

# Precursors\_cci+

## ESA Climate Change Initiative (CCI)



### D3.1 System Specification Document (SSD) Version 2

|               |                                    |
|---------------|------------------------------------|
| Title         | D3.1 System Specification Document |
| Reference     | Precursors_cci+_D3.1_SSD_02_01     |
| Issue         | 02                                 |
| Revision      | 01                                 |
| Status        | Final                              |
| Date of issue | 24/09/2025                         |
| Document type | Deliverable                        |

*This work has received funding from the European Space Agency under Contract No 4000138243 and is the result of the cooperation between the partners of the Precursors\_cci+ consortium.*



Koninklijk Nederlands  
Meteorologisch Instituut  
Ministerie van Infrastructuur en Waterstaat



University  
of Bremen





|                | FUNCTION                          | NAME                                                                                                                                                                                                                                            | DATE                         |
|----------------|-----------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------|
| LEAD AUTHOR(S) | M. Van Roozendael                 | Folkert Boersma<br>Isolde Glissenaar<br>Isidora Anglou<br>Melanie Coldewey-Egbers<br>Isabelle De Smedt<br>Thomas Danckaert<br>Nicolas Theys<br>Lieven Clarisse<br>Cathy Clerbaux<br>Maya George<br>Sora Seo<br>Klaus-Peter Heue<br>Diego Loyola | 24/09/2025                   |
| REVIEWED BY    | Science Leaders                   | M. Van Roozendael<br><br>Folkert Boersma                                                                                                                                                                                                        | 24/09/2025<br><br>24/09/2025 |
|                | ESA Project Officer               | Simon Pinnock                                                                                                                                                                                                                                   | ../../....                   |
| DISTRIBUTED TO | ESA<br>Precursors_cci+ Consortium |                                                                                                                                                                                                                                                 |                              |



## Table of Contents

|                                               |    |
|-----------------------------------------------|----|
| EXECUTIVE SUMMARY                             | 5  |
| 1. PURPOSE AND SCOPE                          | 6  |
| 1.1. Purpose and scope                        | 6  |
| 1.2. Applicable documents                     | 6  |
| 1.3. Reference documents                      | 6  |
| 1.4. List of acronyms                         | 7  |
| 2. SYSTEM OVERVIEW                            | 9  |
| 2.1. System decomposition                     | 10 |
| 2.2. Processing Domain                        | 10 |
| 2.2.1. NO <sub>2</sub> processing system KNMI | 10 |
| 2.2.2. NO <sub>2</sub> processing system DLR  | 10 |
| 2.2.3. HCHO processing system BIRA            | 10 |
| 2.2.4. HCHO processing system DLR             | 11 |
| 2.2.5. CHOCHO processing system BIRA          | 11 |
| 2.2.6. SO <sub>2</sub> processing system BIRA | 11 |
| 2.2.7. CO processing system LATMOS            | 11 |
| 2.2.8. NH <sub>3</sub> processing system ULB  | 11 |
| 2.3. Product Handling Domain                  | 11 |
| 2.4. Management Domain                        | 11 |
| 2.4.1. Production management                  | 11 |
| 2.4.2. Algorithm Development                  | 12 |
| 3. PROCESSING COMPONENTS                      | 12 |
| 3.1. NO <sub>2</sub> processing               | 12 |
| 3.2. HCHO processing                          | 14 |
| 3.3. SO <sub>2</sub> processing               | 17 |
| 3.4. CHOCHO processing                        | 19 |
| 3.5. CO processing                            | 21 |
| 3.6. NH <sub>3</sub> processing               | 22 |
| 4. PROCESSING FACILITIES                      | 24 |



|      |                               |    |
|------|-------------------------------|----|
| 4.1. | Processing facility at BIRA   | 24 |
| 4.2. | Processing facility at KNMI   | 24 |
| 4.3. | Processing facility at DLR    | 24 |
| 4.4. | Processing facility at ULB    | 25 |
| 4.5. | Processing facility at LATMOS | 25 |
| 5.   | DATA FLOW FOR ECV PRODUCTION  | 25 |

## Table of Figures and Tables

|                                                                                 |    |
|---------------------------------------------------------------------------------|----|
| Figure 1: Precursors_cci+ System Decomposition into Domains.....                | 9  |
| Figure 2: Overall ECV Production Scenarios for NO <sub>2</sub> columns .....    | 12 |
| Figure 3: Overall ECV Production Scenarios for HCHO columns.....                | 15 |
| Figure 4: ECV production scenario for CHOCHO columns .....                      | 19 |
| Figure 5: ECV production scenario for CO columns .....                          | 21 |
| Figure 6: ECV production scenario for NH <sub>3</sub> columns. ....             | 22 |
| Table 1: Information on NO <sub>2</sub> L2 processing. ....                     | 13 |
| Table 2: L3 Products processed for NO <sub>2</sub> and where to find them ..... | 14 |
| Table 3: Information on HCHO L2 processing. ....                                | 16 |
| Table 4: Information on HCHO L3 processing. ....                                | 16 |
| Table 5: Information on SO <sub>2</sub> L2 processing. ....                     | 18 |
| Table 6: Information on SO <sub>2</sub> L3 processing. ....                     | 18 |
| Table 7: Information about CHOCHO L2 processing.....                            | 20 |
| Table 8: Information about CHOCHO L3 processing.....                            | 20 |
| Table 9: Information on CO L3 processing. ....                                  | 22 |
| Table 10: Information on CO L3 merged processing.....                           | 22 |
| Table 11: Information on NH <sub>3</sub> pre-processing. ....                   | 23 |
| Table 12: Information on the NH <sub>3</sub> L2 processing. ....                | 23 |
| Table 13: Information on the NH <sub>3</sub> L3 processing. ....                | 23 |
| Table 14: Information on the NH <sub>3</sub> L3 merged processing.....          | 23 |
| Table 15: HPDA clusters hosted at the Leibniz Supercomputing Centre.....        | 24 |
| Table 16: NO <sub>2</sub> processing .....                                      | 26 |
| Table 17: HCHO processing .....                                                 | 26 |
| Table 18: SO <sub>2</sub> processing .....                                      | 27 |
| Table 19: CHOCHO processing .....                                               | 27 |
| Table 20: CO processing .....                                                   | 27 |
| Table 21: NH <sub>3</sub> processing .....                                      | 28 |



## Executive Summary

This document is the second version of the SSD, which contains a complete description of the systems at the end of the second cycle of the project.

