Precursors_cci+

ESA Climate Change Initiative (CCI)

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1 Purpose and scope

1.1 Purpose

The Algorithm Development Plan (ADP) is a working document designed as a project management tool and organized to provide ESA with suitable information on technical developments planned during all development cycles. The ADP is not intended to be a public document.

1.2 Scope

The ADP version 2 is an update of the initial ADP written at the start of the project. It reports on the status of the algorithm developments performed during the first two cycles of the project and includes plans for the third project cycle as part of the project extension until the end of 2026. The document covers all aspects of the retrieval algorithms including forward models used for the retrieval, treatment of a-priori information, cloud correction approaches, surface reflectance treatment, etc. Note that the list of planned developments is informative and not meant to be binding, since modifications to the original plans can happen in the course of the project according to needs.

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

[AD-2] CCI Data Policy v1.1. Available online at: https://climate.esa.int/sites/default/files/CCI_Data_Policy_v1.1.pdf

1.4 Reference documents

[RD-1] GCOS Climate Monitoring 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-128, March 2009 (WMO/TD No. 1488). Available online at: https://library.wmo.int/index.php?lvl=notice_display&id=12884#.Yw4rL7RByUk

[RD-3] Quality assurance framework for earth observation (QA4EO): http://qa4eo.org

[RD-4] The Global Observing System for Climate: Implementation Needs, GCOS-200, October 2016. Available online at: https://gcos.wmo.int/en/gcos-implementation-plan

[RD-5] Status of the Global Observing System for Climate, GCOS-195, October 2015. Available online at: https://library.wmo.int/index.php?lvl=notice_display&id=18962#.Yw4r8LRByUk

[RD-6] 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-7] 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: https://www.iso.org/sites/JCGM/GUM-JCGM100.htm

[RD-8] Merchant, C., et al., 2017, Uncertainty information in climate data records from Earth observation, Earth Syst. Sci. Data Discuss., vol. 9, p511-527

1.5 List of acronyms

AC-SAF	Satellite Application Facility on Atmospheric Composition Monitoring
ADP	Algorithm Development Plan
AK	Averaging Kernel
AMF	Air-mass factor
ATBD	Algorithm Theoretical Basis Document
BIRA-IASB	Royal Belgian Institute for Space Aeronomy
BIRA-IR	BIRA-IASB Infrared Team
BIRA-SYN	BIRA-IASB Synergy Team
BIRA-UVVIS	BIRA-IASB UV-Vis Team
BIRA-MOD	BIRA-IASB Tropospheric Modeling Team
CAMS	Copernicus Atmospheric Monitoring Service
C3S	Copernicus Climate Change Monitoring Service
CCI	ESA Climate Change Initiative
CCI+	Climate Change Initiative Extension (CCI+), is an extension of the CCI over the period 2017-2024.
CEOS	Committee on Earth Observation Satellites
CMUG	Climate Modeling User Group
CHOCHO	Glyoxal
CO	Carbon monoxide
COBRA	COvariance-Based Retrieval Algorithm
CRDP	Climate Research Data Package
CRG	Climate Research Group

DLR	German Aerospace Centre
DOAS	Differential Optical Absorption Spectroscopy
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
FCDR	Fundamental Climate Data Record
FRESCO	Fast Retrieval Scheme for Clouds from the Oxygen A band
GCOS	Global Climate Observation System
GE-LER	Geometry-Dependent effective Lambertian Equivalent Reflectivity
GEMS	Geostationary Environmental Satellite Instrument
GEO	Geostationary orbit
GOME	Global Ozone Monitoring Instrument (aboard ERS-2)
GOME-2	Global Ozone Monitoring Instrument – 2 (aboard MetOp-A, -B and -C)
HCHO	Formaldehyde
IASI	Infrared Atmospheric Sounding Interferometer
IUP-UB	Institute of Environmental Physics, University of Bremen
HRI	Hyperspectral Range Index
KNMI	Royal Netherlands Meteorological Institute
L2	Level-2 (orbit-based) data product
L3	Level-3 (gridded) data product
LEO	Low Earth Orbit
LER	Lambertian Equivalent Reflectivity
LUT	Look-up table
Metop	Meteorological Operational Platform (EUMETSAT)
MOPITT	Measurement of Pollution in the Troposphere
MPIC	Max Planck Institute for Chemistry , Mainz
NASA	National Aeronautics and Space Administration
NH_3	Ammonia
NN	Neural Network
NO_2	Nitrogen dioxide
NRT	Near-Real Time
OCRA	Optical Cloud Recognition Algorithm)
OMI	Ozone Monitoring Instrument (aboard EOS-Aura)
PCA	Principal Component Analysis
QA4ECV	Quality Assurance for Essential Climate Variables
QA4EO	Quality Assurance framework four Earth Observation
R&D	Research and Development
ROCINN	Retrieval of Cloud Information using Neural Networks
SAF	Satellite Application FacilityQA4EO
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric
S5P	Sentinel-5 Precursor

