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Ozone_cci+



**System Specification Document
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Executive Summary

The System Specification Document (SSD, deliverable D3.1) specifies the design of the operational system that generates and provides the Ozone ECV data products for CCI+. It includes an overall description of the main functions and scenarios. It consists of already available subsystems distributed over several organizations.

The products created in this context are ozone Essential Climate Variables, which are used for an assessment of the status of the ozone layer, climate forcing, health impact and other environmental issues.



SSD - System Specification Document

This document specifies the system requirements for the CCI+ O3 system.

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1 Introduction

1.1 Scope and Applicability

This document describes the operational Ozone_cci+ production system that handles the complete production processes and product provision procedures for the CCI+ Ozone ECV products. It also includes information regarding lifecycle and possible hardware solutions. The system specification in this document has been derived from the Algorithm Development Plan [AD3] of the Ozone_cci+ project.

The system specification does not include specifications needed for the product validation processes.

The processing system consists of a decoupled and fully distributed system spread over several organizations where each contributor uses pre-existing systems for the generation of the committed ozone data sets. Based on this architecture, the following ECV parameters will be generated:

The production processes shall ensure the generation of the following ozone ECV parameters:

- Total ozone from UV nadir instruments,
- Low vertical resolution ozone profiles from nadir sensors and
- Ozone profiles from limb and occultation instruments
- Tropospheric ozone from (combined) nadir, limb, and occultation instruments

1.2 Definitions, Acronyms and Abbreviations

Terms, definitions and abbreviations are collected within this document.

1.2.1 Terms and Definitions

Nominal Operation	The day to day operations, 98% of the time the system is operational
Ozone_cci+	ESA project for the development of the CCI ECV Ozone
Processor	Software implementing retrieval algorithms and running in the Ozone_cci+ system to produce intermediate or ECV products
Status Feedback	Automated status reports generated by the Ozone_cci+ system and provided to the Ozone_cci+ operator

1.2.2 Abbreviations

API	Application Programming Interface
ADM	Algorithm Development Management
CCI	Climate Change Initiative
CCI+	Climate Change Initiative +
CRG	Climate Research Group
CMUG	Climate Modelling User Group
ECMWF	European Centre for Medium-Range Weather Forecasts
ECV	Essential Climate Variable
ESA	European Space Agency
LP	Limb Profile
MZM	Monthly Zonal Mean



NP	Nadir Profile
O3	Ozone
O3TC	Ozone Total Column
O3NP	Ozone Nadir Profile
O3LP	Ozone Limb Profile
OS	Operating System
PDU	Product Dissemination Unit
PSD	Product Specification Document
PM	Production Management
UML	Unified Modeling Language
VALT	Validation Team or Group
VQM	Validation & QA Management
SET	System Engineering Team within the Ozone_cci+ project
tbc	to be collected
tbd	to be defined (shall be defined later if the information is available)
TC	Total Column
TrOC	Tropospheric Ozone Column

1.3 Applicable Documents

- [AD1] CCI Data Standards v2.3, ref: CCI-PRGM-EOPS-TN-13-0009, 26 July 2021, available online at: https://climate.esa.int/media/documents/CCI_DataStandards_v2-3.pdf
- [AD2] CCI Data Policy v1.1, ref: CCI-PRGM-EOPS-TN-13-0019, 12 July 2013, available online at: https://climate.esa.int/media/documents/CCI_Data_Policy_v1.1_NpCLUbi.pdf
- [AD3] Ozone_cci+ Algorithm Development Plan (ADP) v2.1, ref: Ozone_cci+_D2.3_ADP_v2.1_20231004, 4 October 2023, available online at: https://climate.esa.int/media/documents/Ozone_cci_D2.3_ADP.v2.1.pdf
- [AD4] Ozone_cci+ System Specification Document (SSD) v2.0, 7 April 2022, available online at: https://climate.esa.int/documents/1730/SSD_Ozone_cci_2.0_draft_v1.pdf

1.4 Reference Documents

- [RD1] 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: <http://library.wmo.int>

1.5 Document Overview

Chapter 2 contains the purpose and the scope of the Ozone_cci+ system.

Chapter 3 describes the design approach.

Chapter 4 gives an overview about the Ozone_cci+ system.

Chapter 5 lists the fundamental operations and the main operational scenarios.



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Chapter 6 shows the component decomposition.

Chapter 7 gives an overview about the input, intermediate and output products which are handled during CCI+ phase.



2 General Description

2.1 Relation to Current Projects

The Ozone_cci+ project (2019-present) further develops the ozone ECVs generated in the previous phases of the Ozone_cci project (2010-2017). In Ozone_cci+, the following new sensors are taken into consideration

- GOME2-C
- S5P
- POAM-III
- SAGE-III-M
- SAGE-III-ISS

2.2 Function and Purpose

The operational Ozone_cci+ system shall generate and update the ozone ECVs as specified in the ADP ([AD3]). The ECVs shall be based on existing ECVs from previous Ozone CCI phases and shall be extended by existing level 1 and/or level 2 data and auxiliary data. Level 2 processing and re-processing shall be possible if required in order to generate the new ozone ECV output products.

2.3 Relation to other Systems and End Users

The Ozone_cci+ system requires interfaces to organizations which provide level 1 and ancillary data for generating the ECV products, and to organizations which provide ground-based reference data for validation procedures. The output products shall be provided to the predefined end users.



3 Design Approach

This chapter describes the approaches used for the descriptions of the scenarios, system components and interfaces. UML diagrams are used for the description of the design. Additionally, non-UML diagrams and techniques are used where appropriate. The most often used diagrams are the context diagram and the sequence diagram.

3.1 Component Description Approach

Typically, the context diagram is used in the overview of each design document to describe the usage environment of the system or the system components. Data/control flow diagrams are used where complex structures of components or elements interact together.

After decomposition of Ozone_cci+ system into individual subsystems and components each of those subsystems is described as follows:

- Description
- Components or Processors
- Functions
- Interfaces
- Hardware

3.2 Scenario Description Approach

Sequence diagrams are used to describe the main usage scenarios relying on the functionality provided by the actors like operators, the system, components or elements.

Scenarios are sequences of events and activities for different use cases of a system. They describe the functions of a system on a certain level of abstraction. The scenarios are described for the Ozone_cci+ system, using the following approach:

- First, a short description is given on how the corresponding scenario is initiated and its purpose and scope.
- Optionally a sequence diagram is given and
- Finally, the flow of actions is described in a bulleted list, as an explanation to the sequence diagram.

3.3 Interface Description Approach

Each interface may consist of one or more interface items. The interface items are subdivided according to inputs and outputs of the subsystem.

An interface item covers an individual file, product or a method which is exchanged between components. A file or a product is easily understood as an interface item. A method is based on the concept of a client/server model.

The System Specification document lists all existing internal and external interfaces and interface items.

The PSD describes the format and content of the ECV output products.

Each interface item is specified by a fixed set of fields. Products are special kinds of interface items insofar as they are archived or distributed to users and / or external entities (e.g. validation systems). Therefore, a product specification is required to inform its users about the specific properties and performance characteristics of these products and to provide a detailed format specification which in general is much more sophisticated than for a normal interface item.



4 System Overview

The design of the Ozone_cci+ System is fundamentally influenced by the separation of the system functionality in three functional domains:

- Processing Domain
- Product Handling Domain
- Management Domain

Each functional domain in the functional decomposition is implemented by one or more dedicated service components. The functional domain and their components will be introduced in the subsections following this introduction.

The **Processing Domain** groups the functions regarding the product processing.

The Ozone_cci+ production system is defined by the use of already existing processing systems which are spread over different organizations. Each processing system is responsible for the production of one or more complete data sets which are either final or which are used by a subsequent processing step.

The **Product Handling Domain** is reduced to the provision of the generated data sets on an ftp server at BIRA (<ftp://ftp-ae.oma.be/esacci/ozone>) and CCI Open Data Portal (<https://climate.esa.int/en/projects/ozone/data>) in order to provide intermediate data sets to subsequent Ozone_cci+ processing systems and to provide all generated output products via online access to the users.

The **Management Domain** groups the management functions for the organization of the production and dissemination.

The Processing and the Product Handling Domains are subdivided into technical components. However, the Management Domain is substituted into administrative components.

4.1 System Decomposition

Figure 4-1 shows the technical and administrative components of the Ozone_cci+ system. The administrative components in the Management Domain and the Product Handling Domain are responsible for specific organisational operations. The technical components (yellow rounded rectangles) of the Processing Domain are provided by the specific science teams.

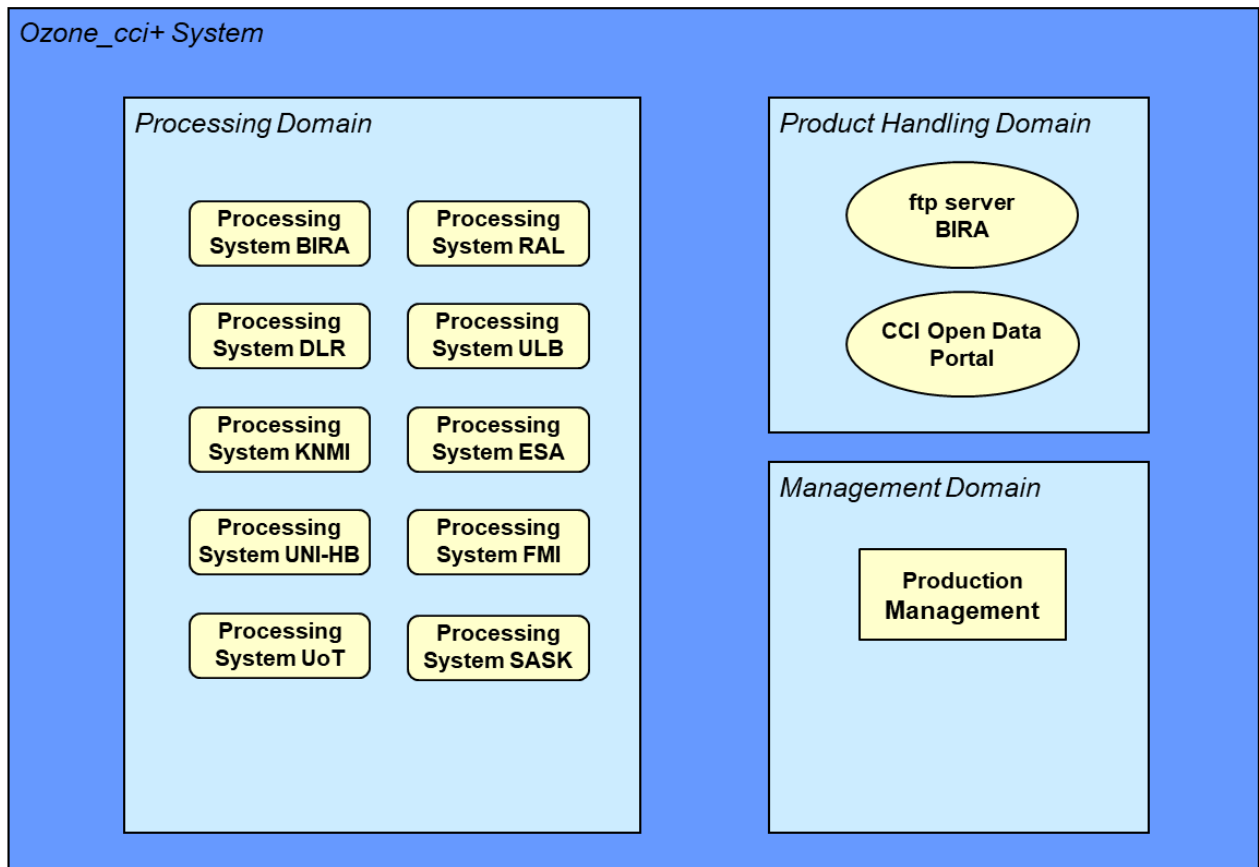


Figure 4-1 Ozone_cci+ System Decomposition into Domains

A detailed description of the functionality of the Ozone_cci+ components is described in chapter 6. An overview about their main functionalities is given in the following subchapters.

