



Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

TITLE:

# Ozone\_cci+



# System Specification Document SSD

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Date of issue: 2022-04-07

Version: **02.00** 

Deliverable: D3.1

WP Manager: M. Wolfmüller

WP Manager Organization: DLR-EOC

Other partners:

BIRA, DLR, FMI, KNMI, RAL, ULB, UNI-HB, UoSASK, UoT



Reference: Ozone\_cci+\_DLR\_SS\_02\_00

# DOCUMENT PROPERTIES

Title SSD

Reference Ozone\_cci+\_DLR\_SS\_02\_00

Issue 2

Revision 00

Status Draft

Date of issue 2022-04-07

Document typeSystem Specification Document

	FUNCTION	NAME	DATE	SIGNATURE
LEAD AUTHOR	WP Manager SSD	M. Wolfmüller	07/04/2022	Original in hands of PM
CONTRIBUTING AUTHORS				
		Ronald van der A		
		Christophe Lerot		
		Melanie Coldewey-Egbers		
		Catherine Wespes		
		Richard Siddans, Barry Latter		
		Viktoria Sofieva		
		Alexei Rozanov, Carlo Arosio		
		Cris Roth, Daniel Zawada		
		Patrick Sheese		
REVIEWED BY		Diego Loyola		
ISSUED BY	WP Manager SSD	M. Wolfmüller		





Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

# DOCUMENT CHANGE RECORD

Issue	Revision	Date	Modified items	Observations
01	00	27/10/2020	-	Creation of document
01	00	22/12/2020	all	Insertion of contributions from the project members
01	00	29/01/2021	several	Insertion of contributions from the document review by the project members
02	00	07/04/2022	several	Insert contributions from project members



Issue: 02 - Revision: 00 - Status:Draft

Date of issue: 2022-04-07

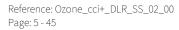
Reference: Ozone\_cci+\_DLR\_SS\_02\_00

# 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 serveral organizations.

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







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

# TABLE OF CONTENTS

1	Introduction	9
1.1	Scope and Applicability	g
1.2		
1	1.2.1 Terms and Definitions	
1	1.2.2 Abreviations	g
1.3	3 Applicable Documents	10
1.4	Reference Documents	10
1.5	Document Overview	10
2 (	General Description	12
2.1	Relation to Current Projects	12
2.2	2 Function and Purpose	12
2.3	Relation to other Systems and End Users	12
3 [	Design Approach	13
3.1	Component Description Approach	13
3.2	Scenario Description Approach	13
3.3	Interface Description Approach	13
4 9	System Overview	14
4.1	System Decomposition	14
4	4.1.1 Processing Domain	15
4	4.1.2 Product Handling Domain	16
4	4.1.3 Management Domain	17
4.2	2 Main Internal Interfaces	17
4.3	B Ozone_cci/cci+ Users	18
5 5	Scenarios (Use Cases)	19
5.1	Fundamental Operations and Scenarios	19
5	5.1.1 Production of Ozone Total Column ECV Parameter	
5	5.1.2 Production of Nadir Ozone Profile ECV Parameter	23
5	5.1.3 Production of Limb Ozone Profile ECV Parameter	23
_	5.1.4 Online Access to Ozone ECV Products	24



Issue: 2 - Revision: 00 - Status: Draft

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00 Page: 6 - 45

6 Sub	system and Subsystem Components	25
6.1	Processing Facilities for Nadir Ozone_cci+ Products	25
6.1.1	Processing Facility at BIRA	26
6.1.2	Processing Facility at DLR	28
6.1.3	Processing Facility at RAL	
6.1.4	Processing Facility at KNMI	
6.1.5	Processing Facility at ULB	
6.2 I	Processing Facilities for Limb Ozone_cci+ Products	34
6.2.1	Processing Facility at FMI	35
6.2.2	Processing Facility at UNI-HB	37
6.2.3	Processing Facility at UoT	
6.2.4	Processing Facility at UoSASK	40
6.3 I	Management Domain	41
6.3.1	Production Management (PM)	41
6.3.2	Algorithm/Processor Development Management (AM)	
7 Data	a Flow for ECV Production	43