SoW	Statement of Work
STREAM	STRatospheric Estimation Algorithm from Mainz
SZA	Solar Zenith Angle
TEMIS	Tropospheric Emission Monitoring Internet Service
TIR	Thermal Infrared spectral range
TROPOMI	Tropospheric Monitoring Instrument (aboard Sentinel-5 Precursor)
TOA	Top-of-atmosphere
ULB	Université Libre de Bruxelles
UPAS	Universal Processor for UV/Vis Atmospheric Sensors
UV-Vis	Ultraviolet and visible spectral range
WP	Work Package

2 Algorithm development plan

2.1 Overview

The general objective of the project is to develop and demonstrate new long-term multi-mission data sets for six important precursors of ozone and aerosol ECVs, namely: NO_2, HCHO, CO, SO_2, NH_3 and glyoxal. The purpose of algorithm developments is to progress towards meeting requirements specified by GCOS for these variables, and more importantly to address requirements expressed by users for these data products. Algorithm developments are addressed in two successive cycles of activities, as requested by ESA.

In the first cycle, the focus will be on L2 data product developments for all trace gases. More specifically for UV-Vis gases (NO_2, HCHO and SO_2), a round-robin intercomparison of retrieval approaches in use in the community will be performed with the aim of defining a common baseline applicable in a consistent way to all historical and current sensors. This exercise will bring together retrieval experts active in QA4ECV, AC-SAF as well as the Sentinel 4 and 5/5P projects. One key motivation of the round-robin is to reconcile retrieval approaches that were so far independently developed in the QA4ECV and AC-SAF projects, with the aim to harmonise products from all sensors including GOME-2 data records operationally produced within the AC-SAF. An outcome of this activity will be the implementation of new/updated retrieval baselines in the AC-SAF, consistent with the CCI ones. Next to the round-robin intercomparison, specific L2 developments will also take place for each target molecule as detailed in section 2.2 below.

In the second cycle, algorithmic developments will progressively evolve from L2 to L3 data products, the latter being obtained by spatial and temporal aggregation of L2 data from single and multiple sensors. In doing so, the team will address questions such as bias correction between different satellites, long-term drifts, the handling of the varying spatial resolutions and overpass times of the sensors, or the impact of the varying sampling characteristics of the data sets. Given the generic nature of the problems associated with data aggregation and merging techniques, an internal consultation will be organized bringing together all the retrieval experts available in the project. Possible methods and approaches will be discussed and evaluated/tested for implementation in this project, considering the characteristics of the different trace gases and the level of maturity of corresponding L2 data sets. Based on these developments, final retrieval baselines will be defined and applied for a large-scale processing.

In the third cycle, the range of the activities carried out under the baseline Precursors_cci portfolio will be extended in two ways. First, we will extend the round-robin of UV-Vis trace retrievals to deepen important aspects of the retrievals. This concerns the treatment of bidirectional surface reflectivity effects on both trace gas and cloud retrievals as well as details of the separation between tropospheric and stratospheric layers of the atmosphere, which both critically impact the accuracy and interpretation of NO_2 measurements from space. Second, new capabilities extending the scope of our CDRs will be introduced. First a new CDR focusing on volcanic SO_2 emissions will be developed. Second, a set of trace gas data products

will be derived from existing GEO sonders using algorithms developed in the first phases of the project. The aim is to integrate them, after validation, in the current CDR data sets. This will provide new information on the diurnal variation of the target trace gases (NO_2, HCHO, SO_2, CO and NH_3).

2.2 Detailed development plan for each trace gas product

2.2.1 Round-robin on NO_2, HCHO and SO_2 retrievals

Round-robin activities during the first development cycle (Jul 2022 – Dec 2023)

At project start, a variety of different retrievals exist for each of the three UV-Vis trace gases of interest. For both historical and practical reasons, the retrievals also vary from instrument to instrument, which limits the usability of the datasets as consistent climate data records. In the context of the QA4ECV project (2014-2018) as well as with the AC SAF, significant efforts were performed to harmonise and optimize NO_2 and HCHO data products, but these developments were independent from each other and did not address the same list of sensors. This motivates the organisation of a round-robin of UV-Vis trace gas retrieval algorithms. This activity will develop over the first project cycle and will be coordinated by IUP-UB.

For NO_2 and HCHO retrievals, the overall approach is to take data from two existing climate data sets for the same instrument (GOME-2A) and to compare all aspects of the retrievals thoroughly. Results from the earlier projects will be used and re-evaluated in the light of recent developments from the TROPOMI projects and from the literature. A limited set of options will be evaluated for each of the retrieval steps (see details given in specific sections below) to come to recommendations for all of them which can then be implemented as project baselines. For SO_2, the round-robin takes a slightly different form and concentrates on an evaluation of two different but similarly performant algorithms (COBRA and PCA) as well as on an analysis of different retrieval options to deal with strong volcanic signals.

The choice of time periods to be evaluated will be the first step of the round robin. A combination of two approaches is foreseen: (1) selection of individual days in all four seasons for which global comparisons can be performed and (2) selection of smaller regions for which time series can be analysed. This approach allows evaluation of spatial dependencies as well as long-term changes with reasonable computational effort.