4.1.1 Processing Domain

The Processing Domain consists of:

- Processing System BIRA
- Processing System DLR
- Processing System FMI
- Processing System KNMI
- Processing System RAL
- Processing System UNI-HB
- Processing System ULB
- Processing System UoT
- Processing System SASK
- Processing System ESA

Some components of the individual processing systems are also used in the framework of the EU Copernicus Climate Change Service (C3S) ozone project. A description of the required input datasets and a detailed description of the algorithms is provided in the C3S ATBD (https://datastore.copernicus-climate.eu/documents/satellite-ozone/C3S2_312a_Lot2_ATBD_O3_latest.pdf)



4.1.1.1 Processing System BIRA

This processing system generates the L2 TC products for GOME2-A, -B, -C, OMI and OMPS-NM.

4.1.1.2 Processing System DLR

This processing system generates (a) L3 TC products for GOME2-A, -B, -C, OMI, OMPS-NM, and S5P, (b) L3 NP products for GOME2-A, -B and OMI, (c) the merged L3 TC (GTO-ECV) and NP (GOP-ECV) products, and (d) the merged TrOC product (GTTO-ECV).

4.1.1.3 Processing System RAL

This processing system generates the L2 NP products for GOME, GOME2-A, -B, -C, OMI and S5P.

4.1.1.4 Processing System KNMI

This processing system generates the assimilated L4 TC product (MSR).

4.1.1.5 Processing System ULB

The L2 processing system generates the L2 NP products for IASI-A, -B and -C. This processing system, implemented at Eumetsat and ingesting the reprocessed Eumetsat L1C (doi:10.15770/EUM_SEC_CLM_0014 for reprocessed IASI/Metop-A L1C until December 2016. From 2017 and for other IASI satellites, NRT datasets which have no dois are used) and L2 inputs, produces the Climate Data Record (CDR) L2 NP products for IASI-A and -B. The L3 processing system generates the L3 NP products obtained from the merged L2 NP products for IASI-A, -B and -C.

4.1.1.6 Processing System FMI

This processing system generates L3 monthly zonal mean products for OSIRIS, ACE, OMPS-LP, MLS, POAM-III, SAGE-III-M and SAGE-III-ISS and the merged SAGE-CCI-OMPS+, MEGRIDOP, and LIMB-HIRES products.

4.1.1.7 Processing System UNI-HB

This processing system generates L2 HARMOZ products for SABER, MLS, OMPS-LP and SAGE-III-ISS.

4.1.1.8 Processing System SASK

This processing system generates L2 HARMOZ products for OSIRIS and OMPS-LP.

4.1.1.9 Processing System UoT

This processing system generates L2 HARMOZ products for ACE.

4.1.1.10 Processing System ESA

The required S5P L2 TC products are obtained from the operational S5P offline processing system.

4.1.2 Product Handling Domain

Product management is mainly provided by the ftp server at BIRA for an online access of all generated Ozone_cci+ output products.

The users access predefined data sets directly via a ftp pickup point. The product provision is organized using a predefined hierarchical directory structure containing the CCI+ projects, product types and directory paths which are defined within the PSDs. The CCI+ products are also available via the CCI Open Data Portal (<https://climate.esa.int/en/projects/ozone/data>).



4.1.3 Management Domain

4.1.3.1 Production Management

Production Management provides tools and procedures for the operator to handle the system processes and to allow data access to the users. It is an organizational component which is responsible for the organization, monitoring and operation of all defined production and dissemination processes. The production processes itself are individually defined and handled by the processing systems in its organisations. The user access to the data is described on the Ozone CCI web page <https://climate.esa.int/en/projects/ozone>.

4.1.3.2 Algorithm Development

This component is responsible to trigger and organize the whole work which is necessary to bring a new algorithm/processor into operation. This includes the development, testing, installation and system update and the validation. These procedures and tasks are defined and handled by the ALGT Teams 1-3 and are coordinated via the Core Management Team and the Science Leader.

4.2 Main Internal Interfaces

Figure 4-2 shows the main information which are exchanged by the internal interfaces. The green boxes within the specific Processing Systems identifies the involved data processors.

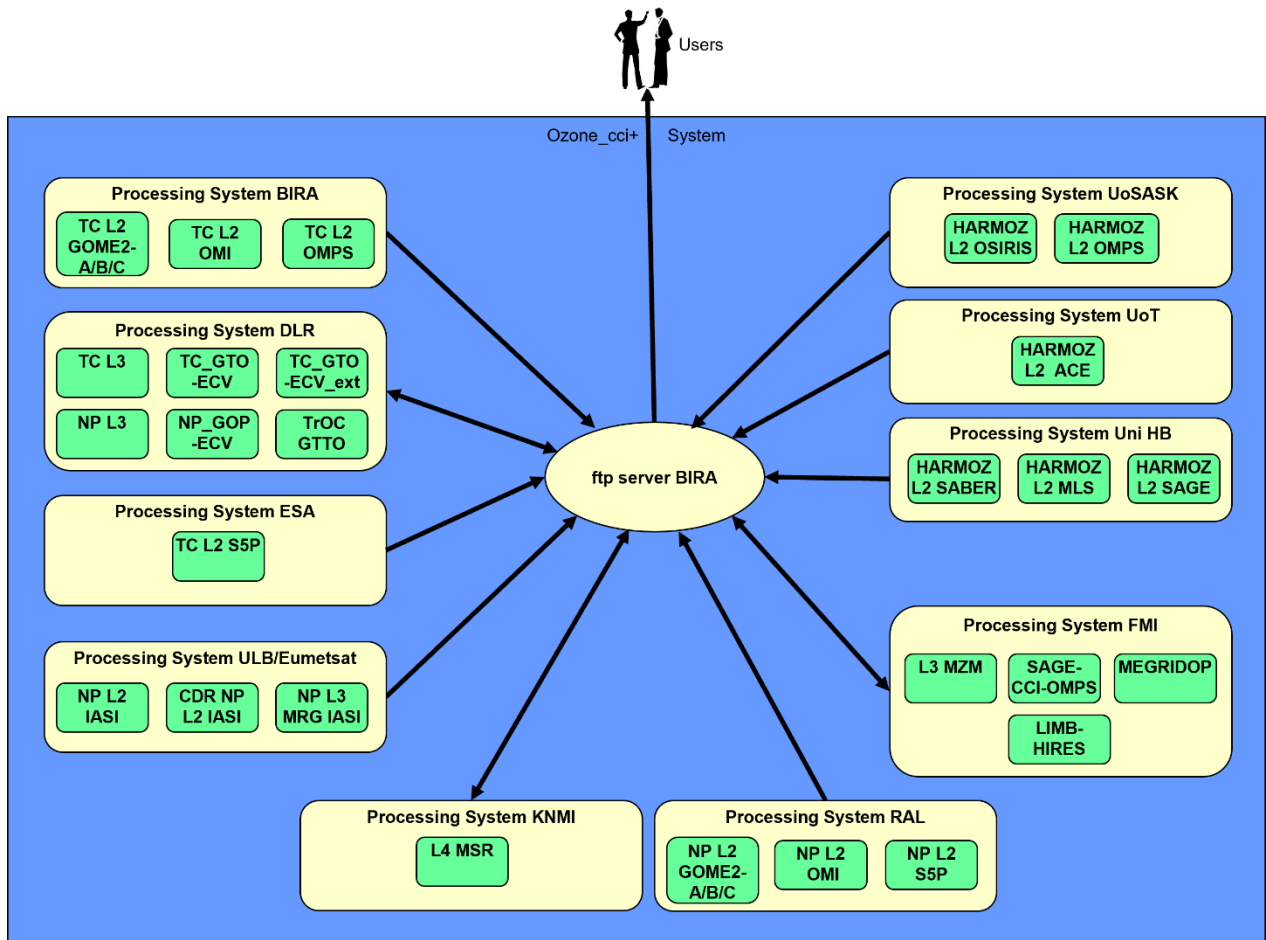


Figure 4-2 Ozone_cci+ System Decomposition with main Internal Interfaces



A detailed description of the interfaces and interface items is given in chapter 6. The main internal interfaces are the interfaces to transfer the output products generated from one processing system to a subsequent processing system which needs these generated output products. The ftp server at BIRA provides the interfaces to transfer these products. In practice, these product transfers are often handled directly by the production operators between the involved processing systems.

4.3 Ozone_cci/cci+ Users

The Ozone_cci+ system interacts with the following users/operators:

- **Ozone_cci+ System Operator**
For each Ozone_cci+ processing system the system operator is responsible for the installation, configuration and acceptance testing of the processors into the specific processor system.
- **Ozone_cci+ Production Operator (Member of Production Management)**
The production operator is responsible to organize, schedule, execute and monitor all defined production processes within a specific processing system. He shall be able to start, restart, stop or cancel all predefined processing or reprocessing scenarios. He generates reports and monitors the data provision and dissemination and handles all defined QA processes.
- **Ozone_cci+ System Engineer (Member of Algorithm/Processor Development Management)**
The System Engineer is responsible to exchange processors or algorithms of the Ozone_cci+ system which are developed by the scientists.
- **Ozone_cci+ Scientist (Member of Algorithm/Processor Development Management)**
The scientist develops algorithms/processors for the production and the quality control of the produced ECV products.
- **ECV User (external)**
The ECV end user searches and downloads the ECV data products from the Ozone_cci+ system.



5 Scenarios (Use Cases)

5.1 Fundamental Operations and Scenarios

This chapter describes the overall scenarios of the Ozone_cci+ system which are necessary to ensure the required ECV parameter production. The following tables give an overview about all products which will be generated by the Ozone_cci+ system.

Level 2 Data Product	Processing Facility	Processing Results
TC_L2_GOME2-A	L2 Processing System BIRA	Processing of new products available after CCI: processing of data until 2021
TC_L2_GOME2-B	L2 Processing System BIRA	Processing of new products available after CCI: processing of data until 2021
TC_L2_GOME2-C	L2 Processing System BIRA	Processing of new products available after CCI: processing of data until 2021
TC_L2_OMI	L2 Processing System BIRA	Processing of new products available after CCI: processing of data until 2021
TC_L2_OMPS	L2 Processing System BIRA	Processing of new products available after CCI: processing of data until 2021
TC_L2_S5P	L2 Processing System ESA	The offline operational algorithm is based on the CCI scientific algorithm GODFIT used for other sensors
NP_L2_GOME2-A	L2 Processing System RAL	No further processing in CCI+ (ICDR provided in C3S)
NP_L2_GOME2-B	L2 Processing System RAL	No further processing in CCI+ (ICDR provided in C3S)
NP_L2_GOME2-C	L2 Processing System RAL	1 year, selected based on instrument performance
NP_L2_OMI	L2 Processing System RAL	No further processing in CCI+ (ICDR provided in C3S)
NP_L2_S5P	L2 Processing System RAL	1 year, selected based on instrument performance
NP_L2_IASI-A	L2 Processing System ULB	Processing of FORLI-O3 products from IASI-A from 2008 to present
NP_L2_IASI-B	L2 Processing System ULB	Processing of FORLI-O3 products from IASI-B from 2012 to present
NP_L2_IASI-C	L2 Processing System ULB	Processing of FORLI-O3 products from IASI-C from 2019 to present
CDR_NP_L2_IASI-A / -B	CDR L2 Processing System Eumetsat	Processing of IASI O3 CDR products from IASI-A and IASI-B from 2008 to 2022 for 4 days per month.
HARMOZ_OSIRIS_L2	LP L2 Processing System SASK	Processing of data from 2001 to present



