospheric ozone at high vertical resolution (Operoz), 2015, ESA Expro contract 4000112948/14/NL/JK. Available at: https://media.suub.uni-bremen.de/bitstream/elib/4650/1/operoz_final_report_20150301_pdfa.pdf

1.5 Acronyms

ACE-FTS	Atmospheric Chemistry Experiment – Fourier Transform Spectrometer
ADP	Algorithm Development Plan
BIRA-IASB	Royal Belgian Institute for Space Aeronomy
CCD	Convective Cloud Differential
CCI	Climate Change Initiative
CDR	Climate Data Record
CHORA	Cloud Height and Ozone Reference Analysis
C3S	Copernicus Climate Change Service
DLR	German Aerospace Centre
ECMWF	European Centre for Medium-range Weather Forecast
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
GAW	Global Atmosphere Watch
GCOS	Global Climate Observation System
GOME	Global Ozone Monitoring Experiment
GOME-2	Global Ozone Monitoring Experiment – 2
GOMOS	Global Ozone Monitoring by Occultation of Stars
GOP	GOME-type Ozone Profile
GTO	GOME-type Total Ozone
GTTO	GOME-type Tropical Tropospheric Ozone
IASI	Infrared Atmospheric Sounding Interferometer
IR	Infrared
IUP-UB	Institute of Environmental Physics, University of Bremen
JPSS	Joint Polar Satellite System
KNMI	Royal Netherlands Meteorological Institute
MetOp	Meteorological Operational Platform (EUMETSAT)
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
MLS	Microwave Limb Sounder
NASA	National Aeronautics and Space Administration
NDACC	Network for the Detection of Atmospheric Composition Change
OMI	Ozone Monitoring Instrument
OMPS	Ozone Mapping and Profiler Suite
OSIRIS	Optical and Spectroscopic Remote Imaging System
PSD	Product Specifications Document
RAL	Rutherford Appleton Laboratory

R&D	Research & Development
S5P	Sentinel-5 Precursor
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Cartography
Suomi-NPP	Suomi National Polar-orbiting Partnership
TOMS	Total Ozone Mapping Spectrometer
TROPOMI	Tropospheric Ozone Monitoring Instrument
ULB	Université Libre de Bruxelles
URD	User Requirements Document
UV	Ultraviolet

2 Introduction

2.1 Summary of user requirements for ozone ECV data products

Data product and algorithm developments in Ozone_cci+ are driven by GCOS. The goal of the Global Climate Observing System (GCOS, https://gcos.wmo.int/en/home) is to provide continuous, reliable, comprehensive data and information on the state and behaviour of the global climate system. GCOS focuses on satellite and in situ observations for climate in the atmospheric domain. Long-term consolidated data sets based on different satellite instruments are the foundation for improved model quality evaluation, allowing a more detailed insight into individual dynamical and chemical processes.

Long-term consolidated data sets are mainly required for: (1) monitoring the Earth climate system on longer (decadal) time scales; (2) investigation of long-term changes as well as of short-term variability; (3) improved description of processes in numerical models for more robust assessment of future evolution.

Table 1 summarizes the requirements established within GCOS for the Ozone ECV.

Table 1: GCOS Target Requirements for the Ozone ECV (GCOS, 2022).

Goal / Breakthrough / Threshold	Profile			Column		
	Tropo	UT + LS	US + Meso	Tropo	Strato	Total
Horizontal resolution (km)	1/20/100	10/50/200	20/100/500	5/20/100	20/100/500	20/100/500
Vertical resolution (km)	1/3/5	0.5/1/3	1/3/10	-	-	-
Time resolution	1h/6h/30d	6h/1d/30d	6h/1d/30d	1h/6h/30d	1h/1d/30d	1h/1d/30d
Timeliness	1h/1d/30d	6h/1d/30d	6h/1d/30d	1h/1d/30d	6h/1d/30d	1h/1d/30d
Uncertainty (%, 2σ)	2/5/10	2/5/10	5/10/15	5/10/15	1/3/5	1/2/3
Stability (%/dec)	1/2/3	1/2/3	1/2/3	1/2/3	1/2/3	1/2/3

The horizontal and vertical resolution and observation frequency are mainly justified on the commonly used (standard) resolution of currently available and used model systems. For the troposphere regional models are often used which have a much higher horizontal resolution. The required horizontal resolution (i.e., 50-100 km) is generally too high; for most climate applications it would be sufficient to have 100-300 km.