To come to qualified recommendations for selection of baseline approaches, validation will be used where possible. In other cases, aspects such as plausibility of results, consistency between instruments and over time, traceability of inputs and approaches, availability of input data for the full time series, and practical considerations such as complexity and computational cost of different options will be considered. The feasibility of implementing recommendations in the operational TROPOMI algorithms for NO_2, SO_2, and HCHO will be limited, as these retrievals are developed and maintained in an operational environment, and

follow their own cycles of improvement. The final decision will be taken by all participants of the round robin including the validation team in consensus. The WP leader will have the last word in the improbable case that no agreement can be found. Reasons for the choices will be documented for traceability.

Table 2-1: List of round-robin activities during the first development cycle

Task ID	Description	Contributors	Status
RR-T01	Collection of existing satellite data sets	IUP-UB, BIRA-UVVIS, KNMI, DLR	Closed
RR-T02	Collection of validation reference measurements	BIRA-SYN	Closed
RR-T03	For NO_2, HCHO: comparison of slant columns	IUP-UB, BIRA-UVVIS, KNMI, DLR	Closed
RR-T04	For SO_2: Comparison of COBRA and PCA results	BIRA-UVVIS	Closed
RR-T05	For all gases: Systematic comparison of effects of different choices for ○ stratospheric correction / background correction ○ cloud correction approaches ○ surface reflectivity data bases ○ a-priori profiles used	IUP-UB, BIRA-UVVIS, KNMI, DLR	Closed
RR-T06	For SO_2: Special evaluation of results for volcanic SO_2 signals	BIRA-UVVIS	Closed
RR-T07	For each of the products and components, derive consensus recommendation for CDR based on validation data (where available), consistency analysis and expert judgment	IUP-UB, BIRA-UVVIS, KNMI, DLR	Closed

Round-robin activities during the third development cycle (Jul 2025 – Dec 2026)

In the third cycle, the round-robin activities will be extended with (1) a more advanced treatment of the directional surface reflectance, and (2) the development of an improved NO_2 background correction scheme focusing on the case of GEO sensors (GEMS). The scope of this activity is to generate improved methodologies for stratospheric NO_2 correction and air mass factor calculations that can be used to refine NO_2 and CHOCHO algorithms (since both gases are retrieved in the same wavelength range).

Concerning the directional surface reflectance, the KNMI DLER and DLR GE-LER databases (available at both 440 nm and 340 nm) will be intercompared with the aim to highlight their strengths and weaknesses and evaluate the way they impact cloud and trace gas retrievals. The impact of the directional surface reflectivity on cloud parameters from FRESCO and OCRA-ROCINN will also be evaluated. The update from using coarse-scale LER surface reflectance climatologies to high-resolution directional LER database is anticipated to substantially impact cloud parameters and trace gas AMFs.

As regards the stratospheric NO_2 correction, specific challenges for geostationary satellites will be investigated: in particular (1) the fact that fewer remote regions are covered, and (2) the diurnal cycle of stratospheric NO_2 matters more than for LEO, since measurements are performed for varying local time. Planned activities include the development of an observation-based algorithm for the estimation of stratospheric NO_2, similar as STREAM, and application to GEMS data. Various intercomparisons will be conducted involving the GEMS operational product (NO_2 v3.0), the GEMS IUP-UB using STREAM, and the baseline GEMS IUP-UB using model data for the stratospheric correction. The level and spatial patterns of the tropospheric columns will be checked for plausibility over remote regions as well as the diurnal cycles of stratospheric and tropospheric columns. The goal will be to identify potential problems/biases in stratospheric correction for GEMS and quantify the uncertainty of tropospheric columns over clean regions due to stratospheric correction.

Table 2-2: List of round-robin activities during the third development cycle

Task ID	Description	Contributors	Status
RR-T08	Advanced treatment of directional LER	KNMI, DLR	Open
RR-T09	Improved NO_2 background correction scheme	MPIC, KNMI, IUP-UB	Open

2.2.2 NO_2 development plan

Detailed tasks planned during the first development cycle (Jul 2022 – Dec 2023)

In the first phase of the project, the focus will be on the NO_2 Round Robin exercise based on the GOME-2A sensor. The reason is that two different, state-of-science approaches exist for this sensor: the QA4ECV-algorithm processed by KNMI (and also the basis for the operational S5P algorithm) and the AC SAF algorithm processed by DLR. Improving our understanding of the main differences between these two independent approaches and their algorithmic impacts has good potential to achieve harmonization between AC SAF and QA4ECV efforts within the ESA CCI+ project. The NO_2 Round Robin will address all steps of the retrieval algorithm: spectral fitting, stratosphere-troposphere separation, and the AMF calculation, including the selection of input parameters.