Level 2 Data Product	Processing Facility	Processing Results
HARMOZ_ACE_L2	LP L2 Processing System UoT	Processing of data from 2004 to present
HARMOZ_OMPS_L2	LP L2 Processing System SASK	Processing of data from 2012 to present
HARMOZ_SABER_L2	LP L2 Processing System UNI-HB	Processing of data from 2002 to present
HARMOZ_MLS_L2	LP L2 Processing System UNI-HB	Processing of data from 2004 to present
HARMOZ_SAGE-III-ISS_L2	LP L2 Processing System UNI-HB	Processing of data from 2017 to present
HARMOZ_OMPS_L2	LP L2 Processing System UNI-HB	Processing of data from 2012 to present

Table 5-1 Level 2 Products

L3/L4 Data Product	Processing Facility	Processing Results
TC_L3_GOME2-A	L3 Processing System DLR	Processing of new products available after CCI: processing of data from 2019-present
TC_L3_GOME2-B	L3 Processing System DLR	Processing of new products available after CCI: processing of data from 2019-present
TC_L3_GOME2-C	L3 Processing System DLR	Processing of new products: processing of data from 2019-present
TC_L3_OMI	L3 Processing System DLR	Processing of new products available after CCI: processing of data from 2019-present
TC_L3_OMPS	L3 Processing System DLR	Processing of new products available after CCI: processing of data from 2019-present
TC_L3_S5P	L3 Processing System DLR	Processing of new products from S5P: processing of data from 2018-present
TC_GTO-ECV	L3 Processing System DLR	Merging of the new processed TC L3 products to the existing GTO-ECV: Processing of data from 2007-present
TC_GTO-ECV_ext	L3 Processing System DLR	Merging of GTO-ECV and MERRA2 to GTO-ECV_ext: Processing of data from 1980-present
TC_L4_MSR	L4 MSR Processing System KNMI	Monthly mean total ozone on a 0.5 degree resolution grid for the data from 1957-2020. The time period of 1957 till 2020 will be assimilated resulting in a global ozone field on a grid 0.5 by 0.5 degree.
NP_L3_GOME2-A	L3 Processing System DLR	Processing of data from 2007-present
NP_L3_GOME2-B	L3 Processing System DLR	Processing of data from 2013-present



L3/L4 Data Product	Processing Facility	Processing Results
NP_L3_OMI	L3 Processing System DLR	Processing of data from 2004-present
NP_GOP-ECV	L3 Processing System DLR	Merging of the new processed NP L3 products to the new GOP-ECV: processing of data from 1995-present
NP_L3_MRG_IASI-A,-B,-C	L3 Processing System ULB	Processing of merged FORLI-O3 products from IASI-A, -B, -C from 2008 to present.
MZM_OSIRIS_L3	LP L3 Processing System FMI	Processing of new products available after CCI. The updates are yearly. This dataset contributes to C3S
MZM_ACE_L3	LP L3 Processing System FMI	Processing of new products available after CCI. The updates are yearly. This dataset contributes to C3S
MZM_OMPS_L3	LP L3 Processing System FMI	Processing of new products available after CCI. The updates are yearly. This dataset contributes to C3S
MZM_SABER_L3	LP L3 Processing System FMI	Processing of new products available after CCI. The updates are yearly. This dataset contributes to C3S
MZM_MLS_L3	LP L3 Processing System FMI	Processing of new products available after CCI. The updates are yearly. This dataset contributes to C3S
MZM_POAM-III_L3	LP L3 Processing System FMI	Processing of the all available data from 1998-2005
MZM_SAGE-III-M_L3	LP L3 Processing System FMI	Processing of all available data from 2002-2005
MZM_SAGE-III-ISS_L3	LP L3 Processing System FMI	Processing of products from new sensor SAGE-III-ISS, data from 2017 to present
SAGE-CCI-OMPS	LP L3 Processing System FMI	The dataset is extended after CCI, with yearly updates. The SAGE-CCI-OMPS dataset contributes to C3S.
MEGRIDOP	LP L3 Processing System FMI	The new dataset, which includes data from 2001 to present. MEGRIDOP substitutes the Merged Lat x Lon dataset, which was developed in CCI.
LIMB-HIRES	LP L3 Processing System FMI	The new merged dataset of ozone profiles with spatial resolution 1°x1°

Table 5-2 Level 3 and Level 4 Products



5.1.1 Production of Ozone Total Column ECV Parameter

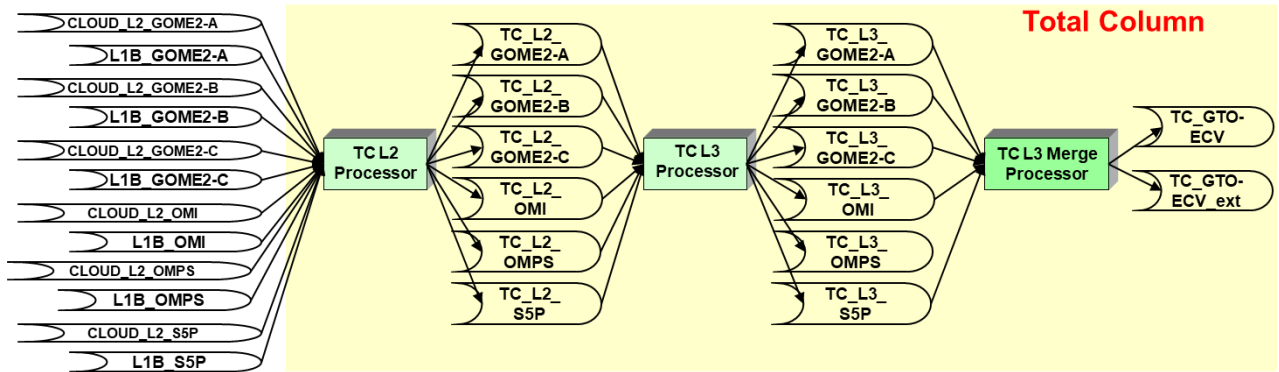


Figure 5-1 Overall ECV Production Scenarios for Ozone Total Column

5.1.1.1 Processing Scenario for TC Products

The system should be able to run the following processing steps:

- Step 1
Ingest L1 input products from GOME2-A, GOME2-B, GOME2-C, OMI and OMPS.
L1 products are consolidated orbits from ascending node to ascending node.
- Step 2 (TC L2 Processor)
Generate and archive L2 intermediate products for GOME2-A, GOME2-B, GOME2-C, OMI and OMPS using the GODFIT algorithm.
One L2 product is generated for each L1 product.
- Step 3
Ingest L2 input products from S5P from Copernicus ESA operational product.
- Step 4 (TC L3 Processor)
Generate and archive L3 intermediate products for GOME2-A, GOME2-B, GOME2-C, OMI, OMPS and S5P.
L3 products are gridded monthly means of a single sensor generated with all L2 products of a given month.
- Step 5 (TC L3 Merge Processor)
Generate and archive output TC_GTO-ECV and TC_GTO-ECV_ext.
TC_GTO-ECV products are monthly means of merged L3 products from GOME2-A, GOME2-B, GOME2-C, OMI and S5P. The L3 products of OMPS are not included in GTO-ECV.
TC_GTO-ECV_ext products are monthly means of merged L3 products from TC_GTO-ECV and MERRA-2 reanalysis. No AUX data is needed for the TC L3 Merge Processor.

5.1.1.2 Partial Reprocessing Scenario for Total Column

- The system should be able to run independently single steps from the full processing scenario in order to reprocess intermediate and/or final products, i.e. partial reprocessing by running steps 2.+3.+4.+5., or by running steps 4.+5., or by running only step 5.
Optionally it may be decided to provide a possibility to restrict the processing according to a given time range.



5.1.2 Production of Nadir Ozone Profile ECV Parameter

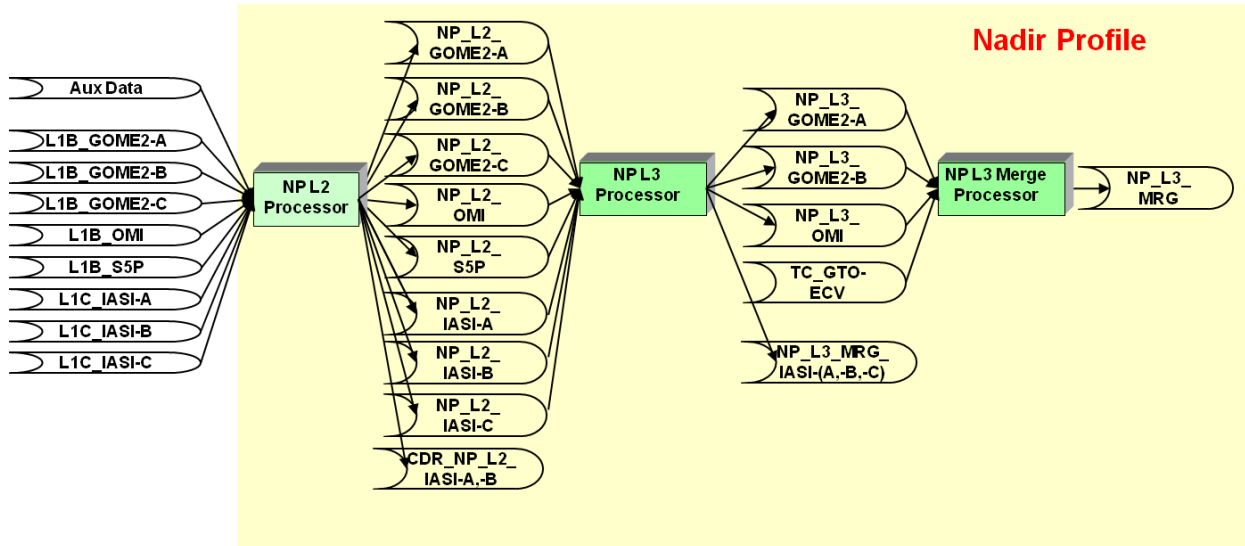


Figure 5-2 Overall ECV Production Scenarios for Nadir Profile

5.1.2.1 Full Processing Scenario for Nadir Profile

The system should be able to run the following processing steps:

- Step 1
Ingest L1B input products from GOME2-A, GOME2-B, GOME2-C, OMI, S5P, IASI-A, IASI-B and IASI-C and necessary auxiliary data products (Eumetsat operational Level-2 data and ECMWF data).
L1 products are consolidated orbits from ascending node to ascending node.
- Step 2 (NP L2 Processor)
Generate and archive L2 intermediate products for GOME2-A, GOME2-B, GOME2-C, OMI, S5P, IASI-A, IASI-B and IASI-C.
One L2 product is generated for each L1 product
- Step 3 (NP L3 Processor)
Generate and archive L3 intermediate products for GOME2-A, GOME2-B, OMI, and IASI.
- Step 4 (NP L3 Merge Processor)
Generate and archive merged L3 products for the nadir ozone profiles based on all L3 products.

5.1.2.2 Partial Reprocessing Scenario

- The system should be able to run independently single steps from the full processing scenario in order to reprocess intermediate and/or final products, i.e. partial reprocessing by running steps 2.+3.+4., or by running only step 3.+4., or by running only step 4.