Issue: 2 - Revision: 00 - Status: Draft

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00 Page: 7 - 45

# Figures

Figure 4-1 Ozone_cci+ System Decomposition into Domains	15
Figure 4-2 Ozone_cci+ System Decomposition with main Internal Interfaces	18
Figure 5-1 Overall ECV Production Scenarios for Ozone Total Column	22
Figure 5-2 Overall ECV Production Scenarios for Nadir Profile	23
Figure 5-3 ECV Production Scenarios for harmonized MZM Limb Products	24
Figure 6-1 Processing Facilities for TC	25
Figure 6-2 Processing Facilities for NP	26
Figure 6-3 Processing Facilities for LP	35



Issue: 2 - Revision: 00 - Status: Draft

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00 Page: 8 - 45

# Tables

Table 5-1 L2 Products	20
Table 5-2 Level 3 and L4 Products	21
Table 7-1 Data_Flow	44



Issue: 2 - Revision: 00 - Status: Draft

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 9 - 45

# 1 Introduction

# 1.1 Scope and Applicability

This document describes the operational Ozone\_cci+ production system in order to handle 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

# 1.2 Definitions, Acronyms and Abbreviations

Terms, definitions and abbreviations are collected within this document.

# 1.2.1 Terms and Definitions

Term	Explanation of the term	
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 Abreviations

abbreviation Explanation of the abbreviation (tbc)
API Application Programming Interface
ADM Algorithm Development Management

CCI Climate Change Initiative
CCI+ Climate Change Initiative +
CRG Climate Research Group

CMUG CCI Climate Modelling User Group

ECMWF European Centre for Medium-Range Weather Forecasts

ECV Essential Climate Variable



Issue: 2 - Revision: 00 - Status: Draft

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 10 - 45

ESA European Space Agency
HMI Human Machine Interface

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

# 1.3 Applicable Documents

[AD1] Data Standards Requirements for CCI Data Producers. Latest version at time of writing is v1.2: ref. CCI-PRGM-EOPS-TN-13-0009, 9 March 2015, available online at: http://cci.esa.int/sites/default/files/CCI\_Data\_Requirements\_Iss1.2\_Mar2015.pdf

[AD2] CCI Data Policy v1.1. Available online at: https://earth.esa.int/documents/10174/1754357/RD-7\_CCI\_Data\_Policy\_v1.1.pdf

[AD3] Algorithm Development Plan (ADP) v1.0, Available online at:

[AD4] SSD, Ozone\_cci System Specification Document, available from http://www.esa-ozone-cci.org/?q=documents [public/deliverables]System Requirements Document from Phase 2

# 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 contents the purpose and the scope of the Ozone\_cci+ system.



Issue: 2 - Revision: 00 - Status: Draft

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 11 - 45

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.

Chapter 6 shows the component descoposition.

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



Issue: 2 - Revision: 00 - Status: Draft

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 12 - 45

# 2 General Description

# 2.1 Relation to Current Projects

The Ozone\_cci+ project further develops the ozone ECVs generated in the Ozone\_cci projects of phase I and II. 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 Ozone CCI phase II 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 ancilliary 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.



Reference: Ozone\_cci+\_DLR\_SS\_02\_00



Issue: 2 - Revision: 00 - Status: Draft

Date of issue: 2022-04-07

Page: 13 - 45

# 3 Design Approach

This chapter describes the approaches used for the descriptions of the scenarios, system components and interfaces. UML diagrames 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.





Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 14 - 45

# 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 the 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 administrational components.