Table 2-3: List of NO_2 development tasks planned during the first development cycle

Task ID	Description	Contributors	Status
NO2-T01	Compare GOME-2A slant columns from AC SAF and QA4ECV (provided by KNMI) for multiple days, and assess differences	DLR, KNMI	Closed
NO2-T02	Intercompare STREAM and data assimilation stratospheric NO_2 columns from GOME-2A (and if feasible from TROPOMI) for a number of selected days. For those days, compare stratospheric NO_2 estimates with independent validation data on stratospheric NO_2 columns.	KNMI, DLR, BIRA-SYN	Closed

NO2-T03	Compare GOME-2A cloud parameters from the AC-SAF (OCRA-ROCINN) and QA4ECV (FRESCO+) approaches for multiple days. Assess differences and their impact on tropospheric NO2 AMFs	KNMI, DLR	Closed
NO2-T04	Evaluate currently available surface reflectance climatologies (from GOME-2A, OMI and S5P) and their fitness-for-purpose in terms of consistency, robustness, resolution, and temporal degradation to serve as a priori input parameters in the NO_2 algorithm	IUP-UB, KNMI, DLR	Closed
NO2-T05	Compare and evaluate different options for a priori NO_2 profiles to be used in the NO_2 algorithm. A priori vertical distributions from TM5-MP, CAMS, and the AC-SAF will be assessed in terms of spatial resolution, vertical layering, seasonality and trends	IUP-UB, KNMI, DLR	Closed

Planned developments for the second development cycle (Jan 2024 – Jun 2025)

Based on the outcome of the Round Robin activities performed in phase 1, final algorithm choices will be made, and the selected scheme will be applied to the multi-satellite data record.

From the resulting L2 single-mission datasets, L3 data sets will be generated. This will be achieved by spatial and temporal binning of the data according to a format compliant with CCI guidelines.

- DLR will develop functional methods to homogenize the individual L3 NO_2 dataset for the morning sensors GOME, SCIAMACHY, and GOME-2A/B/C, and to generate a merged product.
- KNMI will develop methods to generate a consistent L3 dataset for the afternoon sensors OMI and S5P, as well as GOME, SCIAMACHY and GOME-2A for comparison with the DLR set. IUP-UB will guide the DLR and KNMI L3 approaches in terms of consistency and fitness-for-purpose in accounting for bias correction and long-term drifts between the satellites, spatial resolution differences, different overpass times, and sampling issues (e.g. row anomaly, cloud cover).

Table 2-4: List of NO_2 development tasks planned during the second development cycle

Task ID	Description	Contributors	Status
NO2-T06	Based on lessons learned from the round robin, validation and user requirements, final set-up of the NO_2 L2 algorithm including the selection of the spectral fitting approach, stratosphere-troposphere separation scheme, and selected ancillary datasets: albedo database, choice of a priori profiles time	KNMI, DLR, IUP-UB	Closed

	series, choice on the cloud product and cloud correction technique.		
NO2-T07	Updated L2 algorithm for each satellite instrument (GOME, SCIAMACHY, OMI, TROPOMI) (lead: KNMI) and an updated version of the AC-SAF GOME-2 algorithm (lead: DLR).	KNMI, DLR	Closed
NO2-T08	Investigation of inter-satellite consistency.	KNMI, DLR	Closed
NO2-T09	The L3 algorithms will be developed in parallel. This part of the work will address questions such as the correction of inter-sensor biases and long-term drifts, the handling of the different spatial resolutions and of the different overpass times. We will consider the possibility to include auxiliary data in support to users (orbit-level time, uncertainties, sampling rates). We will also consider feedback from C3S and CAMS users to match their needs in terms of format and required information. The expected output is an updated version of the L3 algorithms.	KNMI, DLR	Closed

Planned developments for the third development cycle (July 2025 – Dec 2026)

The objective is to develop NO_2 retrieval algorithms for the GEMS geostationary sensors and make them consistent with the NO_2 retrieval baseline used for LEO sensors in the first phases of the project.

Table 2-5: List of NO_2 development tasks planned during the third development cycle

Task ID	Description	Contributors	Status
NO2-T10	Evaluation of existing GEMS L2 NO_2 products	IUP-UB	Open
NO2-T11	Calculation of look-up tables of altitude-dependent AMFs for NO_2 (440 nm) suitable for the GEO geometry and comparison between MONKI and SCIATRAN LUTs	KNMI, IUP-UB	Open
NO2-T12	Application of the CCI NO_2 retrieval baseline to GEMS data, and assessment of the consistency with existing products	IUP-UB, KNMI	Open
NO2-T13	Sensitivity studies on GEMS NO_2 retrievals	IUP-UB, KNMI	Open

2.2.3 HCHO development plan

Detailed tasks planned during the first development cycle (Jul 2022 – Dec 2023)

As for NO_2, the focus in the first phase will be on the HCHO round-robin. For HCHO, algorithmic developments build on a solid heritage from the QA4ECV project, the TROPOMI L2 processor development and the AC SAF operational GOME-2 products. The OMI and TROPOMI algorithms have been developed in parallel. The consistency between those two "afternoon" HCHO datasets was studied in detail, and reasons for the remaining differences were identified (De Smedt et al., 2021). The "morning" QA4ECV datasets share mostly the same settings as OMI. However, they have not been validated, and their long-term consistency was not evaluated yet. The GOME-2 AC SAF HCHO products differ from the QA4ECV and TROPOMI retrievals on several aspects that need to be revisited. These products have the advantage to be operational and to cover the three GOME-2 instruments.

The development activities for the HCHO algorithm are closely aligned with the Round Robin activity. Except for GOME-2, they will mainly focus on air mass factors and background correction, because of the high level of maturity of the slant column retrievals reached in the QA4ECV and TROPOMI products.