5.1.3 Production of Limb Ozone Profile ECV Parameter

The production scenarios of the Limb Profile products can be subdivided into the following scenarios:

- Production of L2 harmonized Limb Profiles (L2_HARMOZ).
- Production of L3 monthly zonal mean data (L3_MZM).
- Production of the SAGE-CCI-OMPS merged dataset
- Production of the MEGRIDOP merged dataset
- Production of LIMB-HIRES dataset

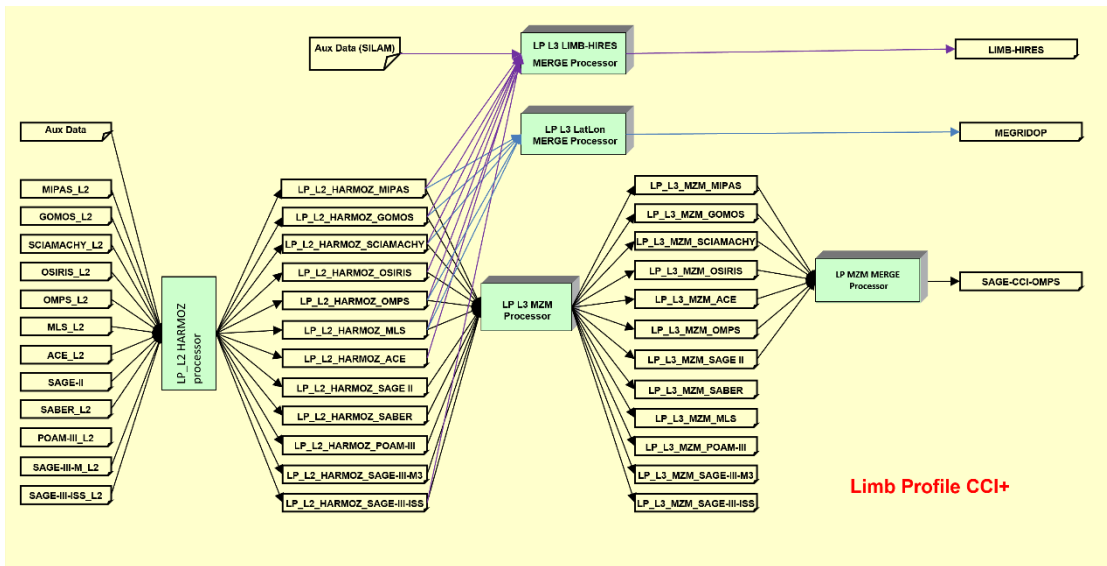


Figure 5-3 ECV Production Scenarios for harmonized MZM and merged Limb Products

5.1.3.1 Full Processing Scenario for the harmonized Limb Profile Products

The production chain for the harmonized MZM Limb Ozone Profile is shown in Figure 5-3.

The system should be able to run the following processing steps:

- Generation of the harmonized L2 profiles for OSIRIS, ACE, OMPS, SABER, MLS, POAM-II, SAGE-II-M3 and SAGE-II-ISS using the sensor specific LP_L2 HARMOZ processor
- Screening the original Level 2 profiles for invalid data
- Interpolation to the HARMOZ pressure grid
- Saving the data in the netcdf format (mandatory and optional parameters)
- Generation of the gridded and merged MZM L3 products
- Creation of Level 3 data from each individual instrument. Computing parameters and uncertainties associated with the Level 3 data
- Creation of merged data based on individual L3 data for SAGE-CCI-OMPS product.
- Creation of merged data based on individual L2 data for MEGRIDOP product.
- Creation of merged data based on individual L2 data for LIMB-HIRES product.
- Creating netcdf files

5.1.4 Production of Limb Tropospheric Ozone ECV Parameter

The production scenarios of the tropospheric ozone products can be subdivided into the following scenarios:

- Production of tropospheric ozone column based on combination of total ozone column from OMI and GTO and stratospheric ozone column derived from several datasets of ozone profiles by limb and occultation instruments.

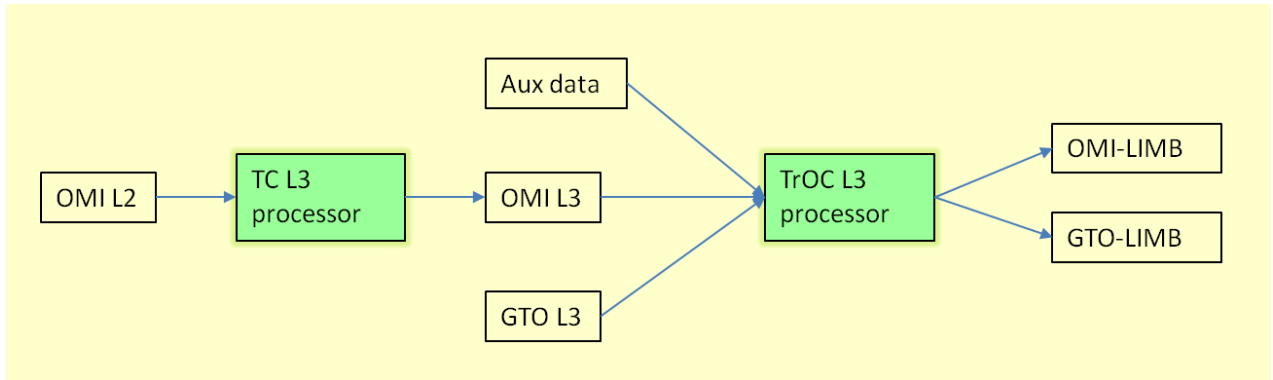


Figure 5-4 ECV Production Scenarios for Tropospheric Ozone Products from Limb sensors

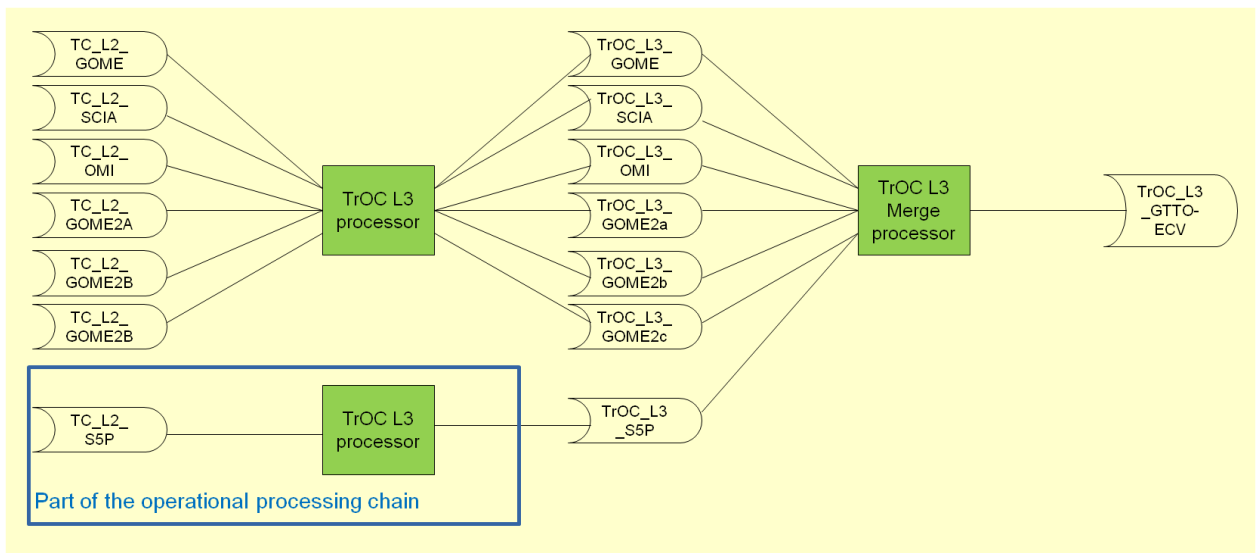


Figure 5-5 ECV Production Scenarios for Tropospheric Ozone Products from Nadir sensors

The production chain for the Tropospheric Ozone from Limb sensors is shown in Figure 5-4.

The system should be able to run the following processing steps:

For OMI-LIMB and GTO-LIMB datasets

- Creation/collection of clear-sky total ozone column from nadir instruments
- Creating high-horizontal resolution stratospheric ozone column by combining ozone profiles from several limb instruments (done in LIMB dataset production)
- Production of OMI-LIMB and GTO-LIMB tropospheric ozone column

5.1.5 Production of Tropical Tropospheric Ozone ECV Parameter

The production chain of the tropical tropospheric ozone column ECV is shown in Figure 5-5. The system should be able to run the following processes:

- Generate the monthly tropical tropospheric ozone column from the total columns of GOME, SCIAMACHY, OMI and GOME-2 (A, B, C) based on the CCD approach.
- Read the operational S5P TTOC data and calculate monthly mean and grid to the same resolution as for GOME-2 to GOME-2.



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- Creation of harmonised data sets for the individual instruments.
- Creation of a merged dataset based on the harmonised data.

5.1.6 Online Access to Ozone ECV Products

The ECV products are provided by the FTP Server at BIRA see Section 4.1.2 Product Handling Domain.



6 Subsystem and Subsystem Components

This chapter describes the further subsystem and component decomposition including their functions, interfaces and interface items which are exchanged between them. The production workflows described in Section 5.1 are handled via already existing processing facilities in different organizations. The online access is provided by a central ftp server at BIRA. The following chapters describe how the Ozone_cci+ system is composed of physical subsystems including their components. The different subsystems are the specific processing facilities of the involved organizations and the data services at BIRA. Components are the specific processors in order to execute the required algorithms which are necessary to generate the required products.

6.1 Processing Facilities for Nadir Ozone_cci+ Products

The following processing facilities are used for the generation of all required nadir Ozone_cci products:

- Processing Facility at BIRA
- Processing Facility at DLR
- Processing Facility at KNMI
- Processing Facility at RAL
- Processing Facility at ULB
- Processing Facility at ESA