It should be noted that the GCOS target requirements also refer to requirements for future (operational) observations.

As part of the User Requirements Document (URD) produced during Ozone_cci+ Phase 1, achievable user and data requirements have been specified for ozone ECV products derived from existing observations having known attributes and covering the past 30 years. Although they are likely to be revised in the course of the current project, the latter requirements have been used as a reference for prioritisation in CCI+.

2.2 Priorities for new algorithm developments

As stated in the ESA SoW, CCI+ capitalises on the success of the CCI programme element to date. The objective is therefore to continue the successful achievements on research, development and assessment of pre-operational ECV processing systems, with the goal of transferring them into operational production outside CCI.

CCI actively coordinates with other European initiatives (e.g., C3S or EUMETSAT) with the aim to ensure an optimal uptake of the R&D performed under CCI in the operational production of ECVs outside CCI, and to assess the R&D that is needed for the evolution of the climate services.

The scope of CCI+ Phase 2 covers four main themes:

- Continued development of nine new ECVs, which started in CCI+ Phase 1.
- New R&D on ECVs that were started in CCI between 2010 and 2015.
- Cross-ECV scientific exploitation.
- Supporting activities on Knowledge Exchange.

The general criteria put forward by ESA for new R&D on existing ECV are the following:

- Match GCOS requirements and improve cross-ECV consistency.
- Add new sensors (e.g., Sentinels).
- Difficult ECVs required by GCOS.
- Extend ECV length and develop corrections for future instrument degradation.
- Further develop multi-mission time-series to fill gaps.
- Improve uncertainty estimates.
- Develop better merged products.
- Perform algorithm round robins.

Having these general criteria in mind, specific priorities were identified for new R&D activities on ozone data records:

- Generally speaking : maximize the impact of new developments on the C3S ozone portfolio.
- Develop complementary tropospheric ozone CDRs.
- Integrate new sensors into existing CDRs (Sentinel-5 Precursor, JPSS-2 OMPS).
- Integrate more historical data sets into existing CDRs, with a focus on making a significant impact on the applicability of the resulting new data sets for climate analysis and trend studies.

- Improve the accuracy and precision of the existing ozone data products at level-2 and level-3.
- Improved the characterization of the uncertainties of the existing data products.
- Strive to design new algorithms or approaches to maximize the information content of the observations in critical altitude ranges (e.g., troposphere and lower stratosphere), as well as in critical regions of the globe (e.g., in polar regions).

These criteria and the consideration of the available resources for new developments have guided us in performing a trade-off analysis leading to the selection of the activities outlined in the next sections.

3 Algorithm Development Plan

3.1 Overview

Algorithm developments planned in this project aim at improving and enhancing the current portfolio of ozone data products generated in previous phases of the CCI programme. The emphasis has been put on enhancing data records suitable for inclusion in the C3S service delivery.

Efforts will concentrate on (1) adding new EO sensors, (2) adding tropospheric ozone CDRs, (3) extending existing data records in time both backward and forward, (4) reducing uncertainties in critical observational conditions, (5) improving the characterization of the data sets, through improved error budget analysis and better identification of various sources of biases.

Table 2 presents a tentative overview of the planned distribution of efforts on algorithm developments during the two contractual phases of the projects. Detailed descriptions of the planned activities are given in the following subsections. Activities in grey will lead to data products that are available on request, but these will not be in the formal Ozone_cci+ data release.

Table 2: Overview of ozone algorithm developments planned over the two contractual phases (CP-1, CP-2). Activities in grey will not lead to an official CCI data product, but these products can be made available on request.