# 4.1 System Decomposition

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



Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 15 - 45

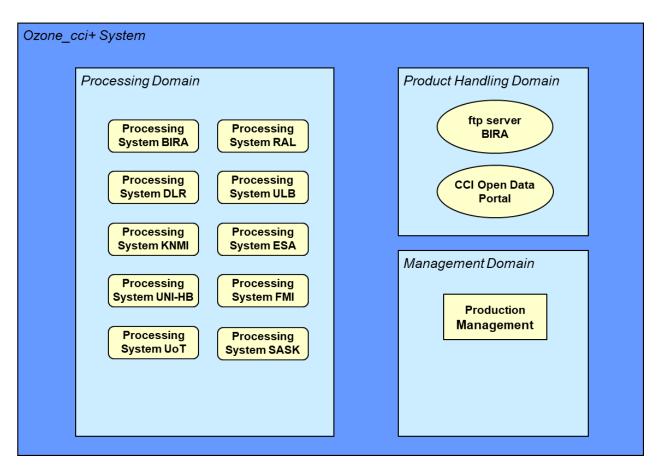


Figure 4-1 Ozone\_cci+ System Decomposition into Domains

A detailed description of the functionality of the Ozone\_cci+ components are 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 Servce (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/C3S\_312b\_Lot2.1.1.2\_201902\_ATBD\_O3\_v1.1a.pdf)



Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00 Page: 16 - 45

# 4.1.1.1 Processing System BIRA

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

# 4.1.1.2 Processing System DLR

This processing system generates (a) L3 TC products for GOME2-A, -B, -C, OMI, OMPS, and S5P, (b) L3 NP products for GOME2-A, -B and OMI, and (c) the Merged L3 TC and NP products.

# 4.1.1.3 Processing System RAL

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

# 4.1.1.4 Processing System KNMI

This processing system generates the L4 Monthly mean total ozone products.

# 4.1.1.5 Processing System ULB

This processing system generates the L2 NP products for IASI-A, -B and -C. The Climate L2 NP products for IASI-A (and possibly -B and -C), developed at ULB, is implemented on the CICLAD-IPSL computing facility).

# 4.1.1.6 Processing System FMI

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

# 4.1.1.7 Processing System UNI-HB

This processing system generates L2 HARMOZ products for SABER, MLS, POAM-III, SAGE-III-M and SAGE\_III-ISS.

#### 4.1.1.8 Processing System SASK

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

# 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).





Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 17 - 45

# 4.1.3 Management Domain

# 4.1.3.1 Production Management

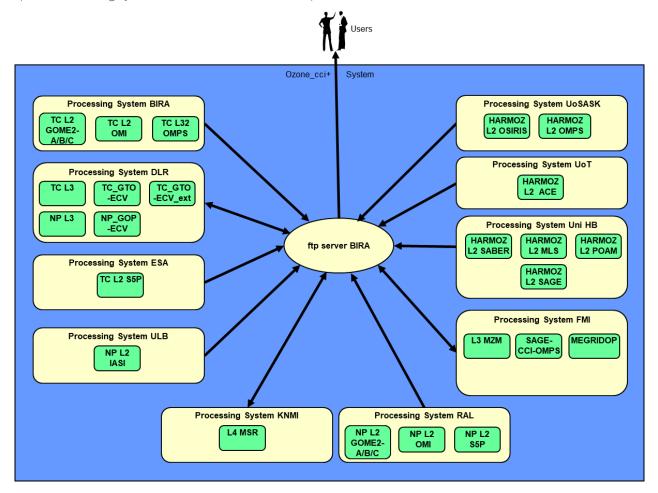
Production Management provides tools and procedures for the operator to handle the system processes and to allow data access to the users. It is an organizational component which is responsible for the organization, monitoring and operation of all defined production and dissemination processes. The production 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 (CRG) 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.





Issue: 2 - Revision: 00 - Status: Draft

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 18 - 45

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 for these products transfer. In practices these products 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.



Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 19 - 45

# 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 be generated by the Ozone\_cci+ system.

L2 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 from GOME2-C 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
Climate_NP_L2_IASI-A (- B, -C)	Climate L2 Processing System ULB	Processing of FORLI-Clim-O3 products from IASI-A from 2008 to present over selected stations.





Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00 Page: 20 - 45

HARMOZ_OSIRIS_L2	LP L2 Processing System SASK	Processing of data from 2001-11 to present
HARMOZ_ACE_L2	LP L2 Processing System UoT	Processing of data from 2004-02 to present
HARMOZ_OMPS_L2	LP L2 Processing System SASK	Processing of data from 2012-02 to present
HARMOZ_SABER_L2	LP L2 Processing System UNI-HB	Processing of data from 2002-01 to present
HARMOZ_MLS_L2	LP L2 Processing System UNI-HB	Processing of data from 2004-08 to present
HARMOZ_POAM-III_L2	LP L2 Processing System UNI-HB	Processing of data from 1998-04 to 2005-12
HARMOZ_SAGE-III-M_L2	LP L2 Processing System UNI-HB	Processing of data from 2002-06 to 2005-11
HARMOZ_SAGE-III-ISS_L2	LP L2 Processing System UNI-HB	Processing of data from 2017-06 to present

Table 5-1 L2 Products

L3/L4 Data Product	Processing Facility	Processing Results
TC_L3_GOME2-A	9	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
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



Issue: 2 - Revision: 00 - Status: Draft

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00 Page: 21 - 45

		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
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
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	no further processing because no new data available
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 LatLon dataset, which was developed in CCI.

Table 5-2 Level 3 and L4 Products

Issue: 2 - Revision: 00 - Status: Draft

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 22 - 45

# 5.1.1 Production of Ozone Total Column ECV Parameter

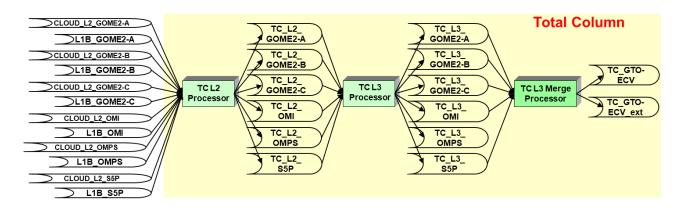


Figure 5-1 Overall ECV Production Scenarios for Ozone Total Column

# 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.

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 23 - 45

# 5.1.2 Production of Nadir Ozone Profile ECV Parameter

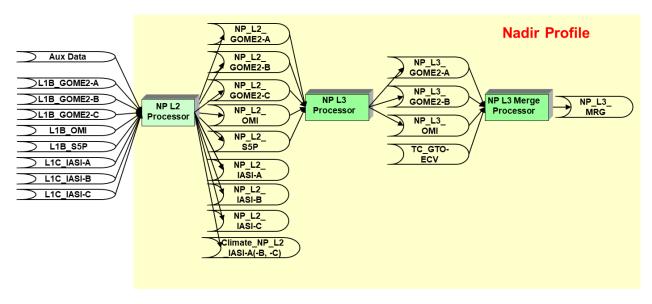


Figure 5-2 Overall ECV Production Scenarios for Nadir Profile

# 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 and OMI.

• 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 products
- Production of the MEGRIDOP products



Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 24 - 45

# 5.1.3.1 Full Processing Scenario for the harmonized Limb Profile Products

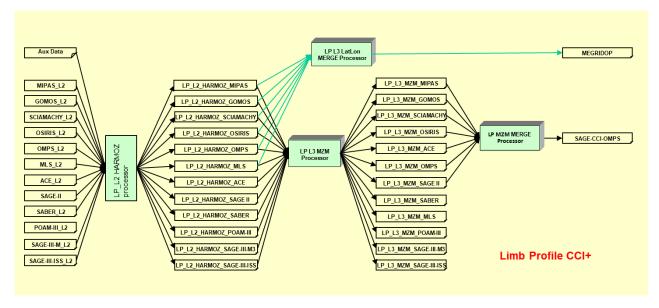


Figure 5-3 ECV Production Scenarios for harmonized MZM Limb Products

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 L3 data for MEGRIDOP product.
- Creating netcdf files

# 5.1.4 Online Access to Ozone ECV Products

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



Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 25 - 45

# 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 chapter 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 ESA