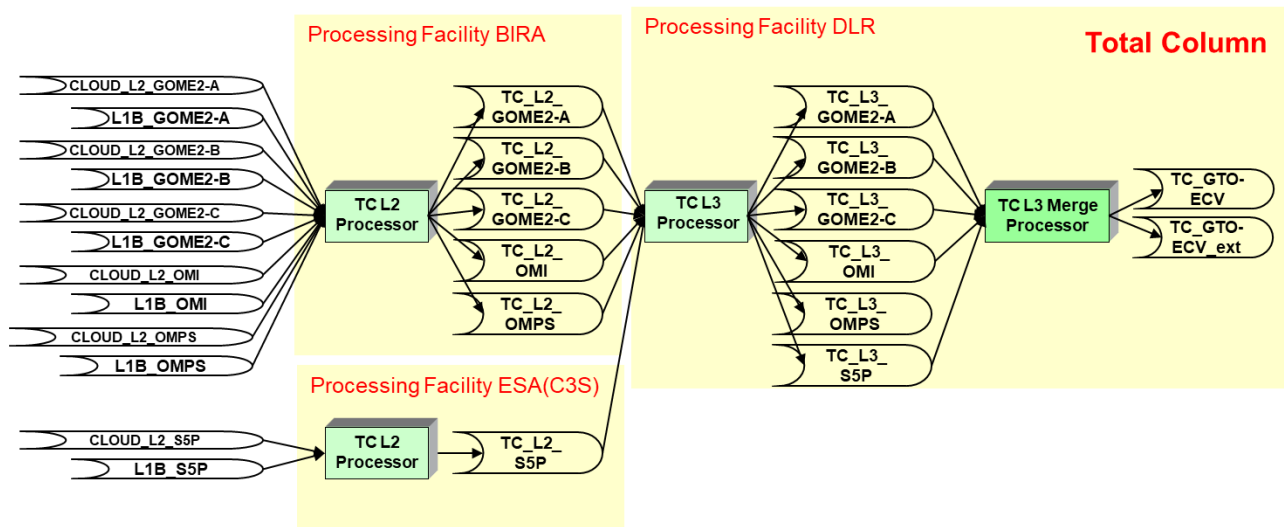


Figure 6-1 Processing Facilities for TC

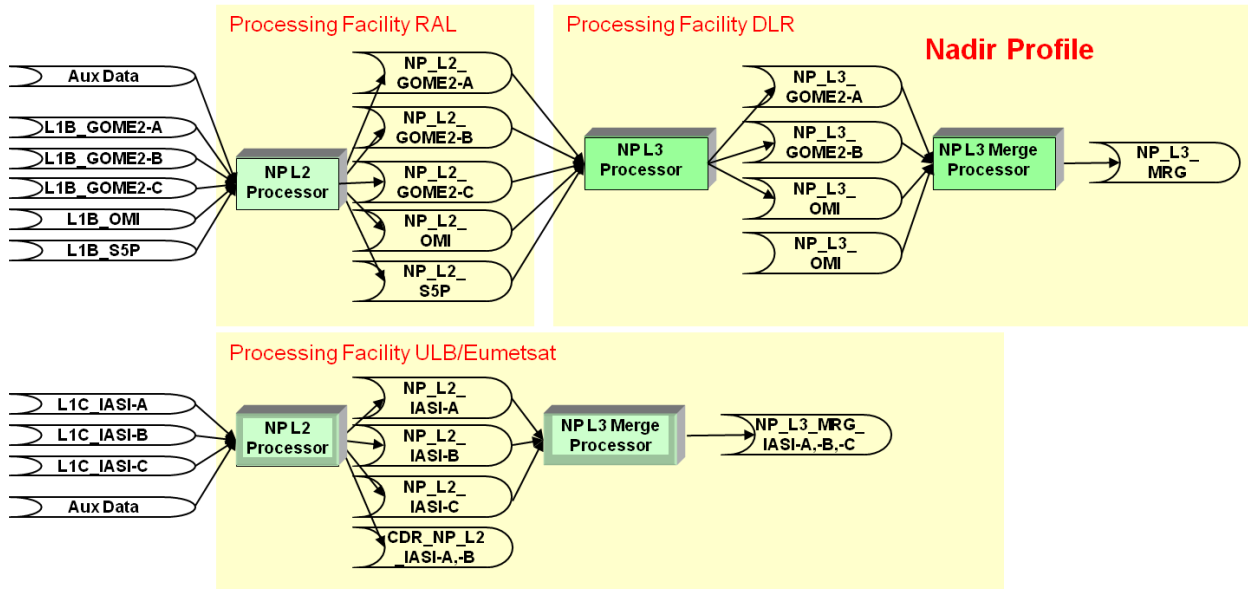


Figure 6-2 Processing Facilities for NP

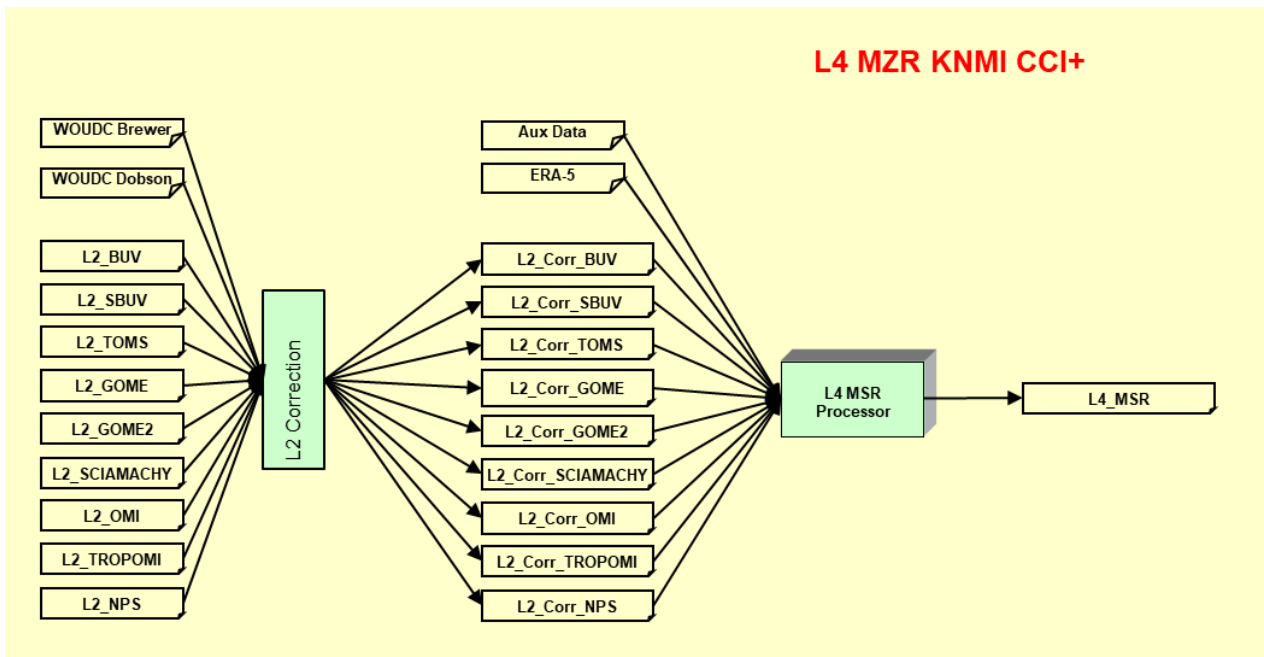


Figure 6-3 Processing Facilities for L4 MSR

6.1.1 Processing Facility at BIRA

6.1.1.1 Description

This processing facility provides the processors:

- TC L2 Processor



6.1.1.2 Processors

Title	TC L2 Processor
Name	GODFIT V4
Description	The processor ingests binary or HDF level 1 data (GOME, SCIAMACHY, GOME-2, OMI or OMPS) on orbit basis as well as required auxiliary data, and produces a level 2 O3 total column product. The L2 processing is orbit oriented. One L1 orbit results in one L2 orbit product.
Used Algorithm	GODFIT V34

6.1.1.3 Functions

The processing facility provides the following functions:

- Generation of TC_L2_GOME2-A, B, C products from GOME2 L1B products
- Generation of TC_L2_OMI products from OMI L1B products
- Generation of TC_L2_OMPS products from OMPS L1B products
- Transfer all generated and validated TC_L2 products to the FTP Server and/or the processing facility at DLR

6.1.1.4 Interfaces and Interface Items

Inputs

- TC_L1B_GOME2-A, B, C original L1B GOME2 products
- CLOUD_L2_GOME2-A, B, C cloud L2 products for GOME2
- TC_L1B_OMI original LB OMI products
- CLOUD_L2_OMI cloud L2 products for OMI
- TC_L1B_OMPS original LB OMPS products
- CLOUD_L2_OMPS cloud L2 products for OMPS
- Auxiliary Data
- Coordinates product for OMI

Outputs:

- TC_L2_GOME2-A
- TC_L2_GOME2-B
- TC_L2_GOME2-C
- TC_L2_OMI
- TC_L2_OMPS

6.1.1.5 Hardware Environment

The technical characteristics of the used system are:

- Central file servers for scientific and operational datasets:
- Approximately 1.2 PB. storage for datasets
- scratch volume on HPC: 100TB
- processing done on HPC at BIRA (Central high performance computing server, shared with BIRA's Space-Pole partners RMI and ROB: HA Linux cluster with 2688 computing cores, 112 compute nodes for HPC and operational tasks). Processors that are used for the TC L2 processing depends on the availability on the HPC. Scheduler is PBSPro



- on HPC in total 224 cpu's
- 88 nodes with 60 GB, 24 nodes with 250 GB
- Intern connectivity ensured by ethernet over InfiniBand.
- State-of-the-art compilers (Fortran 90/95, C/C++, etc.), data analysis tools (IDL, MatLab, etc.) and general purpose software.
- The jobs run on the HPC and typically one cpu is reserved with at walltime of 7 hours to process (from L1 to L2) a single day. The number of cpu's that is used at the same time depends on the current load of the HPC. No parallel programming (MPI, OpenMP,...) is used in the code.

6.1.2 Processing Facility at DLR

6.1.2.1 Description

This processing facility provides the processors:

- TC L3 Processor
- TC L3 Merge Processor
- NP L3 Processor
- NP L3 Merge Processor
- TrOC L3 Processor
- TrOC L3 Merge Processor

6.1.2.2 Processors

Title	TC L3 Processor
Name	UCAS
Description	Level 3 processing: monthly regrid level 2 data, output to netCDF CF
Used Algorithm	existing Universal Climate processor for Atmospheric Spectrometers (UCAS)

Title	TC L3 Merge Processor
Name	UCAS
Description	ECV processing: monthly mean merge GOME, SCIA, GOME-2-A,B,C, OMI and S5P, output to netCDF CF
Used Algorithm	existing Universal Climate processor for Atmospheric Spectrometers (UCAS)

Title	NP L3 Processor
Name	UCAS
Description	Level 3 processing: monthly regrid level 2 data, output to netCDF CF
Used Algorithm	existing Universal Climate processor for Atmospheric Spectrometers (UCAS)



Title	NP L3 Merge Processor
Name	UCAS
Description	ECV processing: monthly mean merge GOME, SCIA, GOME2-A,B and OMI, output to netCDF CF
Used Algorithm	existing Universal Climate processor for Atmospheric Spectrometers (UCAS)

Title	TrOC L3 Processor
Name	UCAS
Description	Level 3 processing: monthly regrid level 2 data, output to netCDF CF
Used Algorithm	existing Universal Climate processor for Atmospheric Spectrometers (UCAS)

Title	TrOC L3 Merge Processor
Name	UCAS
Description	ECV processing: monthly mean merge GOME, SCIA, GOME2-A,B,C, OMI, and S5P; output to netCDF CF
Used Algorithm	existing Universal Climate processor for Atmospheric Spectrometers (UCAS)

6.1.2.3 Functions

The processing facility provides the following functions:

- Generation of TC_L3_GOME products from TC GOME L2 products
- Generation of TC_L3_SCIA products from TC SCIA L2 products
- Generation of TC_L3_GOME2-A products from TC GOME2-A L2 products
- Generation of TC_L3_GOME2-B products from TC GOME2-B L2 products
- Generation of TC_L3_GOME2-C products from TC GOME2-C L2 products
- Generation of TC_L3_OMI products from TC OMI L2 products
- Generation of TC_L3_OMPS products from TC OMPS L2 products
- Generation of TC_L3_S5P products from TC S5P L2 products
- Generation of TC_L3_MRG products (TC_GTO-ECV is generated) from all TC L3 products except TC_L3_OMPS, and TC_GTO-ECV_ext is generated from TC_GTO-ECV and MERRA-2 reanalysis.
- Transfer all generated and validated TC_L3_MRG products to the FTP Server

The processing facility provides the following additional functions for Phase 2:

- Generation of NP_L3_GOME products from NP GOME L2 products
- Generation of NP_L3_SCIA products from NP SCIA L2 products
- Generation of NP_L3_GOME2-A products from NP GOME2-A L2 products
- Generation of NP_L3_GOME2-B products from NP GOME2-B L2 products
- Generation of NP_L3_OMI products from NP OMI L2 products
- Generation of NP_L3_OMPS products from NP OMPS L2 products
- Generation of NP_L3_MRG products (NP_GOP-ECV) from all generated NP L3 products
- Transfer all generated and validated NP_L3_MRG to the FTP Server



The processing facility provides the following additional functions for tropospheric ozone in Phase 2:

- Generation of TrOC_L3_GOME products from TC GOME L2 products
- Generation of TrOC_L3_SCIA products from TC SCIA L2 products
- Generation of TrOC_L3_GOME2-A products from TC GOME2-A L2 products
- Generation of TrOC_L3_GOME2-B products from TC GOME2-B L2 products
- Generation of TrOC_L3_OMI products from TC OMI L2 products
- Generation of TrOC_L3_GOME2-C products from TC GOME2-C L2 products
- Generation of TrOC_L3_S5P products from TC S5P L2 products
- Generation of TrOC_L3_MRG merged products (TrOC_GTTO-ECV) from all generated TrOC L3 products
- Transfer all generated and validated TrOC_L3_MRG to the FTP Server