The System Specification Document (SSD, deliverable D3.1) describes the processing system used to generate and distribute the ESA Precursors\_cci+ ECV data products. It includes an overall description of the main functionalities of the system, as well as detailed specifications of the processing components, processing facilities and the data flow for ECV production. The Precursors\_cci+ system consists of well-established subsystems distributed over several organizations.

# 1. Purpose and scope

## 1.1. Purpose and scope

This document describes the Precursors\_cci+ operational production system, i.e. the various systems and subsystems used to process and distribute the CCI+ Precursors ECV products. It also includes information regarding lifecycle and hardware solutions in place.

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 data products.

The species being generated include total columns of the following short-lived atmospheric trace gases: nitrogen dioxide (NO<sub>2</sub>), sulphur dioxide (SO<sub>2</sub>), carbon monoxide (CO), formaldehyde (HCHO), ammonia (NH<sub>3</sub>) and glyoxal (CHOCHO). The data records originate from measurements from the satellite sounders IASI A/B/C, MOPITT, TROPOMI, OMI, ERS2-GOME, GOME-2 A/B/C and SCIAMACHY.

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

## 1.2. Applicable documents

[AD-1] Data Standards Requirements for CCI Data Producers. Latest version at time of writing is v1.2: ref. CCI-PRGM-EOPS-TN-13-0009, 9 March 2015, available online at: [https://climate.esa.int/media/documents/CCI\\_DataStandards\\_v2-3.pdf](https://climate.esa.int/media/documents/CCI_DataStandards_v2-3.pdf)

[AD-2] CCI Data Policy v1.1. Available online at: [https://climate.esa.int/sites/default/files/CCI\\_Data\\_Policy\\_v1.1.pdf](https://climate.esa.int/sites/default/files/CCI_Data_Policy_v1.1.pdf)

## 1.3. Reference documents

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

[RD-2] Guideline for the Generation of Satellite-based Datasets and Products meeting GCOS Requirements, GCOS Secretariat, GCOS-128, March 2009 (WMO/TD No. 1488). Available online at: [https://library.wmo.int/index.php?lvl=notice\\_display&id=12884#.Yw4rL7RByUk](https://library.wmo.int/index.php?lvl=notice_display&id=12884#.Yw4rL7RByUk)

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

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



- [RD-5] Status of the Global Observing System for Climate, GCOS-195, October 2015. Available online at: [https://library.wmo.int/index.php?lvl=notice\\_display&id=18962#.Yw4r8LRByUk](https://library.wmo.int/index.php?lvl=notice_display&id=18962#.Yw4r8LRByUk)
- [RD-6] Hollmann, R., et al., The ESA climate change initiative: Satellite data records for essential climate variables. American Meteorological Society. Bulletin, Vol. 94, No. 10, 2013, p. 1541-1552.
- [RD-7] Joint Committee for Guides in Metrology, 2008, Evaluation of measurement data — Guide to the expression of uncertainty in measurement (GUM), JCGM 100: 2008. Available online at: <https://www.iso.org/sites/JCGM/GUM-JCGM100.htm>
- [RD-8] Merchant, C., et al., 2017, Uncertainty information in climate data records from Earth observation, Earth Syst. Sci. Data Discuss., vol. 9, p511-527

## 1.4. List of acronyms

|                 |                                                                         |
|-----------------|-------------------------------------------------------------------------|
| BIRA-IASB       | Royal Belgian Institute for Space Aeronomy                              |
| CAMS            | Copernicus Atmospheric Monitoring Service                               |
| CCI             | ESA Climate Change Initiative                                           |
| CO              | Carbon monoxide                                                         |
| COBRA           | COvariance-Based Retrieval Algorithm                                    |
| DLR             | German Aerospace Centre                                                 |
| DOAS            | Differential Optical Absorption Spectroscopy                            |
| ECMWF           | European Centre for Medium-range Weather Forecast                       |
| ECV             | Essential Climate Variable                                              |
| EO              | Earth Observation                                                       |
| ESA             | European Space Agency                                                   |
| EU              | European Union                                                          |
| EUMETSAT        | European Organisation for the Exploitation of Meteorological Satellites |
| GCOS            | Global Climate Observation System                                       |
| GOME            | Global Ozone Monitoring Instrument (aboard ERS-2)                       |
| GOME-2          | Global Ozone Monitoring Instrument – 2 (aboard MetOp-A, -B and -C)      |
| IASI            | Infrared Atmospheric Sounding Interferometer                            |
| HRI             | Hyperspectral Range Index                                               |
| KNMI            | Royal Netherlands Meteorological Institute                              |
| LUT             | Look-up table                                                           |
| Metop           | Meteorological Operational Platform (EUMETSAT)                          |
| MOPITT          | Measurement of Pollution in the Troposphere                             |
| NASA            | National Aeronautics and Space Administration                           |
| NH <sub>3</sub> | Ammonia                                                                 |
| NN              | Neural Network                                                          |
| NO <sub>2</sub> | Nitrogen dioxide                                                        |





|           |                                                                  |
|-----------|------------------------------------------------------------------|
| NRT       | Near-Real Time                                                   |
| OCRA      | Optical Cloud Recognition Algorithm)                             |
| OMI       | Ozone Monitoring Instrument (aboard EOS-Aura)                    |
| QA4ECV    | Quality Assurance for Essential Climate Variables                |
| SAF       | Satellite Application Facility                                   |
| SCIAMACHY | Scanning Imaging Absorption Spectrometer for Atmospheric         |
| S5P       | Sentinel-5 Precursor                                             |
| TROPOMI   | Tropospheric Monitoring Instrument (aboard Sentinel-5 Precursor) |
| ULB       | Université Libre de Bruxelles                                    |
| IUP-UB    | Institute of Environmental Physics, University of Bremen         |
| UPAS      | Universal Processor for UV/Vis Atmospheric Sensors               |
| UV-Vis    | Ultraviolet and visible spectral range                           |



## 2. System overview

The Precursors\_cci+ system can be separated into three main functional domains:

- Processing Domain
- Product Handling Domain
- Management Domain

Each functional domain is implemented in the form of one or more dedicated service components. Functional domains and their components are introduced in the subsections following this introduction.

The Processing Domain groups the functions related to the processing of the different data products. The Precursors\_cci+ production system relies on well established processing systems 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.