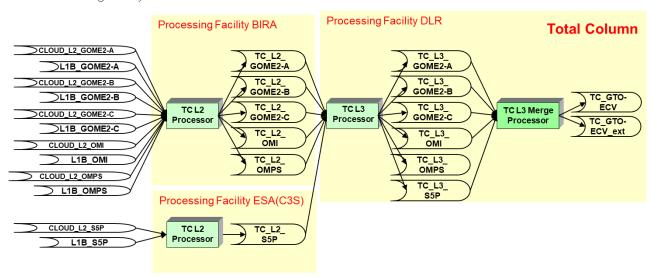


Figure 6-1 Processing Facilities for TC

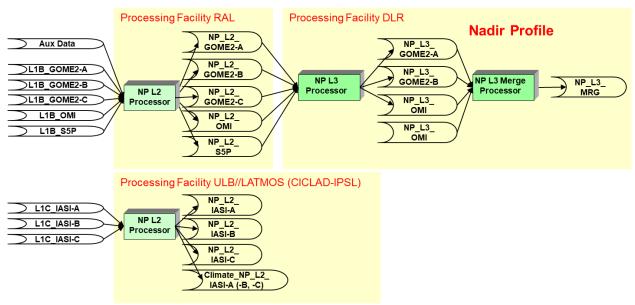


Issue: 2 - Revision: 00 - Status: Draft

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 26 - 45



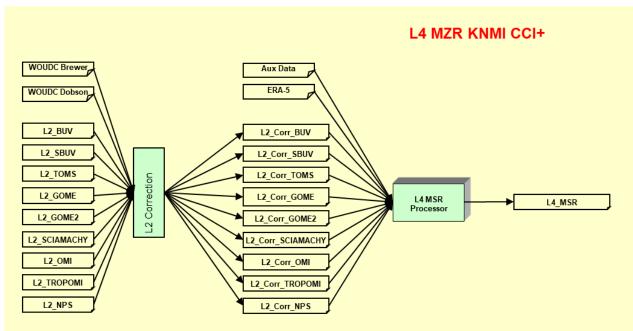


Figure 6-2 Processing Facilities for NP

# 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





Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00 Page: 27 - 45

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
 CLOUD\_L2\_GOME2-A,B,C
 TC\_L1B\_OMI
 CLOUD\_L2\_OMI
 CLOUD\_L2\_OMI
 TC\_L1B\_OMPS
 CLOUD\_L2\_OMPS
 CLOUD\_L2\_OMPS
 Original LB OMI products for OMI
 original LB OMPS products
 cloud L2 products for 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 60GB, 24 nodes with 250GB
- Intern connectivity ensured by ethernet over InfiniBand.

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00 Page: 28 - 45

- 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

# 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)



Issue: 2 - Revision: 00 - Status: Draft

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 29 - 45

#### 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

#### 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



Issue: 2 - Revision: 00 - Status: Draft

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 30 - 45

#### 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

#### 6.1.2.5 Hardware Environment

The technical characteristics of the used system are:

- Linux cluster
- 16 CPUs
- Disc space for L2 input data:
   ~8.5Tb + ~2Tb/year for each additional year
- Disc space for generated L3 data ~200Gb + ~10Gb/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



Issue: 2 - Revision: 00 - Status: Draft

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 31 - 45

# 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 ERA 5 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?
- Cloud product for S5P?

#### 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.
- The processing is performed on 512 dedicated processing cores with frequent access to 2000 more when available. These processors mostly comprise Intel Xeon E5-2650 v2 "Ivy Bridge" (Viglen HX525T2i) each with 16 cores and either 128, 256 or 512Gb memory. In general about 2000 individual orbits (or PDU's) run concurrently on the system.
- Typically 4Gb RAM and 2 Gb disc space will be used by each job.