6.1.2.4 Interfaces and Interface Items

Inputs

- TC_L2_GOME Total Column L2 GOME products
- TC_L2_SCIA Total Column L2 SCIA products
- TC_L2_GOME2-A Total Column L2 GOME2-A products
- TC_L2_GOME2-B Total Column L2 GOME2-B products
- TC_L2_GOME2-C Total Column L2 GOME2-C products
- TC_L2_OMI Total Column L2 OMI products
- TC_L2_OMPS Total Column L2 OMPS products
- TC_L2_S5P Nadir Profile L2 S5P products
- NP_L2_GOME Nadir Profile L2 GOME products
- Np_L2_SCIA Nadir Profile L2 SCIA products
- NP_L2_GOME2-A Nadir Profile L2 GOME2-A products
- NP_L2_GOME2-B Nadir Profile L2 GOME2-B products
- NP_L2_GOME2-C Nadir Profile L2 GOME2-C products
- NP_L2_OMI Nadir Profile L2 OMI products
- NP_L2_S5P Nadir Profile L2 S5P products

Outputs:

- TC_GTO-ECV the merged ozone total column ozone L3 products
- TC_GTO-ECV_ext the merged total ozone column L3 product from TC_GTO-ECV and MERRA-2
- NP_GOP-ECV the merged nadir profile ozone L3 products
- TrOC_GTTO-ECV the merged tropical tropospheric ozone L3 products

6.1.2.5 Hardware Environment

The technical characteristics of the used system are:

- Linux cluster
- 16 CPUs
- Disk space for L2 input data: ~8.5 TB + ~2 TB/year for each additional year
- Disk space for generated L3 data: ~200 GB + ~10 GB/year for each additional year
- RAM 0.5 GB



- Processors used in Python

6.1.3 Processing Facility at RAL

6.1.3.1 Description

This processing facility provides the processors:

- NP L2 Processor

6.1.3.2 Processors

Title	NP L2 Processor
Name	RAL Ozone Profile Algorithm
Description	Ozone profiles are derived from nadir observations (Level 1b data) from GOME, SCIAMACHY, GOME-2-A, B, C, OMI and S5P with an ozone profile Retrieval algorithm from RAL on an orbit basis. One L1 orbit results in one L2 orbit product.
Used Algorithm	RAL Ozone Retrieval Scheme

6.1.3.3 Functions

The processing facility provides the following functions:

- Generation of NP_L2_GOME products from GOME L1B products
- Generation of NP_L2_SCIA products from SCIA L1B products
- Generation of NP_L2_GOME2-A products from GOME2-A L1B products
- Generation of NP_L2_GOME2-B products from GOME2-B L1B products
- Generation of NP_L2_GOME2-C products from GOME2-C L1B products
- Generation of NP_L2_OMI products from OMI L1B products
- Generation of NP_L2_S5P products from S5P L1B products
- Transfer all generated and validated NP_L2 products to the FTP Server

6.1.3.4 Interfaces and Interface Items

Inputs

- NP L1B_GOME original NP L1B GOME products
- NP L1B_SCIA original NP L1B SCIA products
- NP L1B_GOME2-A original NP L1B GOME2-A products
- NP L1B_GOME2-B original NP L1B GOME2-B products
- NP L1B_GOME2-C original NP L1B GOME2-C products
- NP L1B_OMI original NP L1B OMI products
- NP L1B_S5P original NP L1B GOME2-B products
- Auxiliary Data
 - ECMWF ERA5 meteorological data
 - FRESCOv6 and/or OCRA/ROCINN cloud products for GOME, SCIAMACHY and GOME2-A,B,C
 - Coordinates product for OMI.
 - KNMI O2-O2 cloud product for OMI (OMCLD v3)
 - Operational L2__CLOUD product for S5P (v2)



Outputs:

- NP_L2_GOME Nadir Profile L2 GOME products
- NP_L2_SCIA Nadir Profile L2 SCIA products
- NP_L2_GOME2-A Nadir Profile L2 GOME2-A products
- NP_L2_GOME2-B Nadir Profile L2 GOME2-B products
- NP_L2_GOME2-C Nadir Profile L2 GOME2-C products
- NP_L2_OMI Nadir Profile L2 OMI products
- NP_L2_S5P Nadir Profile L2 S5P products

6.1.3.5 Hardware Environment

The technical characteristics of the used system are:

- The Nadir Profile L2 processing is performed on the JASMIN facility located at the Rutherford Appleton Laboratory (RAL) in the UK.
- JASMIN provides a high-speed interface between a Quobyte+Panasas data repository (e.g. containing L1 and meteorological data) and the dedicated processing cluster, in addition to local temporary output product storage.
- JASMIN CPU are a mix of: Intel Xeon E5-2640-v4 "Broadwell" (20core, 256Gb), Intel Xeon Gold-5118 "Skylake" (24core, 248Gb), and AMD (EPYC) (48core, 1024Gb); total cores: ~10,000, single user access max is 2,000.
- Typically 4 GB RAM and 2 GB disk space will be used by each job.
- Additional backup of RSG cluster: Intel(R) Xeon(R) Gold 6230 CPU @ 2.10GHz (40core/80thread, 128GB); total cores: 1,000/2,000 thread

6.1.4 Processing Facility at KNMI

6.1.4.1 Description

This processing facility provides the processors:

- MSR2 Processor

6.1.4.2 Processors

Title	MSR2 Processor
Name	TM-DAM
Description	The processor uses total ozone columns from various satellites (BUV, SBUV, TOMS, GOME, GOME2, SCIAMACHY, OMI, TROPOMI, NPS), ERA 5 meteorological data, WOUDC Brewer and Dobson observation data as input. To generate Monthly mean total ozone on a 0.5 degree resolution grid for the years 1957-2020 as output.
Used Algorithm	TM-DAM

6.1.4.3 Functions

The processing facility provides the following functions:

- Generation of ground-based corrected L2 products
- Generation of the L4 MSR products by assimilating the corrected L2 products
- Transfer all generated and validated L4_MSR products to the FTP Server



6.1.4.4 Interfaces and Interface Items

Inputs

- Total ozone columns from various satellites (BUV, SBUV, TOMS, GOME, GOME2, SCIAMACHY, OMI, TROPOMI, NPS), ERA 5 meteorological data of ECMWF, WOUDC Brewer and Dobson observations.

Outputs:

- L4_MSR Monthly mean total ozone on a 0.5 degree resolution grid

6.1.4.5 Hardware Environment

The technical characteristics of the used system are:

- It runs at a national research cloud computing facility (SURF) on a single virtual machine
- Preprocessing takes place at a dedicated workstation with all input data (meteo, satellite) locally stored.
- Used resources: 1 CPU, 8 GB RAM and 200 GB disc space
- The MSR algorithm is not parallelized and therefore runs on 1 CPU. In addition, the assimilation has to run sequentially, since it uses the results of the previous day as starting point of the next time step. This makes the processing relatively slow.

6.1.5 Processing Facility at ULB/Eumetsat

6.1.5.1 Description

The processing facility at ULB provides the processors:

- NP L2 Processor
- NP L3 Merge Processor

The processing facility at Eumetsat provides the processors:

- CDR NP L2 Processor

6.1.5.2 Processors

Title	NP L2 Processor / CDR NP L2 Processor
Name	FORLI-O3/ IASI-O3 CDR
Description	The processor ingests binary (BUFR) level 1 data (IASI) on PDU basis and produces a level 2 O3 nadir profile product.
Used Algorithm	FORLI-O3 (v20191122)/ FORLI-O3 (v20151001)

Title	NP L3 MERGE Processor
Name	FORLI-O3-MRG
Description	Creation of merged daily mean ozone profiles in 1°x1° latitude-longitude bins using the FORLI-O3 data from the three IASI instruments.
Used Algorithm	Merging is performed by computing weighted mean data according to the retrieval uncertainties. The details are in the User Manual.

6.1.5.3 Functions

The processing facility provides the following functions:



- Generation of NP_L2_IASI-A, B, C products from original IASI-A,B,C L1 products
- Generation of CDR_NP_L2_IASI-A, B products from reprocessed IASI-A,B L1C products
- Generation of NP_L3_MRG_IASI-A,-B,-C products from NP_L2_IASI-A, B, C products
- Transfer all generated and validated CDR NP_L2/NP_L3_MRG IASI products to the FTP Server

6.1.5.4 Interfaces and Interface Items

Inputs

In FORLI-O3:

- Original L1C IASI-A products
- Original L1C IASI-B products
- Original L1C IASI-C products
- Auxiliary Data:
 - IASI L2 meteorological data
 - FORLI look-up tables
 - orography/emissivity

In IASI-O3-CDR:

- Reprocessed L1C IASI-A and -B products
- Auxiliary Data:
 - Reprocessed IASI L2 meteorological data
 - FORLI look-up tables
 - orography/emissivity

In FORLI-O3-MRG:

- NP_L2_IASI-A, B, C products

Outputs:

- NP_L2_IASI-A
- NP_L2_IASI-B
- NP_L2_IASI-C
- CDR_NP_L2_IASI-A & -B
- NP_L3_MRG_IASI-A,-B,-C

6.1.5.5 Hardware Environment

At ULB:

- 3 PC INTEL Servers each one includes:
 - 32 or 8GB RAM
 - 36 or 12TB storage (RAID-6)
 - ARCH x86_64
- 3 NAS SYNOLOGY servers with a total of:
 - 20GB RAM
 - 162 TB storage (RAID-5)
 - DSM 6
- 1 LINUX CLUSTER including:
 - Torque/Maui PBS scheduler
 - 29 nodes totaling 493 threads, running ArchLinux x86_64



A specific number of thread per job (PDU) is attributed to each species retrieved using the FORLI algorithm (e.g. 6 for O3). In order to assure both the forward and the backward processings (to provide a full homogenous dataset in case of development of an improved version), the daily processing of the IASI data for the O3 retrieval can use up to 18 jobs in parallel.

At Eumetsat:

EUMETSAT's mass data reprocessing system used for this dataset is an HTCondor cluster of 25 Intel servers running 64 bit Centos 7. The total system comprises 600 (non-HT) cores and 9.6TB RAM. Primary storage is on a central Dell Isilon NAS cluster with 5PB of capacity.

6.2 Processing Facilities for Limb Ozone_cci+ Products

The following processing facilities are used for the generation of all required nadir Ozone_cci products:

- Processing Facility at FMI
- Processing Facility at UNI-HB
- Processing Facility at UoT
- Processing Facility at UoSask

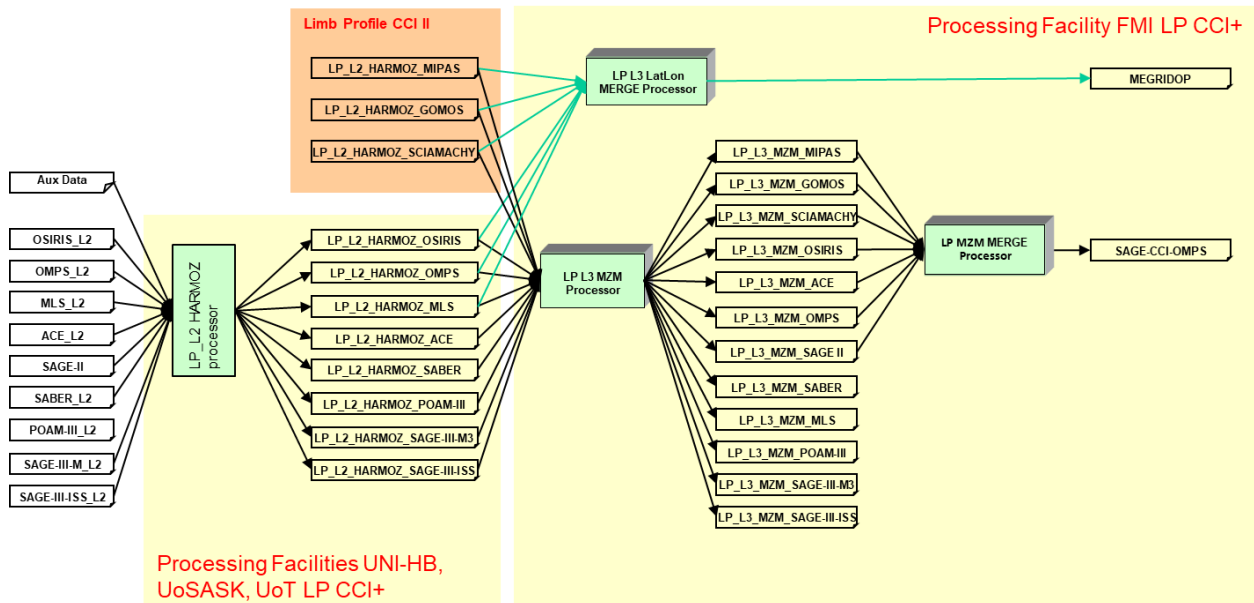


Figure 6-4 Processing Facilities for LP

6.2.1 Processing Facility at FMI

6.2.1.1 Description

This processing facility provides the processors:

- LP L3 Processor
- LP MZM MERGE Processor
- LP L3 LatLon MERGE Processor
- LP L3 LIMB-HIRES MERGE Processor
- TC L3 OMI Processor
- TrOC L3 Processor



6.2.1.2 Processors

Title	LP L3 Processor
Name	FMI-LP-MZM
Description	Creating monthly zonal mean data for each instrument using the HARMOZ level 2 data. Evaluation of uncertainties associated with the L3 data
Used Algorithm	FMI-LP-MZM

Title	LP MZM MERGE Processor
Name	FMI-LP-MMZM
Description	Creation of merged monthly zonal mean data using the MZM data from individual instruments. Evaluation of associated uncertainties.
Used Algorithm	Merging is performed by computing weighted mean data according to the total uncertainties. The details are in the User Manual.