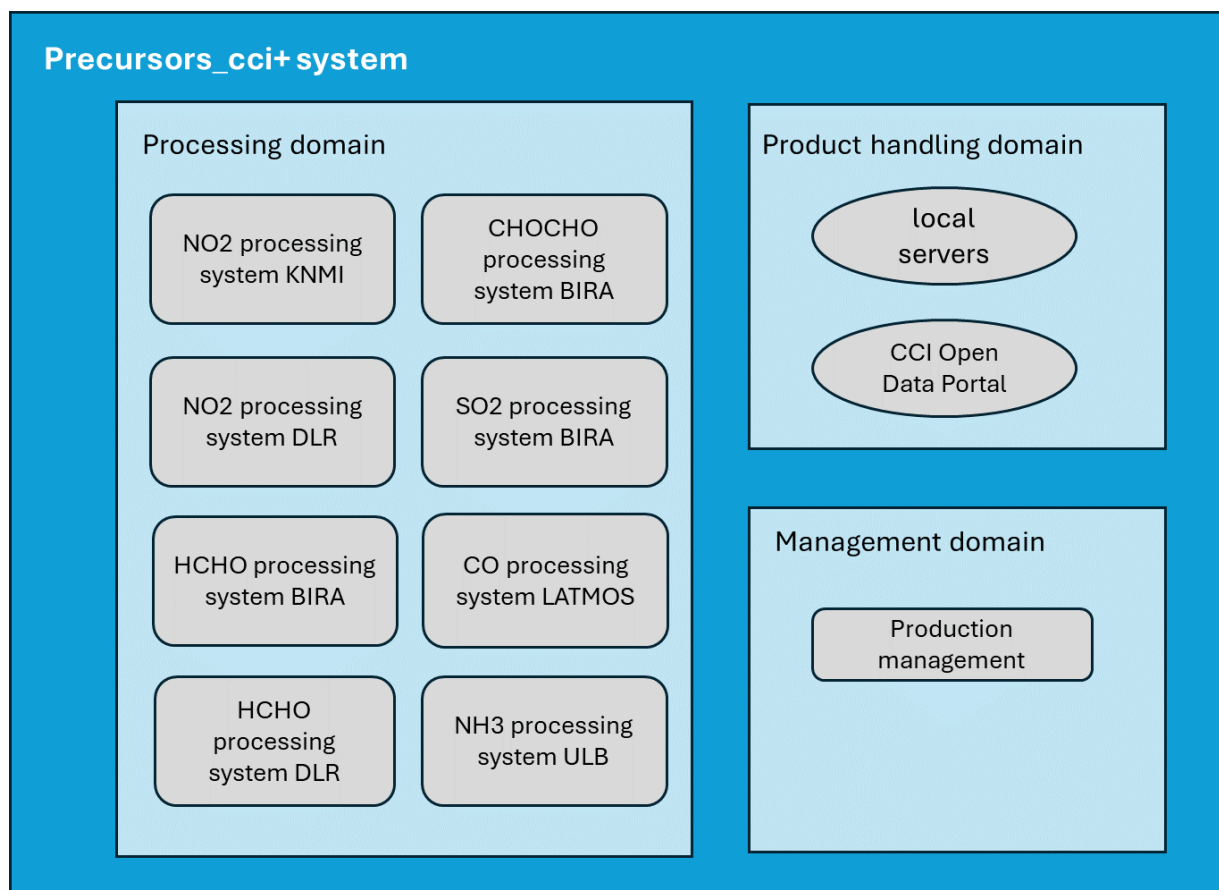


Figure 1: Precursors\_cci+ System Decomposition into Domains

The Product Handling Domain is reduced to the provision of the generated (intermediate) data sets on local servers operated by the project partners. Final level-3 products will be delivered to the ESA CCI Open Data Portal (<https://climate.esa.int/en/data/#/dashboard>).

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 the project's administrative components.

## 2.1. System decomposition

Figure 1 displays the technical and administrative components of the Precursors\_cci+ system. The administrative components in the Management Domain and the Product Handling Domain are responsible for specific organisational operations. The technical components (grey boxes) of the Processing Domain are provided by the specific science teams.

A detailed description of the functionality of these components is given in section 3. Their main functionalities are as follows.

## 2.2. Processing Domain

The processing domain consists of:

- NO<sub>2</sub> processing system KNMI
- NO<sub>2</sub> processing system DLR
- HCHO processing system BIRA
- HCHO processing system DLR
- CHOCHO processing system BIRA
- SO<sub>2</sub> processing system BIRA
- CO processing system LATMOS
- NH<sub>3</sub> processing system ULB

### 2.2.1. NO<sub>2</sub> processing system KNMI

This processing system generates the L2 tropospheric NO<sub>2</sub> columns from OMI, TROPOMI, GOME and SCIAMACHY sensors. It also deals with the production of L3 NO<sub>2</sub> data products assembled in afternoon merged data series based on OMI and TROPOMI (afternoon) sensors.

### 2.2.2. NO<sub>2</sub> processing system DLR

This processing system generates the L2 tropospheric NO<sub>2</sub> columns from the GOME, SCIAMACHY, and GOME-2 A/B/C sensors. It also deals with the production of L3 NO<sub>2</sub> data products assembled in morning merged data series based on GOME, SCIAMACHY and GOME-2 A/B/C.

### 2.2.3. HCHO processing system BIRA

This processing system generates the HCHO L2 total columns from OMI, TROPOMI, GOME and SCIAMACHY sensors. It also deals with the production of HCHO L3 data products assembled in morning and afternoon merged data series, respectively based on GOME, SCIAMACHY and GOME-2 A/B/C (morning sensors), and OMI and TROPOMI (afternoon) sensors.

#### 2.2.4. HCHO processing system DLR

This processing system generates the HCHO L2 total columns from the GOME-2 A/B/C sensors.

#### 2.2.5. CHOCHO processing system BIRA

This processing system generates the CHOCHO L2 total columns from the GOME-2 A/B/C and TROPOMI sensors. It also deals with the production of CHCHO L3 data products from the same sensors.

#### 2.2.6. SO<sub>2</sub> processing system BIRA

This processing system generates the SO<sub>2</sub> L2 total columns from the GOME, SCIAMACHY, OMI and TROPOMI sensors. It also deals with the production of a SO<sub>2</sub> merged L3 data products from the same sensors.

#### 2.2.7. CO processing system LATMOS

This processing system generates the CO L3 merged product, which is based on a combination of data from the IASI A/B/C sensors and the MOPITT instrument.

#### 2.2.8. NH<sub>3</sub> processing system ULB

This processing system generates the NH<sub>3</sub> L2 total columns from the IASI A/B/C sensors. It also deals with the production of a NH<sub>3</sub> merged L3 data products from the same sensors.