Table 2-6: List of HCHO development tasks planned during the first development cycle

Task ID	Description	Contributors	Status
HCHO-T01	Analysis of current state-of-the art L2 datasets, known issues and user requirements. Furthermore, the QA4ECV OMI L2 dataset will be extended beyond 2020 (currently provided on the QA4ECV website) (single-mission L2 data sets).	BIRA-UVVIS	Closed
HCHO-T02	A first version of the L3 CDR will be generated, focusing on known issues that can be handled using post-processing techniques (HCHO-T01: improved quality filtering, reported uncertainties, cloud filtering and threshold for cloud correction). Input to the validation and the round-robin.	BIRA-UVVIS	Closed
HCHO-T03	Compare GOME-2A slant columns from AC SAF and QA4ECV (provided by BIRA) for multiple days and assess differences. DOAS settings will be aligned as much as possible. Suggested periods: burning seasons or similar events.	DLR, BIRA-UVVIS	Closed
HCHO-T04	Compare GOME-2A cloud parameters from the AC-SAF (OCRA-ROCINN) and QA4ECV (FRESCO+) approaches for multiple days. Assess differences and their impact on HCHO AMFs. BIRA-SYN will estimate changes in cloud parameters using the Cloudnet network, and their impact on ground-based validation results.	BIRA-SYN, DLR	Closed
HCHO-T05	Evaluate currently available surface reflectance climatologies (from GOME-2A, OMI and S5P) and their fitness-for-purpose in terms of consistency,	BIRA-UVVIS, DLR	Closed

	robustness, resolution, and temporal degradation to serve as a priori input parameters in the HCHO algorithm		
HCHO-T06	Compare and evaluate different options for a priori HCHO profiles to be used in the HCHO algorithm. A priori vertical distributions from TM5-MP, CAMS, and the AC-SAF will be assessed in terms of spatial resolution, vertical layering, seasonality and long-term consistency. BIRA-SYN will make independent validation based on a selection of HCHO profiles measured by MAX-DOAS instruments.	BIRA-UVVIS, KNMI, BIRA-SYN	Closed
HCHO-T07	Harmonization of the background correction procedure, with the aim to mitigate bias and long-term drift of the AC-SAF products (GOME-2) and those from other sensors included in the CDR.	BIRA-UVVIS, DLR	Closed
HCHO-T08	Provide test data processed with an internal version of the improved AC SAF operational algorithm (based on UPAS-2), applied to test days selected for GOME-2A, B and C (HCHO-T03, HCHO-T04, HCHO-T05, HCHO-T06, HCHO-T07).	DLR, BIRA-UVVIS	Closed

Planned developments for the second development cycle (Jan 2024 – Jun 2025)
The development activities for the HCHO algorithm (lead: BIRA-IASB) are closely aligned with the Round Robin activity. Except for GOME-2, they will mainly focus on air mass factors and background correction, because of the high level of maturity of the slant column retrievals reached in the QA4ECV and TROPOMI products.

It is worth mentioning that within the AC-SAF (CDOP-4), L3 CDR developments based on the 3 GOME-2 instruments are foreseen for NO_2 (lead: DLR) and HCHO (lead: BIRA-IASB). Those developments will happen in parallel with the CCI+ activities, and will be coordinated between DLR and BIRA-IASB to be complementary and to be used directly in the CCI+ CDR.

Table 2-7: List of HCHO development tasks planned during the second development cycle

Task ID	Description	Contributors	Status
HCHO-T09	Based on lessons learned from the round robin as well as the outcome from validation and user requirements, final set-up of the HCHO L2 algorithm including the selected ancillary datasets: update of the LER database, choice of a priori profiles time series, choice on the cloud product and cloud correction technique.	BIRA-UVVIS, DLR	Closed
HCHO-T10	Updated L2 algorithm for each satellite instrument (GOME, SCIAMACHY, OMI, TROPOMI) (lead: BIRA-	BIRA-UVVIS, DLR	Closed

	IASB) and an updated version of the AC-SAF GOME-2 algorithm (lead: DLR).		
HCHO-T11	Investigation of inter-satellite consistency.	BIRA-UVVIS, BIRA-SYN	Closed
HCHO-T12	The L3 algorithms will be developed in parallel. This part of the work will address questions such as the correction of inter-sensor biases and long-term drifts, the handling of the different spatial resolutions and of the different overpass times. We will consider the possibility to include auxiliary data in support to users (orbit-level time, surface temperature, CCI fire product). We will also consider the feedback from C3S and CAMS users to match their needs in terms of format and required information. The expected output is an updated version of the L3 algorithms.	BIRA-UVVIS, DLR	Closed

Planned developments for the third development cycle (July 2025 – Dec 2026)

The objective is to develop a HCHO retrieval algorithm for GEMS and make it consistent with the HCHO retrieval baseline used for LEO sensors in the first phases of the project.