# 6.1.4 Processing Facility at KNMI

#### 6.1.4.1 Description

This processing facility provides the processors:

MSR2 Processor



Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00 Page: 32 - 45

#### 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 observation.

#### 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:

- Special computing facilities consisting of blades and virtual blades on a central KNMI computing facility
- Intel Xeon CPU 3GHz
- Used resources: 1 CPU, 16 GB RAM and 150 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/ LATMOS (CYCLAD-IPSL)

# 6.1.5.1 Description

The processing facility at ULB provides the processors:

• NP L2 Processor

The processing facility at LATMOS (CYCLAD-IPSL) provides the processors:

• Climate NP L2 Processor

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00 Page: 33 - 45

# 6.1.5.2 Processors

Title	NP L2 Processor/ Climate NP L2 Processor
Name	FORLI-O3/ FORLI-Clim-O3
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/ FORLI-Clim-O3

# 6.1.5.3 Functions

The processing facility provides the following functions:

- Generation of NP\_L2\_IASI-A, B, C products from IASI-A,B,C L1 products
- Transfer all generated and validated NP\_L2\_IASI products to the FTP Server

# 6.1.5.4 Interfaces and Interface Items

#### Inputs

# In FORLI-03:

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

# In FORLI-Clim-O3:

- Reprocessed L1C IASI-A (-B, -C) products
- Auxiliary Data:
  - o ECMWF ERA-5 reanalysis as input for temperature and humidity
  - o FORLI look-up tables
  - o orography/emissivity

# Outputs:

- NP\_L2\_IASI-A
- NP\_L2\_IASI-B
- NP\_L2\_IASI-C
- Climate\_NP\_L2\_IASI-A (-B, -C)

# 6.1.5.5 Hardware Environment

## At ULB:

- 3 PC INTEL Servers each one includes:
  - o 32 or 8GB RAM
  - o 36 or 12TB storage (RAID-6)



Issue: 2 - Revision: 00 - Status: Draft

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 34 - 45

- o ARCH x86\_64
- 3 NAS SYNOLOGY servers with a total of:
  - o -20GB RAM
  - o -162 TB storage (RAID-5)
  - o -DSM 6
- 1 LINUX CLUSTER including:
  - o Torque/Maui PBS scheduler
  - o 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 LATMOS/IPSL:

- One multi-CPU cluster called CICLAD and maintained by IPSL to process the IASI data, including:
  - o 20 Computing nodes 1152 cores
  - o 4 nodes with 32 cores 128Gb AMD Opteron
  - o 16 nodes with 64 cores 256Gb AMD Opteron

# 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



Issue: 2 - Revision: 00 - Status: Draft

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 35 - 45

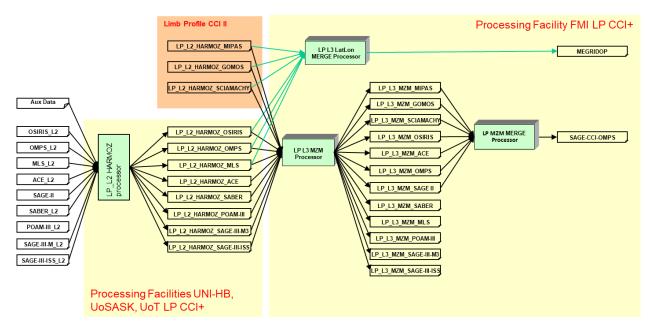


Figure 6-3 Processing Facilities for LP

# 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

# 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	
---------------------------	--



Issue: 2 - Revision: 00 - Status: Draft

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 36 - 45

Name	LP L3 LatLon MERGE Processor  Creating semi-monthly mean ozone profiles in 10°x20° latitude-longitude bins for each sensor. Evaluation of associated uncertainties.	
Description		
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	

# 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)



Issue: 2 - Revision: 00 - Status: Draft

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 37 - 45

 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 POAM-III Processor
- LP L2 SAGE-III-M 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 > mean + 3 mad of the distribution at P > 50 hPa.	
Used Algorithm	harmoz_saber_v20_cv01.py processed with python software	

Title	LP L2 SAGE-III-M Processor	
Name	HARMOZ_SAGE-III-M3	
Description	The processor ingests orbit-wise L2 measurements to produce monthly HARMOZ files. Initial version of the processing, which takes into account the 'Retrieval flag' in L2 data to filter the profiles.	
Used Algorithm	harmoz_sagellIMeteor_v42_cv02.py processed with python software	

Title	LP L2 SAGE-III-ISS Processor	
Name	HARMOZ_SAGE-III-ISS	
Description	The processor ingests orbit-wise L2 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.	



Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 38 - 45

Used Algorithm	harmoz_sageIlliss_v52_cv02.py processed with python software
----------------	--

Title	L2 POAM-III Processor	
Name	HARMOZ POAM-III	
Description	The processor ingests monthly data and interpolates them onto CCI grid by using ECMWF ERA-Interim pressure profiles. The provided quality flag for ozone data is taken into consideration	
Used Algorithm	harmoz_poamIII_v4_cv02.py processed with python software	

Title	P 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 ERA 5information.	
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-M 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\_POAM-III products
- Generation of harmonized LP\_L2\_HARMOZ\_OMPS-LP UBR products
- Transfer all generated and validated LP\_L2\_HARMOZ products for SABER, SAGE-III-M, SAGE-III-ISS, MLS, POAM-III, 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



Issue: 2 - Revision: 00 - Status: Draft

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 39 - 45

SAGE-III-M\_L2 original L2 v4 SAGE-III-M products
 SAGE-III-ISS\_L2 original L2 v5.2 SAGE-III-ISS products

MLS\_L2 original L2 v5 MLS products
 POAM-III\_L2 original L2 v4 POAM-III products

• OMPS-LP UBR L2 original L2 v3.3 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-M2	harmonized Limb Profile L2_HARMOZ products for SAGE-III-M
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_POAM-III	harmonized Limb Profile L2_HARMOZ products for POAM-III
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



Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 40 - 45

• 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



Issue: 2 - Revision: 00 - Status: Draft

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 41 - 45

#### 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 Group (CRG), the relevant science users, relevant instrument teams and relevant space agencies.



Issue: 2 - Revision: 00 - Status: Draft

Date of issue: 2022-04-07

Reference: Ozone\_cci+\_DLR\_SS\_02\_00

Page: 42 - 45

• 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



Issue: 01 - Revision: 00 - Status: Final

Date of issue: 2021-01-29

Reference: Ozone\_cci+\_DLR\_SS\_01\_00 Page: 43 - 45

# 7 Data Flow for ECV Production

The following table gives an overview about the data flow required for the production of the ECVs. The amount of L2, L3 and ECV data is derived from the input data reduced by predefined scaling factors for the several processing steps.