### 2.3. Product Handling Domain

L3 data product management is provided in a decentralised way by the different organisations in charge of data generation. The IASI products come via AERIS (<https://iasi.aeris-data.fr/>), the HCHO products via the BIRA-IASB distribution portal (<https://distributions.aeronomie.be/22d149ff-cc22-4ca6-9b1e-762e09ebe4bb>) and the NO<sub>2</sub> products via the TEMIS web-site (<https://www.temis.nl/airpollution//no2col/cci-no2-tropomi.php>). Note that the final L3 CCI+ products will also be progressively available via the CCI Open Data Portal (<https://climate.esa.int/en/projects/precursors-for-aerosols-and-ozone/>).

### 2.4. Management Domain

#### 2.4.1. Production management

Production Management provides tools and procedures allowing the operator to handle the system and for users to access the data. It is an organizational component 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.

## 2.4.2. Algorithm Development

Algorithm developments include the development, testing, installation and system update and their validation. These procedures and tasks are defined and handled by the project algorithm team.

## 3. Processing components

This section describes the organisation of the processing for each molecule and upon relevance for each sensor involved in the ECV data production. The following aspects are addressed:

- processing chains from L1 to L2 to L3 products
- software tools used at the different steps
- reference to external processing environments
- responsibilities at the different steps of the processing

### 3.1. NO<sub>2</sub> processing

The algorithm to produce NO<sub>2</sub> column ECV parameters is described in detail in the CCI+ precursor ATBD (D2.1 Algorithm Theoretical Basis Document). The overall ECV production for NO<sub>2</sub> column is shown in Figure 2.

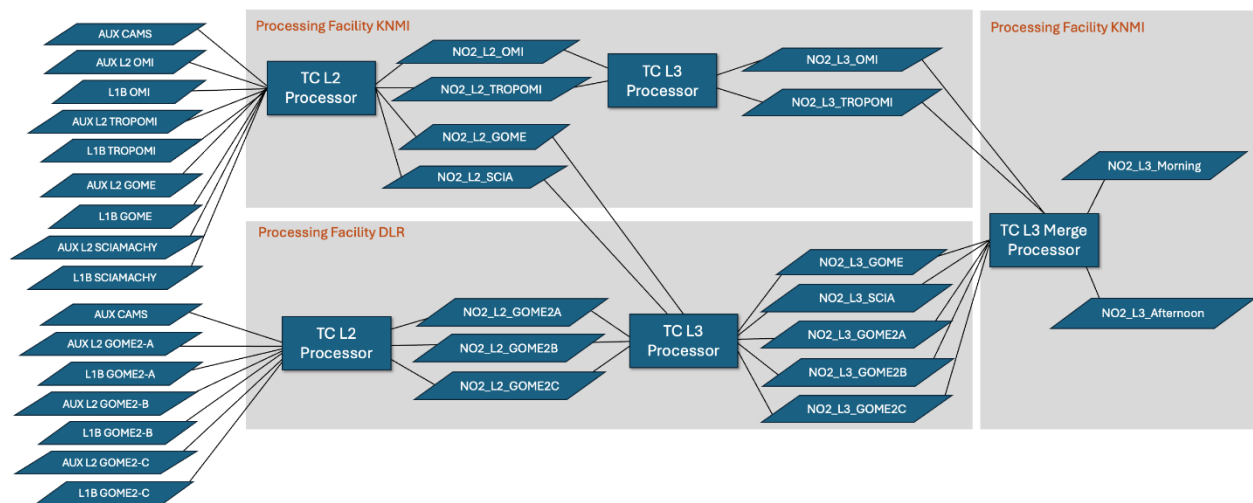


**Figure 2: Overall ECV Production Scenarios for NO<sub>2</sub> columns**

The L2 processing facility located at KNMI provides the following functions:

- Generation of NO<sub>2</sub>\_L2\_GOME product from GOME L1B, GOME auxiliary L2 products (NO<sub>2</sub> SCD and clouds) and TM5-MP auxiliary data. NO<sub>2</sub> SCDs are taken from the QA4ECV GOME L2 NO<sub>2</sub> product.
- Generation of NO<sub>2</sub>\_L2\_SCIA product from SCIA L1B, SCIA auxiliary L2 products (NO<sub>2</sub> SCD and clouds) and TM5-MP auxiliary data. NO<sub>2</sub> SCDs are taken from the QA4ECV SCIAMACHY L2 NO<sub>2</sub> product.



- Generation of NO<sub>2</sub>\_L2\_OMI product from OMI L1B, OMI auxiliary L2 products (NO<sub>2</sub> SCD and clouds) and TM5-MP auxiliary data. NO<sub>2</sub> SCDs are taken from the QA4ECV OMI L2 NO<sub>2</sub> product.
- Generation of NO<sub>2</sub>\_L2\_S5P product from S5P L1B, S5P auxiliary L2 products (NO<sub>2</sub> SCD and clouds) and TM5-MP auxiliary data. NO<sub>2</sub> SCDs are taken from the operational TROPOMI L2 NO<sub>2</sub> product.

The L2 processing facility located at DLR provides the following functions:

- Generation of NO<sub>2</sub>\_L2\_GOME2\_[A/B/C] products from GOME2 L1B, GOME2 auxiliary L2 products (clouds) and CAMS reanalysis auxiliary data. NO<sub>2</sub> SCDs are reprocessed with the AC SAF prototype GOME2 L2 NO<sub>2</sub> algorithm.

The L3 processing facility (located at KNMI) provides the following functions:

- Generation of NO<sub>2</sub>\_L3\_OMI product from NO<sub>2</sub>\_L2\_OMI product.
- Generation of NO<sub>2</sub>\_L3\_S5P product from NO<sub>2</sub>\_L2\_S5P product.

The L3 processing facility (located at DLR) provides the following functions:

- Generation of NO<sub>2</sub>\_L3\_GOME product from NO<sub>2</sub>\_L2\_GOME product.
- Generation of NO<sub>2</sub>\_L3\_SCIA product from NO<sub>2</sub>\_L2\_SCIA product.
- Generation of NO<sub>2</sub>\_L3\_GOME2\_[A/B/C] products from NO<sub>2</sub>\_L2\_GOME2\_[A/B/C] products.