Table 2-8: List of HCHO development tasks planned during the third development cycle

Task ID	Description	Contributors	Status
HCHO-T13	Evaluation of existing GEMS L2 HCHO product(s)	BIRA-UVVIS	Open
HCHO-T14	Application of the CCI HCHO retrieval baseline to GEMS data, and assessment of the consistency with existing product(s)	BIRA-UVVIS	Open
HCHO-T15	Sensitivity studies on GEMS HCHO retrievals	BIRA-UVVIS	Open

2.2.4 SO_2 development plan

Detailed tasks planned during the first development cycle (Jul 2022 – Dec 2023)

Recently, a new algorithm to retrieve SO_2 using the so-called COBRA scheme was developed for TROPOMI (Theys et al., 2021). Those results show that COBRA significantly improves the product quality both in terms of noise and bias, and for this reason we decided to use COBRA as a baseline for SO_2 slant column fitting in CCI+. First comparisons with an experimental SO_2 PCA implementation for TROPOMI (available from NASA) indicates similar and even slightly better performance by COBRA. In this first phase, the focus will therefore be on a round-robin

intercomparison involving both PCA and COBRA algorithms. Other aspects of the retrieval will also be investigated, similarly as for HCHO and NO_2.

Table 2-9: List of SO_2 development tasks planned during the first development cycle

Task ID	Description	Contributors	Status
SO2-T01	Comparison of SO_2 SCDs retrieved from OMI using COBRA and PCA algorithms, for a limited set of data focusing on anthropogenic scenes. Assess differences and eventually come up with improved settings. OMI will also be included as reference point to assess the benefit of COBRA and PCA over a DOAS approach. Data set envisaged for this comparison: one full month in each season of two years, at the beginning and later in the OMI mission to test the impact of the row anomaly.	BIRA-UVVIS, NASA	Closed
SO2-T02	Based on SO2-T01, specific developments addressing (a) the extension of COBRA to alternative windows (used for volcanic eruptions), (b) improvement of the robustness of the covariance data in case of strong contamination by volcanic SO_2 and possibly development of a fallback solution, (c) work towards a proper quality assurance flag, (d) the adaptation of the algorithm to predecessor sensors (GOME-1, SCIAMACHY, OMI).	BIRA-UVVIS	Closed
SO2-T03	Based on the latest developments of SO2-T02, the COBRA spectral fitting step will be tested on GOME-1 and/or SCIAMACHY (preliminary results).	BIRA-UVVIS	Closed
SO2-T04	In conjunction with other trace gases involved in the round-robin, re-evaluation of SO_2 AMF calculation schemes. This will concern: (a) Evaluation of a-priori SO2 profiles from TM5-MP and CAMS in terms of spatial resolution, vertical layering and long-term consistency. BIRA-SYN will make independent validation based on a selection of SO_2 profiles measured by MAX-DOAS instruments. (b) Evaluation of different surface reflectance climatologies in the UV region as well as different possible treatment of snow/ice (important for some SO_2 point sources at high latitudes in Asian countries). (c) Consider application/adaptation of best practices for cloud treatment derived from other molecules (NO_2, HCHO), through a limited number of tests.	BIRA-UVVIS, BIRA-SYN	Closed

SO2-T05	Optimisation of SCD and VCD results for volcanic eruptions, in case of large SO_2 signals through use of different fitting windows avoiding saturation effects. This aspect will be revisited through comparison of SCDs and VCDs from OMI, TROPOMI, GOME-2 by varying the fitting windows used and fitting window selection criteria. The AC-SAF GOME-2 operational products will also be used for this exercise. Data set envisaged for the comparison: maximum 2-5 completed days for a limited number of volcanic events.	BIRA-UVVIS, DLR	Closed

Planned developments for the second development cycle (Jan 2024 – Jun 2025)

From the project schedule, it is anticipated that several of the SO2 Round-robin activities listed above will continue beyond the first contractual phase. In addition to those tasks, further development of the algorithm is planned, essentially to adapt the COBRA scheme to past missions (GOME and SCIAMACHY) and to improve on the airmass factor calculations and error estimates. Once the algorithm is finalized, the production of L2 datasets will be undertaken.

From the resulting L2 single-mission datasets, L3 data sets will be generated. This will be achieved by spatial and temporal binning of the data according to a defined format.

In addition to single-mission L3 SO_2 data, efforts to create merged L3 data will be undertaken for the anthropogenic and volcanic degassing at the level of the expressed user needs.

Table 2-10: List of SO_2 development tasks planned for the second development cycle

Task ID	Description	Contributors	Status
SO2-T06	Improvement of air mass factor calculations. This includes (a) an update of the AMF look-up-table and error analysis module, (b) revisiting the ancillary data and their long-term consistency (following Round-robin outcome).	BIRA-UVVIS	Closed
SO2-T07	Adaptation of the algorithm to predecessor sensors (GOME-1, SCIAMACHY, OMI). This includes (a) the use of a separate tool of wavelength calibration, specific to each sensor, (b) setting up the COBRA framework for each sensor and defining the settings considering the instrumental specificities, (c) applying the air mass factor calculation and error analysis modules to each sensor.	BIRA-UVVIS	Closed
SO2-T08	Definition of L2 output format and production single mission L2 SO_2 products	BIRA-UVVIS	Closed

SO2-T09	Investigation of the inter-satellite consistency of the resulting VCD data records and performing other sat-sat comparisons. Support to validation efforts	BIRA-UVVIS, BIRA-SYN	Closed
SO2-T10	The L3 algorithms will be developed in parallel. This part of the work will address questions such as the correction of inter-sensor biases and long-term drifts, the handling of the different spatial resolutions and of the different overpass times.	BIRA-UVVIS	Closed

Planned developments for the third development cycle (July 2025 – Dec 2026)

Two main activities are planned during the third cycle: (1) to develop a multi-platform SO_2 climate data record focusing specifically on volcanic eruptions, and (2) to develop a GEMS SO_2 retrieval algorithm consistent with the CCI SO_2 retrieval baseline developed for LEO sensors.