Title	LP L3 SMM Processor
Name	LP L3 LatLon MERGE Processor
Description	Creating semi-monthly mean ozone profiles in 10°x20° latitude-longitude bins for each sensor. Evaluation of associated uncertainties.
Used Algorithm	The details are in User manual

Title	LP L3 LIMB-HIRES Processor
Name	LP L3 LIMB-HIRES MERGE Processor
Description	Creating daily mean ozone profiles with the spatial resolution 1°x1° latitude-longitude using data from several limb instruments. Evaluation of associated uncertainties.
Used Algorithm	The details are in User manual

Title	TC L3 OMI Processor
Name	TC L3 OMI Processor
Description	Creating daily mean cloud-free total ozone column with the spatial resolution 1°x1°. Evaluation of associated uncertainties.
Used Algorithm	The details are in User manual



Title	TrOC L3 Processor
Name	TrOC L3 Processor
Description	Creating monthly mean tropospheric ozone column with the spatial resolution 1°x1° latitude-longitude using total ozone column from nadir instruments (OMI, GTO) and stratospheric ozone column from high-resolution limb profile dataset. Evaluation of associated uncertainties.
Used Algorithm	The details are in User manual

6.2.1.3 Functions

The processing facility provides the following functions:

- Generation of the LP_L3_MZM products for all sensors
- Generation of SAGE-CCI-OMPS products
- Generation of MEGRIDOP products
- Transfer all generated and validated LP_L3_MZM, SAGE-CCI-OMPS and MEGRIDOP products to the FTP Server

6.2.1.4 Interfaces and Interface Items

Inputs

- LP_L2_HARMOZ_OSIRIS harmonized Limb Profile L2 products for OSIRIS
- LP_L2_HARMOZ_ACE harmonized Limb Profile L2 products for ACE
- LP_L2_HARMOZ_OMPS harmonized Limb Profile L2 products for OMPS
- LP_L2_HARMOZ_SABER harmonized Limb Profile L2 products for SABER
- LP_L2_HARMOZ_MLS harmonized Limb Profile L2 products for MLS
- LP_L2_HARMOZ_POAM-III harmonized Limb Profile L2 products for POAM-III
- LP_L2_HARMOZ_SAGE-III-M harmonized Limb Profile L2 products for SAGE-III-M
- LP_L2_HARMOZ_SAGE-III-ISS harmonized Limb Profile L2 products for SAGE-III-ISS
- LP_L3_MZM_GOMOS LP L3 Monthly zonal mean GOMOS products from CCI II
- LP_L3_MZM_SCIAMACHY LP L3 Monthly zonal mean SCIAMACHY products from CCI II
- LP_L3_MZM_MIPAS LP L3 Monthly zonal mean MIPAS products from CCI II
- LP_L3_MZM_OSIRIS LP L3 Monthly zonal mean OSIRIS products from CCI II
- Auxiliary Data Ozone profiles from SILAM chemistry-transport model

Outputs:

- LP_L3_MZM_OSIRIS Monthly zonal mean Limb Profile L3 products for OSIRIS
- LP_L3_MZM_ACE Monthly zonal mean Limb Profile L3 products for ACE
- LP_L3_MZM_OMPS Monthly zonal mean Limb Profile L3 products for OMPS
- LP_L3_MZM_SABER Monthly zonal mean Limb Profile L3 products for SABER
- LP_L3_MZM_MLS Monthly zonal mean Limb Profile L3 products for MLS
- LP_L3_MZM_POAM-III Monthly zonal mean Limb Profile L3 products for POAM-III
- LP_L3_MZM_SAGE-III-M Monthly zonal mean Limb Profile L3 products for SAGE-III-M
- LP_L3_MZM_SAGE-III-ISS Monthly zonal mean Limb Profile L3 products for SAGE-III-ISS



- SAGE-CCI-OMPS Merged Monthly zonal mean ozone profiles from several limb instruments (SAGE-II, MIPAS, GOMOS, SCIAMACHY, OSIRIS, OMPS-LP)
- MEGRIDOP Merged gridded dataset of ozone profiles from several limb instruments (OSIRIS, MIPAS, GOMOS, SCIAMACHY, MLS, OMPS-LP) Hardware Environment

The processing facility provides the following functions:

- FMI-CCI software
- Collection of Matlab routines
- The computation of monthly zonal mean and gridded data from individual satellite instruments can be run in parallel. However, these computations are fast, so usually the parallelization is not important. The processing of merged gridded datasets is performed sequentially, without parallelization

6.2.2 Processing Facility at UNI-HB

6.2.2.1 Description

This processing facility provides the processors to convert LP L2 original data into HARMOZ format:

- LP L2 SABER Processor
- LP L2 MLS Processor
- LP L2 SAGE-III-ISS Processor
- LP L2 OMPS-LP UBR Processor

6.2.2.2 Processors

Title	LP L2 SABER Processor
Name	HARMOZ SABER
Description	The processor screens non-physical large values for latitude, longitude, temperature, and local solar time in L2 original profiles. Ozone outliers have been removed, i.e. values $> \text{mean} + 3 \text{ mad}$ of the distribution at $P > 50$ hPa.
Used Algorithm	harmoz_saber_v20_cv01.py processed with python software

Title	LP L2 SAGE-III-ISS Processor
Name	HARMOZ_SAGE-III-ISS
Description	The processor ingests orbit-wise L2 v5.3 measurements to produce monthly HARMOZ files. The altitude-based retrieval flag is used to screen data, whereas the 'Event quality flag' is reported in the files.
Used Algorithm	harmoz_sageIIIiss_v53_cv02.py processed with python software



Title	LP L2 MLS Processor
Name	HARMOZ MLS
Description	Filtering and screening of bad v5 L2 data is performed according to the MLS user guide. The native VMR vs pressure MLS ozone profiles are converted in number density and interpolated at a common altitude grid using ECMWF ERA5 information.
Used Algorithm	harmoz_mls_v5_cv01.py processed with python software

Title	LP L2 OMPS-LP UBR Processor
Name	HARMOZ OMPS-LP UBR
Description	The processor ingests orbit-wise L2 measurements to produce monthly HARMOZ files. Data are screened according to cloud flag, vertical resolution. SAA flag is reported. The dataset includes profiles retrieved in the presence of a polar mesospheric cloud in the FOV (accordingly flagged).
Used Algorithm	harmoz_ompsIUP_cv01.py processed with python software, profiles retrieved at UBR with SCIATRAN

6.2.2.3 Functions

The processing facility provides the following functions:

- Generation of harmonized LP_L2_HARMOZ_SABER products
- Generation of harmonized LP_L2_HARMOZ_SAGE-III-ISS products
- Generation of harmonized LP_L2_HARMOZ_MLS products
- Generation of harmonized LP_L2_HARMOZ_OMPS-LP UBR products
- Transfer all generated and validated LP_L2_HARMOZ products for SABER, SAGE-III-ISS, MLS, and OMPS-LP UBR to the FTP Server and/or to the processing facility at FMI

6.2.2.4 Interfaces and Interface Items

Inputs

- SABER_L2 original L2 v2.0 SABER products
- SAGE-III-ISS_L2 original L2 v5.3 SAGE-III-ISS products
- MLS_L2 original L2 v5 MLS products
- OMPS-LP UBR L2 original L2 v4.0 OMPS-LP UBR products
- Auxiliary Data
 - ECMWF data: Pressure, temperature and altitude. All processors use ERA-5 data.

Outputs:

- LP_L2_HARMOZ_SABER harmonized Limb Profile L2_HARMOZ products for SABER
- LP_L2_HARMOZ_SAGE-III-ISS harmonized Limb Profile L2_HARMOZ products for SAGE-III-ISS
- LP_L2_HARMOZ_MLS harmonized Limb Profile L2_HARMOZ products for MLS
- LP L2 HARMOZ OMPS-UBR harmonized Limb Profile L2_HARMOZ products for OMPS-LP UBR



6.2.2.5 Hardware Environment

The processing facility provides the following functions:

- Local computers and cluster grid engine. Python scripts with HARMOZ codes are run on the IUP cluster facility. Since the data sets are updated every 2 months, scripts are generally not run in parallel. However, they can be parallelized simply by having multiple cores processing single months at the same time.

6.2.3 Processing Facility at UoT

6.2.3.1 Description

This processing facility provides the processors:

- LP L2 ACE Processor

6.2.3.2 Processors

Title	LP L2 ACE Processor
Name	HARMOZ_ACE
Description	ACE-FTS v3.5/3.6 L1 are produced at UoT, then filtered out according to the quality flags provided and interpolated into CCI vertical grid by using the native altitude and pressure grids.
Used Algorithm	Not available

6.2.3.3 Functions

The processing facility provides the following functions:

- Generation of harmonized LP_L2_HARMOZ_ACE products
- Transfer all generated and validated LP_L2_HARMOZ products for ACE to the FTP Server and/or the processing facility at FMI

6.2.3.4 Interfaces and Interface Items

Inputs

- ACE_L2 original L2 ACE products
- Auxiliary Data
 - ECMWF data: Pressure, temperature and altitude. Except for POAM-III, the other processors use ERA-5 data.

Outputs:

- LP_L2_HARMOZ_ACE harmonized LP L2_HARMOZ products for ACE

6.2.3.5 Hardware Environment

The processing facility provides the following functions:

- Servers to process L1 and L2 data.

6.2.4 Processing Facility at UoSASK

6.2.4.1 Description

This processing facility provides the processors:



- LP L2 OSIRIS Processor

6.2.4.2 Processors

Title	LP L2 OSIRIS Processor
Name	HARMOZ_OSIRIS
Description	The processor ingests binary level 1 data (OSIRIS) on orbit basis and produces a level 2 O3 limb profile product, which is then converted into HARMOZ format.
Used Algorithm	SaskMART, SASKTRAN

Title	LP L2 OMPS-LP Processor
Name	HARMOZ_OMPS-LP
Description	The processor ingests binary level 1 data (OMPS-LP) on orbit basis and produces first a L2 O3 limb profile product, which is then converted into HARMOZ format.
Used Algorithm	SASKTRAN

6.2.4.3 Functions

The processing facility provides the following functions:

- Generation of harmonized LP_L2_HARMOZ_OSIRIS and the LP_L2_HARMOZ_OMPS products
- Transfer all generated and validated LP_L2_HARMOZ products for OSIRIS and OMPS LP to the FTP Server and/or the processing facility at FMI

6.2.4.4 Interfaces and Interface Items

Inputs

- OSIRIS_L2 original L2 OSIRIS products
- OMPS-LP L2 original L2 OMPS-LP data produced at UoSask
- Auxiliary Data
 - Pressure profiles from ECMWF for the conversion into HARMOZ format

Outputs:

- LP_L2_HARMOZ_OSIRIS harmonized LP L2_HARMOZ products for OSIRIS
- LP_L2_HARMOZ_OMPS-LP harmonized LP L2_HARMOZ products for OMPS-LP

6.2.4.5 Hardware Environment

The processing facility provides the following functions:

- Special computing facilities consisting of servers at the University of Saskatchewan.