The L3 Merge processing facility (located at KNMI) provides the following functions:

- Generation of NO<sub>2</sub>\_L3\_Morning\_Merge product from NO<sub>2</sub>\_L3\_GOME, NO<sub>2</sub>\_L3\_SCIA and NO<sub>2</sub>\_L3\_GOME2\_[A/B/C] products.
- Generation of NO<sub>2</sub>\_L3\_Afternoon\_Merge product from NO<sub>2</sub>\_L3\_OMI and NO<sub>2</sub>\_L3\_S5P products.

Further information on L2 and L3 processing is given in the tables below:

- Name of the program (versioning)
- Version
- Language
- Responsibility

**Table 1: Information on NO<sub>2</sub> L2 processing.**

| Sensor                                                                                                                                                | Slant Columns                                       | Air Mass Factor                                              | Stratospheric Correction                                              |
|-------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------|--------------------------------------------------------------|-----------------------------------------------------------------------|
| GOME <ul style="list-style-type: none"><li>• Name of the program (versioning)</li><li>• Version</li><li>• Language</li><li>• Responsibility</li></ul> | NLIN (7.55)<br>qa4ecv 1.1<br>Fortran90<br>U. Bremen | S5P_OPER_LUT_NO2AMF_*.nc<br>DAK v3.1<br>Fortran90<br>KNMI/WU | Data assimilation<br>TM5-MP v1.0-<br>DOMINO v3.0<br>Fortran90<br>KNMI |
| SCIAMACHY                                                                                                                                             |                                                     | S5P_OPER_LUT_NO2AMF_*.nc                                     | Data assimilation                                                     |



|                                                                                                                                                           |                                                          |                                                                    |                                                                       |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------|--------------------------------------------------------------------|-----------------------------------------------------------------------|
| <ul style="list-style-type: none"><li>Name of the program (versioning)</li><li>Version</li><li>Language</li><li>Responsability</li></ul>                  | NLIN (7.35-7.37)<br>qa4ecv 1.1<br>Fortran90<br>U. Bremen | DAK v3.1<br>Fortran90<br>KNMI/WU                                   | TM5-MP v1.0-<br>DOMINO v3.0<br>Fortran90<br>KNMI                      |
| GOME2 A, B, C<br><ul style="list-style-type: none"><li>Name of the program (versioning)</li><li>Version</li><li>Language</li><li>Responsability</li></ul> | QDOAS v3.5<br>version AC SAF<br>protoC++/xml<br>DLR      | ACSAF_GOME2_A/B/C_NO2_AMF_*.nc<br>VLIDORT v2.7<br>Fortran90<br>DLR | STREAM<br>(Beirle et al., 2016)<br>MATLAB<br>DLR                      |
| OMI<br><ul style="list-style-type: none"><li>Name of the program (versioning)</li><li>Version</li><li>Language</li><li>Responsability</li></ul>           | QDOAS<br>v3.1<br>C<br>KNMI                               | S5P_OPER_LUT_NO2AMF_*.nc<br>DAK v3.1<br>Fortran90<br>KNMI/WU       | Data assimilation<br>TM5-MP v1.0-<br>DOMINO v3.0<br>Fortran90<br>KNMI |
| TROPOMI<br><ul style="list-style-type: none"><li>Name of the program (versioning)</li><li>Version</li><li>Language</li><li>Responsability</li></ul>       | TROPNLL2DP<br>v2.3.1<br>C++<br>KNMI                      | S5P_OPER_LUT_NO2AMF_*.nc<br>DAK v3.1<br>Fortran90<br>KNMI/WU       | Data assimilation<br>TM5-MP v1.0-<br>DOMINO v3.0<br>Fortran90<br>KNMI |

Table 2: L3 Products processed for NO<sub>2</sub> and where to find them

| NO <sub>2</sub> | Institute | Period    | Generated | Available at: /<br>Expect completion           | doi                             |
|-----------------|-----------|-----------|-----------|------------------------------------------------|---------------------------------|
| OMI             | KNMI      | 2004-2021 | Yes       | <a href="http://www.temis.nl">www.temis.nl</a> | doi:10.21944/cci-no2-omi-l3     |
| TROPOMI         | KNMI      | 2018-2021 | Yes       | <a href="http://www.temis.nl">www.temis.nl</a> | doi:10.21944/cci-no2-tropomi-l3 |
| GOME            | DLR       | 1995-2003 | Yes       | Public release in Oct 2025                     |                                 |
| SCIAMACHY       | DLR       | 2002-2012 | Yes       | Public release in Oct 2025                     |                                 |
| GOME-2A         | DLR       | 2007-2020 | Yes       | Public release in Oct 2025                     |                                 |
| GOME-2B         | DLR       | 2013-2024 | Yes       | Public release in Oct 2025                     |                                 |
| GOME-2C         | DLR       | 2019-2024 | Yes       | Public release in Oct 2025                     |                                 |

### 3.2. HCHO processing

The algorithm to produce HCHO column ECV parameters is described in detail in the CCI+ precursor ATBD (D2.1 Algorithm Theoretical Basis Document). The overall ECV production for HCHO column is schematized in Figure 3.



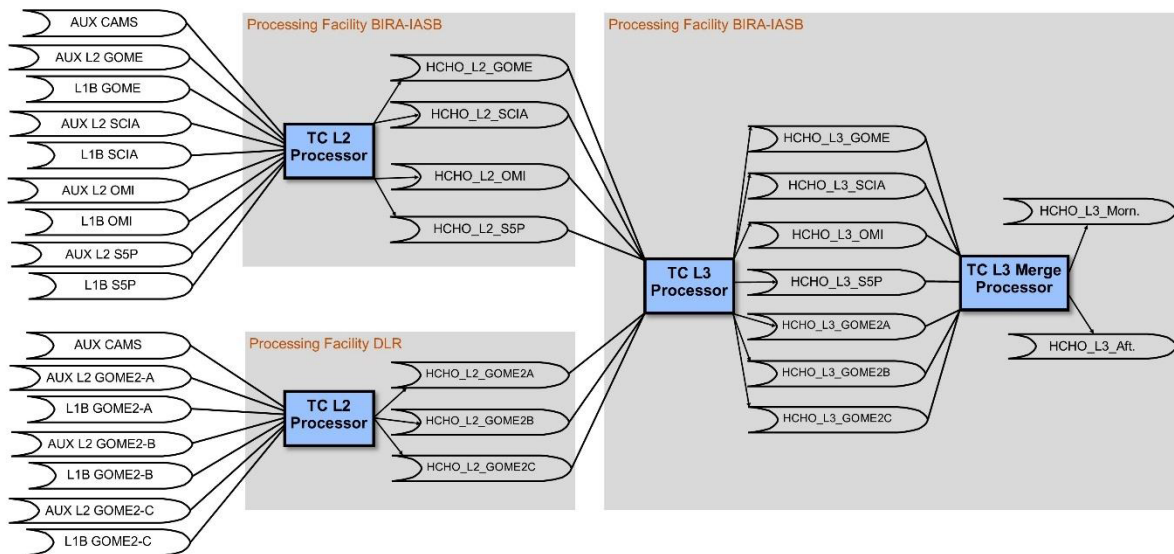


Figure 3: Overall ECV Production Scenarios for HCHO columns

The L2 processing facility located at BIRA-IASB provides the following functions:

- Generation of HCHO\_L2\_GOME product from GOME L1B, GOME auxiliary L2 products (HCHO SCD and clouds) and CAMS auxiliary data. HCHO SCDs are taken from the QA4ECV GOME L2 HCHO product.
- Generation of HCHO\_L2\_SCIA product from SCIA L1B, SCIA auxiliary L2 products (HCHO SCD and clouds) and CAMS auxiliary data. HCHO SCDs are taken from the QA4ECV SCIAMACHY L2 HCHO product.
- Generation of HCHO\_L2\_OMI product from OMI L1B, OMI auxiliary L2 products (HCHO SCD and clouds) and CAMS auxiliary data. HCHO SCDs are taken from the QA4ECV OMI L2 HCHO product.
- Generation of HCHO\_L2\_S5P product from S5P L1B, S5P auxiliary L2 products (HCHO SCD and clouds) and CAMS auxiliary data. HCHO SCDs are taken from the operational TROPOMI L2 HCHO product.

The L2 processing facility located at DLR provides the following functions:

- Generation of HCHO\_L2\_GOME2\_[A/B/C] products from GOME2 L1B, GOME2 auxiliary L2 products (clouds) and CAMS auxiliary data. HCHO SCDs are reprocessed with the AC SAF prototype GOME2 L2 HCHO algorithm.
- Auxiliary data and algorithm settings are harmonized with the GOME, SCIAMACHY, OMI and TROPOMI processors.

The L3 processing facility (located at BIRA-IASB) provides the following functions:

- Generation of HCHO\_L3\_GOME product from HCHO\_L2\_GOME product.
- Generation of HCHO\_L3\_SCIA product from HCHO\_L2\_SCIA product.
- Generation of HCHO\_L3\_GOME2\_[A/B/C] products from HCHO\_L2\_GOME2\_[A/B/C] products.
- Generation of HCHO\_L3\_OMI product from HCHO\_L2\_OMI product.





- Generation of HCHO\_L3\_S5P product from HCHO\_L2\_S5P product.

Further information on L2 and L3 processing is given in Table 3 and Table 4:

- Name of the program (versioning)
- Version
- Language
- Responsibility

**Table 3: Information on HCHO L2 processing.**

| Sensor                                                                                                                                                                     | Slant Columns                                                                     | Air Mass Factor                                                | Background Correction                                            |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|----------------------------------------------------------------|------------------------------------------------------------------|
| <b>GOME</b> <ul style="list-style-type: none"> <li>● Name of the program (versioning)</li> <li>● Version</li> <li>● Language</li> <li>● Responsibility</li> </ul>          | <a href="#">QDOAS (git hub)</a> (1)<br>version qa4ecv 1.2<br>C++/xml<br>BIRA-IASB | Amf_gome_hcho(git)<br>1.2.0<br>python3<br>BIRA-IASB            | bc_gome_hcho(git)<br>1.2.0<br>python3<br>BIRA-IASB               |
| <b>SCIAMACHY</b> <ul style="list-style-type: none"> <li>● Name of the program (versioning)</li> <li>● Version</li> <li>● Language</li> <li>● Responsibility</li> </ul>     | <a href="#">QDOAS (git hub)</a> (1)<br>version qa4ecv 1.2<br>C++/xml<br>BIRA-IASB | Amf_scia_hcho (git)<br>1.0.0<br>Python3<br>BIRA-IASB           | Bc_scia_hcho (git)<br>1.0.0<br>Python3<br>BIRA-IASB              |
| <b>GOME2 A, B, C</b> <ul style="list-style-type: none"> <li>● Name of the program (versioning)</li> <li>● Version</li> <li>● Language</li> <li>● Responsibility</li> </ul> | <a href="#">QDOAS (git hub)</a> (1)<br>version ac saf proto<br>C++/xml<br>DLR     | ACSAF_GOME2_A/B/<br>C_HCHO_AMF_*.nc<br>(git)<br>Python3<br>DLR | ACSAF_GOME2_A/B/C<br>_HCHO_BC_*.nc (git)<br>Python3<br>DLR       |
| <b>OMI</b> <ul style="list-style-type: none"> <li>● Name of the program (versioning)</li> <li>● Version</li> <li>● Language</li> <li>● Responsibility</li> </ul>           | <a href="#">QDOAS (git hub)</a> (1)<br>version qa4ecv 1.2<br>C++/xml<br>BIRA-IASB | Amf_omi_hcho (git)<br>1.2.2<br>python3<br>BIRA-IASB            | bc_omi_hcho.py (git)<br>1.0.2<br>python3<br>BIRA-IASB            |
| <b>TROPOMI</b> <ul style="list-style-type: none"> <li>● Name of the program (versioning)</li> <li>● Version</li> <li>● Language</li> <li>● Responsibility</li> </ul>       | UPAS2<br>version operational<br>3.2.x.x<br>DLR                                    | amf_s5p_hcho (git)<br>1.2.0<br>python3<br>BIRA-IASB            | bc_s5p_hcho (git)<br>4.2.3.dev1+g57ff220<br>python3<br>BIRA-IASB |