Table 2-11: List of SO_2 development tasks planned during the third development cycle

Task ID	Description	Contributors	Status
SO2-T11	Selection of major volcanic eruptions in the timeframe 1995-2022	DLR, BIRA-UVVIS	Open
SO2-T12	Extract SO_2 plume height information from the MSVOLSO2L4 dataset and recalculate VCDs with the proper plume height information	DLR	Open
SO2-T13	Development of homogenization and merging algorithms applicable to the GOME, SCIAMACHY, GOME-2 and TROPOMI sensors	DLR, BIRA-UVVIS	Open
SO2-T14	Evaluation of existing GEMS L2 SO_2 product(s) with respect to the (GCOS) requirements.	BIRA-UVVIS	Open
SO2-T15	Application of the CCI SO_2 retrieval baseline to GEMS data for the spectral fitting (COBRA), AMFs, and assessment of the consistency with existing LEO product(s)	BIRA-UVVIS	Open
SO2-T16	Sensitivity studies on the observed diurnal variation and dependence with ancillary data	BIRA-UVVIS	Open
SO2-T17	Approach to integrate GEMS data (1 year) into the existing CCI SO_2 CDR	BIRA-UVVIS	Open

2.2.5 CO development plan

Detailed tasks planned during the first development cycle (Jul 2022 – Dec 2023)

The first cycle will focus on obtaining two separated CO records (MOPITT and IASI), and to analyse the overlapping time series, which extend from 2007 to now. During this cycle a thorough investigation of the differences between the three IASI CO datasets will be done. Note that in the framework of the EUMETSAT AC-SAF project the IASI CO was reprocessed

backwards, with homogeneous temperature and water vapour profiles. This is a major upgrade as compared to the former IASI CO record that was analysed in the framework of QA4ECV, as the CO time series is now fully consistent over time.

Table 2-12: List of CO development tasks planned during the first development cycle

Task ID	Description	Contributors	Status
CO-T01	Analysis of the entire IASI data record (~ 15 years) produced with consistent temperature, water vapor and cloud products. This product is generated using the FORLI retrieval algorithm (Hurtmans et al, 2012), and distributed through the Eumetcast system (AC SAF). For cloud contamination, the new cloud scheme developed at ULB will be applied (see the NH_3 section).	LATMOS	Closed
CO-T02	Use of the entire MOPITT version 9 data record (2000-now) reprocessed with the latest version of the algorithm (Deeter et al., 2021) for co-localisation with IASI data over ~10 areas representative of different emission activities (city pollution, biomass burning areas, remote ocean, background CO, etc). The differences with IASI retrievals will be assessed.	LATMOS	Closed

Planned developments for the second development cycle (Jan 2024 – Jun 2025)

In the second project cycle, both datasets (IASI and MOPITT) will be combined, using correction factors calculated from the a priori, and weighted according to the associated errors. The removal of clouds will be taken care with a new detection technique, developed in the framework of the IASI-FT EU project (Whitburn et al., 2022). This will improve the robustness of the record.

Gridded L3 total columns will then be produced on monthly timescales at a resolution of 1° x 1°. This will be done by combing MOPITT (2000-now) and for IASI/Metop-A (2007-2021), IASI/Metop-B (2013-now), IASI/Metop-C (2019-now), with correction bias factors and error weighting. As discussed during the negotiation phase and subsequent progress meetings, a comparative study of CO data from IASI, MOPITT, and TROPOMI will also be carried out.

Table 2-13: List of CO development tasks planned during the second development cycle

Task ID	Description	Contributors	Status
CO-T03	Combination of IASI CO and MOPITT CO data, with proper cloud filtering and error weighting. Correction factors will be delivered as a function of latitude and seasons, to match the 2 records as best as possible.	LATMOS	Closed
CO-T04	Generation of L3 IASI-MOPITT combined data, on a 1°x1° grid/monthly averages.	LATMOS	Closed

CO-T05	Comparison study of CO data from IASI, MOPITT, and TROPOMI.	LATMOS	Closed

Planned developments for the third development cycle (July 2025 – Dec 2026)

The objective is to develop a CO retrieval algorithm applicable to the GIIRS-B geostationary sensor, in preparation for IRS.