6.3 Management Domain

6.3.1 Production Management (PM)

The Production Management is an organizational component and has to be done on each processing facility. It is responsible to fulfil the following functions:

- Organization, monitoring and control of all operational production processes. This includes the production of new data as well as the production of reprocessing procedures.



- Organization, monitoring and control of all operational quality control processes.
A quality control process may be a complete QA processing of a processed data set which must be executed independently from the L2, L3 or ECV merge processing. Each processing facility is responsible for quality control of the respective data sets.
Organization, monitoring and control of all operational product procurement processes. This includes the procurement of all needed input data. Detection and elimination of production errors.
Maintenance and update of the Ozone_cci+ components and system according to the common development of the used COTS and the approved pre-operational algorithm versions and Ozone_cci+ component deliveries.
- Maintenance of the resources of the Ozone_cci+ system regarding needed disk space, archive space, available processing nodes, available processing systems
- Monitoring of the Ozone_cci+ system.
This includes the monitoring of logfiles as well the listing of all available Ozone_cci+ products
- Provision of all output products from the Ozone_cci+ project. The simple open public ftp archive makes all output products accessible all time.

6.3.2 Algorithm/Processor Development Management (AM)

The Algorithm/Processor Development Management is an organizational component. It is organized with the help of the ALG-Teams 1, 2 and 3. The ALGT leader and the teams are responsible to fulfil the following functions:

- Definition of algorithm development priorities
Definition of algorithm/processor development priorities in order to control the operational product evolution.
This task has to be coordinated in interaction with the Climate Research Group (CRG) and the CCI Climate Modelling User Group (CMUG), the relevant science users, relevant instrument teams and relevant space agencies.
- Definition of new requirements
Collection and definition of new requirements for the development and improvement of the algorithms
- Coordination of algorithm development
Coordination of the algorithm development, according to the new requirements. This includes the organization of all necessary steps which ensure well defined version-controlled algorithm deliveries.
- Integration of new algorithm versions
Integration of new algorithm versions into the operational system within a pre-operational instance
- Triggering of validation procedure
Assurance of scientific quality of the ECV products triggering a subsequent verification and validation process of the pre-operational instance.
- This validation process is handled by the Validation team



7 Data Flow for ECV Production

7.1 Total Column Products

TC Products	Input Products		
	Gbyte	Gbyte/y	Cover. Years
GOME L1	720,00	45,00	16,00
SCIA L1	17408,00	1450,67	12,00
GOME2-A L1	82500,00	5500,00	15,00
GOME2-B L1	49500,00	5500,00	9,00
GOME2-C L1	16500,00	5500,00	3,00
OMI L1	18000,00	1000,00	18,00
OMPS L1	3700,00	370,00	10,00
S5P L2			
TC_GTO-ECV			
TC_GTO-ECV_ext			
Total	188328,00	19365,67	

TC Products	Intermediate Products L2			
	Factor L1/L2	Gbyte	Gbyte/y	Cover. Years
GOME L1	42,00	17,14	1,07	16



SCIA L1	470,00	37,04	3,09	12
GOME2-A L1	205,00	402,44	26,83	15
GOME2-B L1	205,00	241,46	26,83	9
GOME2-C L1	205,00	80,49	26,83	3
OMI L1	7,90	2278,48	126,58	18
OMPS L1	17,00	217,65	21,76	10
S5P L2		6616,00	1654,00	4
TC_GTO-ECV				
TC_GTO-ECV_ext				
Total		9890,70	1886,99	

TC Products	Intermediate Products L3			
	Factor L1/L3	Gbyte	Gbyte/y	Cover. Years
GOME L1	500	1,44	0,09	16
SCIA L1	16000	1,09	0,12	9
GOME2-A L1	15000	5,50	0,37	15
GOME2-B L1	15000	3,30	0,37	9
GOME2-C L1	15000	1,10	0,37	3
OMI L1	750	24,00	1,33	18
OMPS L1	250	14,80	1,48	10
S5P L2			2,12	4
TC_GTO-ECV	n/a	40,00	1,48	27
TC_GTO-ECV_ext				



Total		91,23	7,72	
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TC Products	ECV Merged Products			
	Factor L1/ECV	Gbyte	Gbyte/y	Cover. Years
GOME L1	1000	0,72	0,05	16
SCIA L1	16000	1,09	0,12	9
GOME2-A L1	15000	5,50	0,37	15
GOME2-B L1	15000	3,30	0,37	9
GOME2-C L1	15000	1,10	0,37	3
OMI L1	750	24,00	1,33	18
OMPS L1	250	14,80	1,48	10
S5P L2		8,48	2,12	4
TC_GTO-ECV		2,17	0,08	27
TC_GTO-ECV_ext		3,20	0,08	40
Total		50,51	6,36	

7.2 Nadir Profile Products

NP Products	Input Products		
	Gbyte	Gbyte/y	Cover. Years
GOME L1	600	37,50	16,00



SCIA L1	10000	1000,00	10,0
GOME2-A L1	40000	2857,14	14,0
GOME2-B L1	24000	3000,00	8
GOME2-C L1	4000	2000,00	2
OMI L1	17352	1020,71	17,0
S5P			
IASI-C L1	20600	5150,00	4,0
IASI-B L1	57500,00	5227,00	11,0
IASI-A L1	61000,00	5083,00	12,0
NP_GOP-ECV			
Total	235002,00	25375,35	

NP Products	Intermediate Products L2			
	Factor L1/L2	Gbyte	Gbyte/y	Cover. Years
GOME L1	1,00	720	45,00	16,00
SCIA L1	5,00	676	75,11	9,00
GOME2-A L1	10,00	1100	81,48	13,50
GOME2-B L1	36,59	656	82,00	8
GOME2-C L1	48,78	82	82,00	1
OMI L1	10,00	6000	352,94	17,0
S5P		Tbd	tbd	1,0
IASI-C L1 (original)	11,00 NP_L2	1939,00	484,00	4,00 (2020-2023)



IASI-B L1 (original)	11,50 (NP_L2)	5055	460,00	11 (2013-2023)
(reprocessed)	19 (CDR_NP_L2)	1100	275,00	4 (2020-2023)
IASI-A L1 (original)	12,00 (NP_L2)	5100	425	12 (2008-2019)
(reprocessed)	18,00 (CDR_NP_L2)	3400	283	12 (2008-2019)
NP_GOP-ECV				
Total		25828	2647,53	

NP Products	ECV Products L3			
	Factor L1/L3-ECV	Gbyte	Gbyte/y	Cover. Years
GOME L1	350	1,71	0,11	16
SCIA L1	12000	0,83	0,09	9
GOME2-A L1	18000	2,22	0,56	4
GOME2-B L1	tbd	Tbd	Tbd	Tbd
GOME2-C L1	tbd	Tbd	Tbd	Tbd
OMI L1	11500	1,51	0,22	7
S5P				
IASI-C L1	n/a	n/a	n/a	
IASI-B L1	n/a	n/a	n/a	
IASI-A L1	n/a	n/a	n/a	
NP_GOP-ECV				
Total		6,28	0,97	



NP Products	ECV Merged Products L3			
	Factor L1/L3 ECV	Gbyte	Gbyte/y	Cover. Years
GOME L1				
SCIA L1				
GOME2-A L1				
GOME2-B L1				
GOME2-C L1				
OMI L1				
S5P				
IASI-A/-B/-C L1	198	704	44	16
NP_GOP-ECV	n/a	0,075	0,003	27
Total		0,075	0,003	

7.3 Limb Profile Products

LP Products	Input Products		
	Gbyte	Gbyte/y	Cover. Years
SCIA L2	27,00	2,84	9,50
MIPAS L2		0,00	10,00



GOMOS L2	0,46	0,05	10,00
OSIRIS L2	9,70	0,42	23,00
ACE L2		0,006	21,00
SABER L2	211,2	9,60	22,00
MLS L2	69,00	3,63	19,00
OMPS	168	14,00	12,00
POAM-III	0,13	0,02	8,00
SAGE-III-M	1,90	0,54	3,50
SAGE-III-ISS	5,40	0,90	6,00
SAGE-CCI-OMPS			
MEGRIDOP			
LIMB-HIRES			
TrOC OMI-LIMB			
TrOC GTO-LIMB			
Total	492,79	31,8	

LP Products	Harmonized LP L2 Products			
	Factor L2/Har.L2	Gbyte	Gbyte/y	Cover. Years
SCIA L2	6,600	4,091	0,431	9,500
MIPAS L2	1,000	0,000	0,000	10,000
GOMOS L2	1,000	0,459	0,046	10,000
OSIRIS L2	1,000	9,700	0,423	23,000
ACE L2	1,000	0,140	0,006	23,000



SABER L2	3,000	67,000	3,000	22,000
MLS L2	1,000	69,000	3,625	19,000
OMPS	15,000	11,000	0,950	12,000
POAM-III	2,700	0,047	0,006	8,000
SAGE-III-M	67,000	0,028	0,008	3,500
SAGE-III-ISS	70,000	0,078	0,013	6,000
SAGE-CCI-OMPS				
MEGRIDOP				
LIMB-HIRES				
TrOC OMI-LIMB				
TrOC GTO-LIMB				
Total		161,5	8,51	

LP Products	LP L3 Products			
	Factor L2/L3-ECV	Mbyte	Mbyte/y	Cover. Years
SCIA L2	753	5,57	0,59	9,5
MIPAS L2	0	5,86	0,59	10,0
GOMOS L2	80	5,86	0,59	10,0
OSIRIS L2	739	5,86	0,59	10,0
ACE L2	0	5,86	0,59	10,0
SABER L2	0	5,86	0,59	10,0
MLS L2	6335	4,69	0,59	8,0
OMPS	0	5,86	0,59	10,0



POAM-III	10	5,86	0,59	10,0
SAGE-III-M	14	5,86	0,59	10,0
SAGE-III-ISS	16	5,86	0,59	10,0
SAGE-CCI-OMPS				
MEGRIDOP				
LIMB-HIRES				
TrOC OMI-LIMB				
TrOC GTO-LIMB				
Total		62,99	6,45	

LP Products	SAGE-CCI-OMPS, MEGRIDOP, LIMB-HIRES Merged Products			
	Factor L3/L3-ECV	Gbyte	Gbyte/y	Cover. Years
SCIA L2				
MIPAS L2				
GOMOS L2				
OSIRIS L2				
ACE L2				
SABER L2				
MLS L2				
OMPS				
POAM-III				



SAGE-III-M				
SAGE-III-ISS				
SAGE-CCI-OMPS		0,05	0,0049	10
MEGRIDOP		0,60	0,0602	10
LIMB-HIRES		15,50	0,9600	16
TrOC OMI-LIMB		0,80	0,0500	16
TrOC GTO-LIMB		0,80	0,0500	16
Total		17,75	1,1250	

7.4 MSR L4 Product

L4 MSR	Input Products		
	Gbyte	Gbyte/y	Cover. Years
L2 Input Products	12000,00	190,48	63
Meteo	14000,00	220,00	63
L4 MSR			
Total	26000,00	410,48	

L4 MSR	L4 MSR Output			
	Factor Inputs/L4 MSR	Gbyte	Gbyte/y	Cover. Years
L2 Input Products				
Meteo				



L4 MSR	52000,00	0,50	0,01	63
Total				

Table 7-1 Data_Flow



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