(1) <https://github.com/UVVIS-BIRA-IASB/qdoas>

**Table 4: Information on HCHO L3 processing.**

| Sensor                                                                                                                                                            | L3 framework                                        | L3 gridding software                                                  |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------|-----------------------------------------------------------------------|
| <b>GOME</b> <ul style="list-style-type: none"> <li>● Name of the program (versioning)</li> <li>● Version</li> <li>● Language</li> <li>● Responsibility</li> </ul> | l3_gome_hcho (git)<br>1.0.0<br>Python3<br>BIRA-IASB | <a href="#">HARP (git hub)</a> (1)<br>Version 1.20<br>C/python<br>S&T |
| <b>SCIAMACHY</b> <ul style="list-style-type: none"> <li>● Name of the program (versioning)</li> <li>● Version</li> <li>● Language</li> </ul>                      | l3_scia_hcho (git)<br>1.0.0<br>Python3              | <a href="#">HARP (git hub)</a> (1)<br>Version 1.20<br>C/python        |





|                                    |                     |                                    |
|------------------------------------|---------------------|------------------------------------|
| • Responsibility                   | BIRA-IASB           | S&T                                |
| GOME2 A, B, C                      |                     |                                    |
| • Name of the program (versioning) | l3_gome2_hcho (git) | <a href="#">HARP (git hub)</a> (1) |
| • Version                          | 1.0.0               | Version 1.20                       |
| • Language                         | Python3             | C/python                           |
| • Responsibility                   | BIRA-IASB           | S&T                                |
| OMI                                |                     |                                    |
| • Name of the program (versioning) | l3_omi_hcho (git)   | <a href="#">HARP (git hub)</a> (1) |
| • Version                          | 1.2.0               | Version 1.20                       |
| • Language                         | Python3             | C/python                           |
| • Responsibility                   | BIRA-IASB           | S&T                                |
| TROPOMI                            |                     |                                    |
| • Name of the program (versioning) | l3_s5p_hcho (git)   | <a href="#">HARP (git hub)</a> (1) |
| • Version                          | 5.0.4               | Version 1.20                       |
| • Language                         | Python3             | C/python                           |
| • Responsibility                   | BIRA-IASB           | S&T                                |

(1) <https://github.com/stcorp/harp>

### 3.3. SO<sub>2</sub> processing

The algorithm to produce SO<sub>2</sub> column ECV parameters is described in detail in the CCI+ precursor ATBD (D2.1 Algorithm Theoretical Basis Document). The overall ECV production for SO<sub>2</sub> column is schematized in Figure 4.

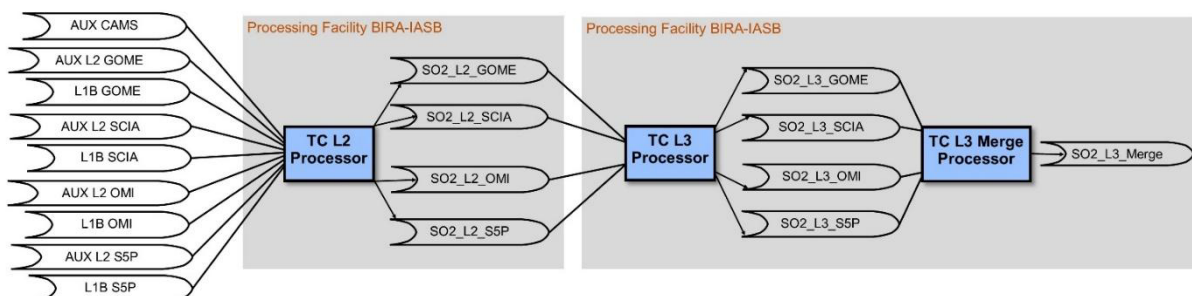


Figure 4: Overall ECV production for SO<sub>2</sub> column.

The L2 processing facility (located at BIRA-IASB) provides the following functions:

- Generation of SO2\_L2\_GOME product from GOME L1B, GOME auxiliary L2 products (clouds and total ozone) and CAMS auxiliary data.
- Generation of SO2\_L2\_SCIA product from SCIA L1B, SCIA auxiliary L2 products (clouds and total ozone) and CAMS auxiliary data.
- Generation of SO2\_L2\_OMI product from OMI L1B, OMI auxiliary L2 products (clouds and total ozone) and CAMS auxiliary data.
- Generation of SO2\_L2\_S5P product from S5P L1B, S5P auxiliary L2 products (clouds and total ozone) and CAMS auxiliary data.

The L3 processing facility (located at BIRA-IASB) provides the following functions:

- Generation of SO2\_L3\_GOME product from SO2\_L2\_GOME product.





- Generation of SO2\_L3\_SCIA product from SO2\_L2\_SCIA product.
- Generation of SO2\_L3\_OMI product from SO2\_L2\_OMI product.
- Generation of SO2\_L3\_S5P product from SO2\_L2\_S5P product.

The L3 Merge processing facility (located at BIRA-IASB) provides the following functions:

- Generation of SO2\_L3\_Merge product from SO2\_L3\_GOME, SO2\_L3\_SCIA, SO2\_L3\_OMI and SO2\_L3\_S5P products.

Further information on L2 and L3 processing is given in Table 5 and Table 6:

- Name of the program (versioning)
- Version
- Language
- Responsibility

**Table 5: Information on SO2 L2 processing.**

| Sensor                                                                                                                                                            | Slant Columns                                              | Air Mass Factor                                     |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------|-----------------------------------------------------|
| <b>GOME</b> <ul style="list-style-type: none"><li>• Name of the program (versioning)</li><li>• Version</li><li>• Language</li><li>• Responsibility</li></ul>      | COBRA GOME SO2<br>Version 8<br>Matlab<br>BIRA-IASB         | amf_gome_so2 (git)<br>1.0.0<br>Python3<br>BIRA-IASB |
| <b>SCIAMACHY</b> <ul style="list-style-type: none"><li>• Name of the program (versioning)</li><li>• Version</li><li>• Language</li><li>• Responsibility</li></ul> | Tbd<br><br>BIRA-IASB                                       | Tbd<br><br>BIRA-IASB                                |
| <b>OMI</b> <ul style="list-style-type: none"><li>• Name of the program (versioning)</li><li>• Version</li><li>• Language</li><li>• Responsibility</li></ul>       | COBRA OMI SO2<br>Version 23<br>Matlab<br>BIRA-IASB         | Amf_omi_so2 (git)<br>1.0.0<br>python3<br>BIRA-IASB  |
| <b>TROPOMI</b> <ul style="list-style-type: none"><li>• Name of the program (versioning)</li><li>• Version</li><li>• Language</li><li>• Responsibility</li></ul>   | l2_s5p_so2: (git)<br>4.1.4<br>python3<br>BIRA-IASB/S5P-PAL | amf_s5p_so2 (git)<br>3.2.0<br>python3<br>BIRA-IASB  |