Algorithm development	Responsible team	Product Level	CP-1				CP-2			
			Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Total ozone developments										
Backward extension of MSR	KNMI	L4								
Nadir profile developments										
Update of L1 & L2 schemes for GOME and GOME-2A	RAL	L2								
Inclusion of Sentinel-5 Precursor	RAL	L2								
Prototype combined retrieval GOME-2A and IASI-A	RAL	L2								
Extension and update of merged GOP-ECV	DLR	L3								
Reprocessing of IASI using FORLI-O3-CDR	ULB	L2								
Prototype merging scheme for IASI based on standard FORLI	ULB	L3								
Limb profile developments										
Extension and updates to homogenized level-2	FMI	L2								
Extension and updates to high-resolution level-3	FMI	L3								
Prototype retrieval of OMPS-LP onboard JPSS-2	IUP-UB	L2								
Prototype merging scheme for OMPS-LP on SNPP and JPSS-2	IUP-UB	L3								
Tropospheric ozone developments										
Merging of tropical GOME-type CCD data (GTTO-ECV scheme)	DLR	L3								
Merging of tropical GOME-type CCD data (CHORA scheme)	IUP-UB	L3								
Global tropospheric ozone column from nadir and multiple limb sensors	FMI	L3								
Nadir-limb matched SNPP/OMPS tropospheric ozone	IUP-UB	L3								

3.2 Total ozone developments

3.2.1 MSR extension backward in time (level-4)

During CCI+ Phase 1, KNMI improved the Multi Sensor Reanalysis (MSR) algorithm for use before 1980 by including a dependency on the chlorine content Cariolle parameterization of the heterogeneous chemistry in the chemical-transport model. In addition, the spatial error correlation was adapted to maximise the effect of ground measurements on the assimilated ozone field. This improved assimilation scheme was applied to observations (including satellite and Dobson stations) in the period 1957-1979 using the ERA-Interim meteorological fields of ECMWF. These meteo fields are at 2° x 3° resolution, resulting in ozone fields at low resolution.

In Phase 2 of CCI+, KNMI will collect the newly processed ERA5 backward extension of meteorological fields for the period 1959 to 1978. Using ERA5, we will reprocess the entire period from 1960-1978 in order to obtain a consistent MSR total ozone data record from 1960 to present, with a single resolution of 0.5° (on an output grid of 1° x 1°). Additional quality control checks will be implemented to verify all ground data in the period 1959-1979.

3.3 Nadir profile developments

3.3.1 Updated level-1 & level-2 schemes for GOME & GOME-2A

Building on the experience of the existing RAL UV ozone processor and requirements of S5P, S4 and S5, a new processor has been developed, which includes better handling of instrument radiometry issues. This new scheme will be applied to existing data instruments, in particular to process new level-1 data.

- update RAL new processor for GOME (v5) and GOME-2A (v7) new level-1 data;
- process and analyse subsets of data with new processor to assess level-2 quality and identify potential further improvements, with the aim of increasing level-2 accuracy and stability to merit full mission reprocessing.

3.3.2 Processing of Sentinel-5P level-2

To mitigate spectrally-dependent errors in UV radiometry for Sentinel-5P, which limit the quality of height-resolved data, along with increased data volumes have required the development of a re-engineered RAL UV ozone processor.

- test data sets will be evaluated against correlative data, with the aim of increasing level-2 accuracy and stability to merit a future processing of the Sentinel-5P mission;
- subsampling (spatial and temporal) necessary to meet realistic computational requirements, while being sufficient for potential multi-mission merging in GOP, will be established.

3.3.3 Prototype combined retrieval of MetOp-A (level-2)

The extended version of RAL's Infrared and Microwave Sounding (IMS) scheme co-retrieves ozone with other atmospheric parameters. Vertical sensitivity of the retrieved ozone profiles is controlled by ozone absorption in the IR (IASI) which differs from, and complements, that in the UV (GOME-2). Combining these two products through optimal estimation should exploit their complementary vertical sensitivities and increase vertical resolution in the troposphere and UTLS from what is achievable from either independently. The addition of slant-column retrieval from GOME-2 visible (Chappuis) band, to enhance near surface sensitivity, will also be considered.

- Generate consistent IMS product for MetOp-A (IASI lv1 v8.x);
- identify appropriate version and sub-set of RAL UV ozone profile product MetOp-A to combine;
- generate level-2 based optimal estimation combination of IR+UV profiles and assess quality;
- consider slant-column retrieval from GOME-2A visible (Chappuis) band and assess suitability for combination with IR+UV product.

