Ozone_cci+

Algorithm Development Plan (ADP)

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Executive Summary

This Algorithm Development Plan (ADP, deliverable D2.3 in Ozone_cci+) 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 and existing ones improved with a focus on ozone data products at different product levels (Table 1).

The present issue summarises the development plans for 2025.

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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 Reference 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

[RD-17] CCI+ Ozone User Requirements Document: ESA Ozone_cci+ User Requirements Document (URD), Ref. Ozone_cci+_D1.1_URD_v5.1, Issue 5, Revision 1, 14/10/2025.

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 Algorithm Development Plan

2.1 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. Efforts will concentrate on (1) improving and extending existing data records forward in time, (2) adding a profile product suitabel for UTLS studies, (3) testing retrievals for the recently launched geostationary sensors, (3) reducing uncertainties and improving the characterization of the data sets, through improved error budget analysis and better identification of various sources of biases.

Table 1 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 part of the public Ozone_cci+ data release.

Table 1: Overview of ozone algorithm developments planned over the 2025-2026 period, coinciding with the third phase of Ozone_cci+. Activities in grey will not lead to a publicly released CCI data product, but these products can be made available on request.

Algorithm development	Responsible team	Product Level	2025				2026			
			Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Total ozone developments										
Adaptation of GODFIT to retrieve OMI Collection 4	BIRA-IASB	L2								
Inclusion of reprocessed OMI Col4 in GTO-ECV	DLR	L3								
Development of cloud-screened GTO-ECV	DLR	L3								
Tropospheric ozone developments										
Inclusion of reprocessed OMI Col4 in GTTO-ECV	DLR	L3								
Application of CHORA CCD scheme to GOME-type sensors	IUP-UB	L3								
Merging of GOME-type CHORA columns	IUP-UB	L3								
Updates and extension of GTO-LIMB	FMI	L3								
Prototype retrieval schemes for GEMS & TEMPO	RAL	L2								
Nadir profile developments										
Updates to S5P retrieval scheme	RAL	L2								
Updates and extension of GOP-ECV	DLR	L3								
Updates and extension of IASI merging scheme	ULB	L3								
Limb profile developments										
Updates and extension of SAGE-CCI-OMPS+	FMI	L3								
Updates and extension of MEGRIDOP	FMI	L3								
Updates and extension of LIMB-HIRES	FMI	L3								
Development of UTLS data record (LIMB-UTLS)	FMI	L3								
Improved retrieval and extension of OMPS-LP onboard N21	IUP-UB	L2								
Development of merging scheme for OMPS on SNPP and N21	IUP-UB	L3								

2.2 Total ozone developments

2.2.1 OMI GODFIT using Collection 4 (level-2)

- Verification of Collection 3 vs Collection 4 OMI L2 total ozone

2.2.2 GTO-ECV (level-3)

- Inclusion of reprocessed OMI Col 4 in GTO-ECV
  - Generation of daily and monthly OMI Col 4 level-3 data based on OMI Col 4 level-2 data (see Sec. 2.2.1)
  - Usage of OMI Col 4 level-3 as a reference and computation of correction factors for GOME, SCIAMACHY, GOME-2A/B/C, and TROPOMI based on comparisons during overlap periods
  - Application of correction factors to daily level-3 data
  - Merging of daily OMI Col 4 level-3 data and adjusted daily level-3 data from other sensors
- Development of clear-sky GTO-ECV for use by GTO-LIMB
  - Generation of daily clear-sky level-3 data for GOME, SCIAMACHY, OMI, GOME-2A/B/C, and TROPOMI
  - Application of existing correction factors to daily clear-sky level-3 (all sensors except for OMI)
  - Merging of daily clear-sky level-3 data (OMI and adjusted GOME, SCIAMACHY, GOME-2A/B/C, and TROPOMI)

2.3 Tropospheric ozone developments

2.3.1 GTTO-ECV (level-3)

- Adapt DLR's CCD algorithm settings to the Collection 4 OMI GODFIT L2 2 data.
- Generate monthly tropospheric ozone column datafiles.
- Update the harmonised and merged GTTO-ECV tropospheric ozone dataset.

2.3.2 CHORA scheme applied to GODFIT total ozone (level-3)

- Apply IUP-UB CHORA algorithm to single-sensor GODFIT total O3 data from OMI, GOME-2 (A,B,C), and TROPOMI
- Develop a merging algorithm based on the method by Sofieva et al. (2017)
- Optimise the horizontal/temporal resolution for the merging of the different sensors and reprocessing

2.3.3 GTO-LIMB (level-3)

- Inclusion of cloud-free GTO-ECV, update of the processor

- Processing a test dataset and its preliminary evaluation (simple analyses of biases by comparison with other datasets)

2.3.4 Geostationary sensors (GEMS, TEMPO; level-2)

- Develop sensor specific corrections starting from the basic algorithm developed via ESA for Sentinel 4 (cfr. ATBD)
- Implement framework for deriving and applying radiometric soft calibration
- Implement and test post-retrieval de-striping algorithm
- Generate sample test datasets for selected days of GEMS and TEMPO
- Assess initial results via comparisons to CAMS and ozone sondes.

2.4 Nadir profile developments

2.4.1 Sentinel-5P (level-2)

- Complete definition of retrieval settings and approach for radiometric soft calibrations of S5P (based on consolidated settings for OMI).
- Generate sub-sets of data for internal testing (verification cf CAMS, checking internal consistency etc).
- Document updates in ATBD

2.4.2 GOP-ECV (level-3)

- Adaption and refinement of GOP-ECV merging scheme for inclusion of updated RAL nadir profile products (v4.10)

2.4.3 Merged IASI (level-3)

- Update of the merging scheme
- Correction of a few bugs
- Refinement of uncertainty calculation: error propagation & standard error of the weighted mean

2.5 Limb profile developments

2.5.1 SAGE-CCI-OMPS+ (level-3)

- Investigation of possibility of inclusion of NASA OMPS-LP into the merged SAGE-CCI-OMPS+ dataset
    - Analyses of deseasonalized anomalies of NASA OMPS-LP
    - Development of the merging algorithm
    - Data processing
- Evaluation of the merged dataset with 3 OMPS-LP datasets included

2.5.2 MEGRIDOP (level-3)

- Investigation of possibility of inclusion of NASA OMPS-LP into the merged MEGRIDOP dataset
    - Analyses of deseasonalized anomalies of NASA OMPS-LP
    - Development of the merging algorithm
    - Data processing
- Evaluation of the merged dataset with 3 OMPS-LP datasets included

2.5.3 LIMB-HIRES (level-3)

- Feasibility study for using MEGRIDOP as a reference for creating LIMB-HIRES
- Study the potential for improvement of the transition in the UTLS using a Bayesian approach
- Exploring the vertical region of the transition
- Validation of LIMB-HIRES data in the UTLS and identifation of valid altitude range.

2.5.4 LIMB-UTLS (level-3)

- Regriding ozone profiles to a tropopause-referenced grid for each instrument
- Computation of monthly mean values from individual instruments and their intercomparisons

2.5.5 OMPS-LP on NOAA-21 (level-2)

- Produce a second version of the OMPS NOAA-21 retrieval, building on top of the preliminary version developed in Phase 2;
- Test retrieval settings to improve the retrieval quality in the middle and lower stratosphere;
- Retrieve aerosol extinction profiles from NOAA-21 observations and use these profiles in the ozone retrievals;
- Test the usage of the side slits of the instrument, by using the UV radiance from the central slit and Vis radiance from the corresponding side slit.

2.5.6 Merged OMPS-LP SNPP and NOAA-21 (level-3)

- Development planned for 2026