Table 2-14: List of CO development tasks planned during the third development cycle

Task ID	Description	Contributors	Status
CO-T06	Adaptation and application to GIIRS-B of a new CO algorithm (in preparation for IRS) based on deep learning techniques and capable to handle huge data flows	LATMOS	Open
CO-T07	Construction of new covariance matrices, based on IASI's heritage	LATMOS	Open
CO-T08	Extraction of meteorological input data from ERA5	LATMOS	Open
CO-T09	Development of cloud flagging approach.	LATMOS	Open

2.2.6 NH_3 development plan

Detailed tasks planned during the first development cycle (Jul 2022 – Dec 2023)

Table 2-15: List of NH_3 development tasks planned during the first development cycle

Task ID	Description	Contributors	Status
NH3-T01	Implementation of a new cloud detection algorithm (replacing the L2 from EUMETSAT by a cloud product that is consistent over the entire time-series). The cloud detection algorithm is currently under development (Whitburn et al., 2022).	ULB	Closed
NH3-T02	Implementation of a novel way to calculate the HRI which will lead to improved consistency over time and between the different instruments (with respect to e.g. instrumental calibrations and changing ambient CO_2 concentrations).	ULB	Closed
NH3-T03	Development of an algorithm for generating L3 gridded data (both on a monthly and daily basis) based on best practices available in the literature.	ULB	Closed
NH3-T04	Implementation of averaging kernels in the ANNI retrieval framework	ULB	Closed

Planned developments for the second development cycle (Jan 2024 – Jun 2025)

In the second cycle, we will investigate the need for tailored corrections to remove residual inconsistencies in the long-term IASI time series and across the different IASI instruments. These will be implemented if required.

Table 2-16: List of NH_3 development tasks planned during the second development cycle

Task ID	Description	Contributors	Status
NH3-T05	Assessment of residual inconsistencies/spurious trends in the long-term time series	ULB	Closed
NH3-T06	Development of second order corrections for all three IASI instruments	ULB	Closed

Planned developments for the third development cycle (July 2025 – Dec 2026)

In the third cycle, the objective is to develop a NH_3 retrieval algorithm applicable to the GIIRS-B geostationary sensor, in preparation for IRS. This activity will be performed by LATMOS, who takes over the NH_3 tasks of ULB in the last cycle of the project.

Table 2-17: NH_3 development tasks planned during the third development cycle

Task ID	Description	Contributors	Status
NH3-T07	Retrieval of NH_3 from the GIIRS-B atmospheric spectra. Required adaptations include mainly those related to instrumental characteristics (spectral range and resolution). Cross validation with IASI at 9:30 AM and PM will allow to optimize the consistency with the IASI CDR record.	LATMOS	Open

2.2.7 Glyoxal development plan

Detailed tasks planned during the first development cycle (Jul 2022 – Dec 2023)

Recently, glyoxal L2 data sets have been produced from OMI (2005-2018), TROPOMI (2018-2021), GOME-2A (2007-2017) and GOME-2B (2013-2020). While the BIRA-IASB algorithm has been directly used for OMI and TROPOMI, the GOME-2 data records have been generated as part of the AC-SAF activities, based on similar retrieval settings. No extension of those GOME-2A/B data sets or application to GOME-2C is planned as part of AC-SAF.

Table 2-18: List of Glyoxal development tasks planned during the first development cycle

Task ID	Description	Contributors	Status
GLY-T01	Application of the BIRA-IASB algorithm to GOME-2C to extend the time series of the mid-morning space glyoxal observations. This implies application of the full retrieval chain, i.e. spectral DOAS fits, AMF computations and application of normalization procedures.	BIRA-UVVIS	Closed

GLY-T02	Homogenization and update of input data for AMF computation: Reprocessing of a priori profiles with the latest version of MAGRITTE from 2005 onwards.	BIRA-TMOD	Closed
GLY-T03	Homogenization and update of input data for AMF computation: Evaluation of reprocessed MAGRITTE profiles (GLY-T02) by comparison with TM5 profiles on a limited period, which will help to better characterize the product uncertainties related to this input data.	IUP-UB	Closed
GLY-T04	Homogenization and update of input data for AMF computation: Investigation of existing state-of-the-art surface reflectance databases and selection considering key aspects such as the spatial resolution or the instrument overpass time. For this, we will take benefit of the outcome of the NO_2 round-robin activities (since NO_2 and glyoxal products are retrieved in the same spectral range).	BIRA-UVVIS	Closed
GLY-T05	Development of air mass factor calculation, background correction and uncertainty analysis tools, generic for all sensors.	BIRA-UVVIS	Closed
GLY-T06	Development of output formats in line with CCI conventions.	BIRA-UVVIS	Closed
GLY-T07	L3: development of single-mission spatial-temporal binning algorithm (v1).	BIRA-UVVIS	Closed

Planned developments for the second development cycle (Jan 2024 – Jun 2025)

Based on the L2 baseline defined in the first project phase, L2 data sets from OMI, TROPOMI and GOME-2 will be reprocessed and will serve as basis to generate L3 data sets for each instrument complemented by a single merged L3 CDR. Optimal methods to produce those data sets and to account for the different spatial resolutions and overpass times or for possible drifts/biases will be investigated in collaboration with the teams responsible for algorithmic developments of other molecules. The spatial and temporal binning of the data will be applied according to a defined format compliant with CCI guidelines.

Table 2-19: List of Glyoxal development tasks planned during the second development cycle

Task ID	Description	Contributors	Status
GLY-T08	Based on lessons learned from preliminary validation, evaluation of inter-satellite consistency and URDs, final set-up of the CHOCHO L2 algorithm including the selected set of ancillary data, refined error analysis modules, improved settings for all algorithmic modules.	BIRA-UVVIS	Closed
GLY-T09	L3: development of single-mission spatial-temporal binning (v2) and multi-mission merged product.	BIRA-UVVIS	Closed

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