3.3.4 Extension and update of the merged GOME-type level-3 data record

During CCI+ Phase 1 the GOME-type Ozone Profile Essential Climate Variable (GOP-ECV) data record has been developed. It covers the period 1995-2020 and combines measurements from five nadir-viewing satellite sensors: GOME, SCIAMACHY, OMI, GOME-2A, and GOME-2B. The ozone profile retrieval is based on the RAL scheme. The merged ozone profiles are harmonised with respect to the merged total ozone data record GTO-ECV (GOME-type Total Ozone Essential Climate Variable).

In the framework of CCI+ Phase 2 the following activities are planned:

- adaption of the existing merging and harmonisation algorithm to include ozone profiles from TROPOMI/Sentinel-5P and GOME-2/MetOp-C in GOP-ECV;
- usage of updated GOME and GOME-2A level-2 ozone profiles in final GOP-ECV data record.

3.3.5 Reprocessing of IASI level-2

The scope of this activity is to retrieve a homogeneous climate data set of level-2 ozone profiles from the three IASI sensors on MetOp-A, -B and -C from 2008 to present, using a dedicated FORLI inversion scheme, namely FORLI-O3-CDR (Climate Data Record). Due to constraints in the computing facility, ozone profiles will be retrieved for an optimised subsample (likely three days per month) in order to reprocess the complete time period of the IASI missions by end of project.

In the framework of CCI+ Phase 2, the following activities are planned:

- adaptation of the standard FORLI-O3 to ingest the fully reprocessed and homogenised IASI level-1c radiances & IASI level-2 CDR temperature and humidity profiles;

- backprocessing of the entire IASI level-1C dataset with FORLI-O3-CDR & negotiating with Eumetsat to produce that FORLI-O3-CDR dataset (with an optimised subsampling) in the course of the CCI+ Phase 2;
- intercomparison of the FORLI-O3-CDR dataset vs the standard FORLI-O3 one and ozone sondes used as reference, to verify the benefit of FORLI-O3-CDR for trend determination.

3.3.6 Prototype merging of IASI level-3

The scope of this activity is to merge the existing ULB IASI-A, -B & -C ozone profile datasets retrieved with the last release of the standard FORLI-O3 inversion scheme. During CCI+ Phase 1, comparisons of ozone measurements by IASI-A, -B and -C showed excellent consistency and stability of the time series.

In the framework of CCI+ Phase 2, the following activities are planned:

- development of a merging scheme of the IASI-A, -B & -C O3 profiles datasets;
- optimization of the spatial resolution for the merging of the three IASI sensors;
- generation of the merged daily (daytime & nighttime) Level-3 ozone profile and associated total O3 column averaging kernel datasets from the three IASI sensors;
- generation of a merged daily Level-3 total and tropospheric O3 columns datasets.

3.4 Limb profile developments

3.4.1 Extension and updates to homogenized level-2

The planned work includes

- revise the a posteriori uncertainty estimation and correction;
- analyse the evolution of biases and uncertainty correction factors;
- develop a method to extend homogenized ozone profile datasets to 2002-2004.

3.4.2 Extension and updates to high-resolution level-3

The planned work includes

- assess and possibly include ACE-FTS data into high-resolution level-3 dataset of ozone profiles;
- generate the daily gap-free high-resolution (1°x1°) dataset of ozone profiles using the level-2 data from seven sensors (Sect. 3.4.1); Special attention will be on the extension to 2002-2004;
- provide netcdf-4 output.

3.4.3 Prototype retrieval of OMPS-LP JPSS-2 (level-2)

The launch of the OMPS-LP instrument onboard the JPSS-2 (re-named NOAA-21) satellite was successfully completed in November 2022. This improves the current availability of limb observations, characterised by several ageing instruments (e.g., Aura MLS and OSIRIS) prior to the launch of ESA's ALTIUS mission (scheduled end 2025). The first OMPS-LP sensor, onboard Suomi-NPP was launched in 2012 and already passed twice its estimated lifetime. IUP-UB will prepare the retrieval of measurements from the new instrument in order to ensure a continuation of the measurement time series in the coming years. The new instrument shares similar characteristics of the currently operating OMPS-LP, in terms of measurement technique, wavelength coverage and resolution.