Meteo L4 MSR

Total

Input Products L4 MSR

L2 Input Products

12000,00

14000,00

26000,00

Gbyte

190,48

410,48

Cover. Years

63,00

63,00

63,00

Gbyte/y

L4 MSR Output Factor Inputs/L4 MSR TITLE: System Specification Document

Issue: 01 - Revision: 00 - Status: Final

Date of issue: 2021-01-29

Reference: Ozone\_cci+\_DLR\_SS\_01\_00 Page: 44 - 45

Input Products T	otal Column			Intermediate Products				Intermediate Pro	ducts L3			ECV Merged Products			
	Gbyte	Gbyte/y	Cover. Years	Factor L1/L2	Gbyte	Gbyte/y	Cover. Years	Factor L1/L3	Gbyte	Gbyte/y	Cover. Years	Factor L1/ECV	Gbyte	Gbyte/y	Cover. Years
GOME L1	720,00	45,00	16,00	42,00	17,14	1,07	16,00	500	1,44	0,09	) 16	1000	0,72	0,05	
SCIA L1	17408,00	1450,67	12,00	470,00	37,04	3,09	12,00	16000	1,09	0,12	2 9	16000	1,09	0,12	
GOME2-A L1	82500,00	5500,00	15,00	205,00	402,44	26,83	15,00	15000	5,50	0,37	7 15	15000	5,50	0,37	
GOME2-B L1	49500,00	5500,00	9,00	205,00	241,46	26,83	9,00	15000	3,30	0,37	7 9	15000	3,30	0,37	
GOME2-C L1	16500,00	5500,00	3,00	205,00	80,49	26,83	3,00	15000	1,10	0,37	7 3	15000	1,10	0,37	
OMI L1	18000,00	1000,00	18,00	7,90	2278,48	126,58	18,00	750	24,00	1,33	3 18	750	24,00	1,33	
OMPS L1	3700,00	370,00	10,00	17,00	217,65	21,76	10,00	250	14,80	1,48	3 10	250	14,80	1,48	
S5P L2	· ·	·			6616,00	1654,00	4,00			2,12	2 4		8,48	2,12	
TC GTO-ECV								n/a	40,00	1,48	3 27		2,17	0,08	
TC GTO-ECV ex	:												3,20	0,08	
Total	188328,00	19365,67			9890,70	1886,99			91,23	7,72	2		50,51	6,36	
nput Products N	adir Profile			Intermediate Products	L2			ECV Products L3				ECV Products			
		Gbyte/y	Cover. Years		Gbyte	Gbyte/y		Factor L1/L3-ECV	Gbyte	Gbvte/v	Cover. Years	Factor L1/L4 ECV	Gbyte	Gbyte/y	Cover. Yea
GOME L1	600	37,50	16,00				16,00	350		, ,			,		
SCIA L1	10000	1000,00	10,0				9,00	12000							
GOME2-A L1	40000	2857.14	14,0			81.48		18000							
GOME2-B L1	24000	3000.00	8			82.00		tbd	tbd	tbd	tbd				
GOME2-C L1	4000	2000.00	2	,				tbd	tbd	tbd	tbd				
OMI L1	17352	1020,71	17.0				17,0	11500							
S5P	1		,-	-,	tbd	tbd	1.0		1,5	-,					
IASI-C L1	8800.00	5866.67	1,50				1,50	tbd	tbd	tbd	tbd				
IASI-B L1	40500,00	5400.00	7.50			480.00	7,50		tbd	tbd	tbd				
IASI-A L1	69200.00	5125.93	13.50			422,22	13,50		tbd	tbd	tbd				
NP GOP-ECV		0.120,00	,	,	0.00,00	,	,		1			tbd	tbd	tbd	tbd
Total	214452.00	26307.94			19154,00	2034,09			6.28	0,97	,		0,00	0	
	,,,,,,	,-			,,,,	,,,,			-, -	.,.			.,	-	
Input Products L	imb Profile			Harmonized LP L2 Pro	ducts			LP L3 Products				SAGE-CCI-OMPS. MEGR	DOP Merge	d Products	
	Gbyte	Gbyte/y	Cover. Years	Factor L2/Har.L2	Gbyte	Gbyte/y	Cover. Years	Factor L2/L3-ECV	Mbvte	Mbvte/v	Cover. Years	Factor L3/L3-ECV	Gbyte	Gbyte/y	Cover, Yea
SCIA L2	27,00	2,84	9,50					753						,,	
MIPAS L2	,,,,,	0,00	10,00				10,00	0	5,86						
GOMOS L2	0,46	0,05	10,00				10,00	80							
OSIRIS L2	5,50	0,42	13,00			0,42	13,00	739	5,86						
ACE L2	3,00	0,00	10,00	1,00		0,00	10,00	0							
SABER L2		0,00	10,00			0,00	10,00	0	5,86						
MLS L2	29,00	3,63	8,00			3,63	8,00	6335							
	,	0,00	10,00			0,00	10,00	0			10,0				
		0.02	8,00				8,00	10	-,	-,-					
OMPS	0,13				-,			14	-,						
OMPS POAM-III	0,13 1,90		3.50	67.00	0.03	0.01	J.5U.	14							
OMPS POAM-III SAGE-III-M	-, -	0,54 0,70	3,50 3,00		0,03	0,01	3,50 3,00	16							
OMPS POAM-III SAGE-III-M SAGE-III-ISS SAGE-CCI-OMPS	1,90 2,10	0,54											0,05	0,0049	
OMPS POAM-III SAGE-III-M SAGE-III-ISS	1,90 2,10	0,54											0,05	0,0049 0,0602	

0,50

Gbyte

52000,00

0,01

Cover. Years

63,00

Gbyte/y



Issue: 01 - Revision: 00 - Status: Final

Date of issue: 2021-01-29

Reference: Ozone\_cci+\_DLR\_SS\_01\_00

Page: 45 - 45