The activities will include:

- adapt the existing IUP-UB ozone profile retrieval chain for OMPS-LP onboard Suomi - NPP to process observations by the instrument onboard NOAA-21;
- adapt the existing IUP-UB ozone retrieval algorithm: the current algorithm fits several spectral ranges in the UV and visible domains to retrieve ozone profiles from cloud top to ~60 km; we anticipate that only minor changes will be needed;
- implement recommendations from the NASA team in charge of level-1 data, especially concerning the pointing corrections.

3.4.4 Prototype merging of OMPS-LP on SNPP and JPSS-2 (level-3)

The scope of this activity is the merging of the existing IUP-UB OMPS-LP SNPP data set with the retrieved ozone profiles from the OMPS-LP instrument onboard NOAA-21. We intend to generate a merged OMPS-LP time series covering the period from 2012 to 2024, in preparation of the replacement of the Suomi-NPP sensor by the NOAA-21 instrument, at the end of its lifetime. This will provide an additional tool for the study of long-term ozone changes.

The activities will include:

- reprocessing of the current OMPS-LP Suomi-NPP data set to improve the long-term drift, by using the newly generated L1G data by the NASA team;
- preliminary intercomparison between the retrieved ozone profiles from OMPS-LP onboard Suomi-NPP and NOAA-21 to evaluate biases and differences;
- development of the merging scheme of the two OMPS-LP time series; based on the fact that both retrieval schemes and the instruments are very similar, a simple debiasing of the two data records will be tested in addition to the merging of deseasonalized anomalies;
- production of the merged OMPS-LP dataset covering the 2012-2024 period.

3.5 Tropospheric ozone developments

3.5.1 Merged tropical tropospheric columns using CCD (GTTO-ECV)

DLR's CCD algorithm will be applied to total O3 data from GOME, SCIAMACHY, OMI, GOME-2 (A,B,C) and S5P. The resulting tropical tropospheric O3 columns will be merged using the GTTO-ECV scheme to obtain a data record from 1995 to 2023.

The planned algorithm improvements include

- processing of CCD for two pressure levels (200 and 270 hPa) and write output in one file;
- test AC-SAF GOME-2 CCD as input for the harmonisation;
- generate climatology with monthly mean as well as 5 years mean values.

3.5.2 Merged tropical tropospheric columns using CCD (CHORA)

The IUP-UB CCD algorithm will also be applied to total O3 data from GOME, SCIAMACHY, OMI, GOME-2 (A,B,C) and S5P. The merging will be done with the algorithm developed by Leventidou et al. (2016, 2018)

- storage of 200 and 270 hPa data similar to the DLR CCD algorithm to make both algorithms better comparable;
- optimisation of horizontal/temporal resolution for the merging of the different sensors;
- optimisation of the merging algorithm;
- computation of the full ozone dataset (monthly average, optimized resolution, e.g. 2° x 2.5°) and storage as netcdf files.

3.5.3 Tropospheric column from nadir and multiple limb sensors (SUNLIT)

The planned work includes

- evaluation of the stratospheric ozone column using the high-resolution dataset of ozone profiles, created as part of the limb WP (Sect. 3.4.2);
- computation of two tropospheric ozone datasets (monthly average, 1° x 1° resolution): OMI-LIMB and GTO-LIMB, using daily gridded total ozone column datasets (OMI and GTO-ECV);
- generating the netcdf-4 data files.

3.5.4 Tropospheric column from limb-nadir matched Suomi-NPP/OMPS

A data set of tropospheric ozone from 2012 to 2018 will be created by applying the Limb-Nadir-Matching (LNM) algorithm to the data from SNPP/OMPS. The ozone total columns retrieved from OMPS-NM and stratospheric ozone vertical profile retrieved from OMPS-LP will be used. Both total ozone columns and stratospheric profiles are retrieved at IUP-UB.

The following activities will be performed:

- retrieval of the full time series of the total ozone column;
- creation of the tropopause height database;
- filtering and extrapolation of the limb ozone profiles (where needed);
- calculation of the stratospheric ozone columns;
- creation of the tropospheric ozone column database;
- assessment of the error budget of the resulting tropospheric ozone columns;
- validation of the results.