**Table 6: Information on SO2 L3 processing.**

| Sensor                                                                                                                                                            | L3 framework                                       | L3 gridding software                                                  |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------|-----------------------------------------------------------------------|
| <b>GOME</b> <ul style="list-style-type: none"><li>• Name of the program (versioning)</li><li>• Version</li><li>• Language</li><li>• Responsibility</li></ul>      | l3_gome_so2 (git)<br>1.2.2<br>Python3<br>BIRA-IASB | <a href="#">HARP (git hub)</a> (1)<br>Version 1.20<br>C/python<br>S&T |
| <b>SCIAMACHY</b> <ul style="list-style-type: none"><li>• Name of the program (versioning)</li><li>• Version</li><li>• Language</li><li>• Responsibility</li></ul> | l3_scia_so2 (git)<br>tbd<br>Python3<br>BIRA-IASB   | <a href="#">HARP (git hub)</a> (1)<br>Version 1.20<br>C/python<br>S&T |





|                                                                                                                                                         |                                                                         |                                                                       |
|---------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------|-----------------------------------------------------------------------|
| <b>OMI</b> <ul style="list-style-type: none"><li>Name of the program (versioning)</li><li>Version</li><li>Language</li><li>Responsability</li></ul>     | l3_omi_so2 (git)<br>1.5.1<br>Python3<br>BIRA-IASB                       | <a href="#">HARP (git hub)</a> (1)<br>Version 1.20<br>C/python<br>S&T |
| <b>TROPOMI</b> <ul style="list-style-type: none"><li>Name of the program (versioning)</li><li>Version</li><li>Language</li><li>Responsability</li></ul> | l3_s5p_so2 (git)<br>version 1.5.5.dev2+gd18242b<br>Python3<br>BIRA-IASB | <a href="#">HARP (git hub)</a> (1)<br>Version 1.20<br>C/python<br>S&T |

(1) <https://github.com/stcorp/harp>

### 3.4. CHOCHO processing

The algorithm to produce CHOCHO column ECV parameters is described in detail in the CCI+ precursor ATBD (D2.1 Algorithm Theoretical Basis Document). Figure 4 provides an overview of the ECV processing chain for CHOCHO columns.

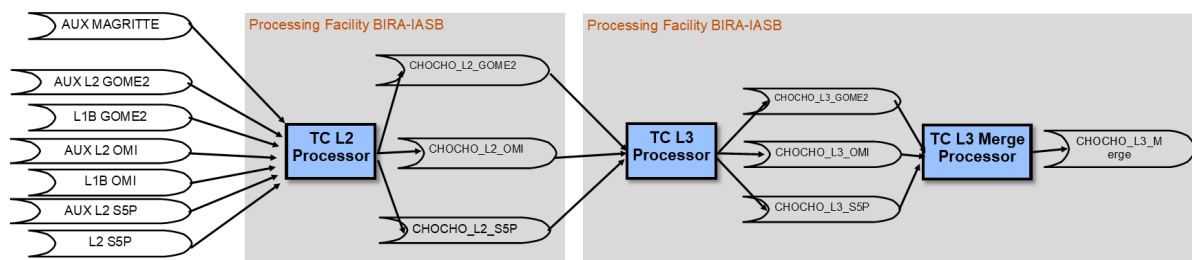


Figure 4: ECV production scenario for CHOCHO columns

The L2 processing facility located at BIRA-IASB provides the following functions:

- Generation of CHOCHO\_L2\_GOME2\_A/B/C products from GOME-2 L1B data, GOME-2 L2 auxiliary data (O2-O2 cloud parameters obtained from the GOME-2 NO2 operational L2 product) and auxiliary data from the Magritte CTM.
- Generation of CHOCHO\_L2\_OMI product from OMI L1B data, OMI L2 auxiliary data (cloud parameters from the O2-O2 OMI L2 cloud product) and auxiliary data from the Magritte CTM.
- Generation of CHOCHO\_L2\_S5P product from S5P L2 data (slant columns obtained from the S5P-PAL CHOCHO product), S5P L2 auxiliary data (cloud parameters from the operational NO2 OFL product).

The L3 processing facility located at BIRA-IASB provides the following functions:

- Generation of CHOCHO\_L3\_GOME2\_A/B/C products from CHOCHO\_L2\_GOME2\_A/B/C products.
- Generation of CHOCHO\_L3\_OMI products from CHOCHO\_L2\_OMI product.
- Generation of CHOCHO\_L3\_S5P products from CHOCHO\_L2\_S5P product.

The L3 merge processing facility located at BIRA-IASB provides the following functions:

- Generation of CHOCHO\_L3\_Morning\_Merge product from CHOCHO\_L2\_GOME2\_A/B/C products.



- Generation of CHOCHO\_L3\_Afternoon\_Merge product from CHOCHO\_L2\_OMI and CHOCHO\_L2\_S5P products.

Detailed information (program name, version, implementation language) about the processing facilities is provided in Table 7 and Table 8.

**Table 7: Information about CHOCHO L2 processing**

| Sensor                                                                                                                                                          | Slant columns                                                          | Air mass factor                                      | Background correction                                   |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------|------------------------------------------------------|---------------------------------------------------------|
| <b>GOME-2</b> <ul style="list-style-type: none"><li>• Name of the program (versioning)</li><li>• Version</li><li>• Language</li><li>• Responsibility</li></ul>  | QDOAS / CHOCHO_GOME2{A,B,C}.xml (git)<br>3.6.5<br>C++/XML<br>BIRA-IASB | chocho_amf (git)<br><br>2.1<br>Python<br>BIRA-IASB   | l2_gome2_chocho (git)<br><br>1.0<br>Python<br>BIRA-IASB |
| <b>OMI</b> <ul style="list-style-type: none"><li>• Name of the program (versioning)</li><li>• Version</li><li>• Language</li><li>• Responsibility</li></ul>     | QDOAS / CHOCHO_CCI+_OMI.xml (git)<br>3.6.5<br>C++/XML<br>BIRA-IASB     | chocho_amf (git)<br><br>1.0.5<br>Python<br>BIRA-IASB | l2_omi_chocho (git)<br><br>1.1.2<br>Python<br>BIRA-IASB |
| <b>TROPOMI</b> <ul style="list-style-type: none"><li>• Name of the program (versioning)</li><li>• Version</li><li>• Language</li><li>• Responsibility</li></ul> | N/A (slant columns obtained from S5P_PAL product)                      | chocho_amf (git)<br><br>1.0.5<br>Python<br>BIRA-IASB | l2_s5p_chocho (git)<br><br>1.0.7<br>Python<br>BIRA-IASB |

**Table 8: Information about CHOCHO L3 processing**

| Sensor                                                                                                                                                                   | L3 framework                                        | L3 gridding software                  |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------|---------------------------------------|
| <b>GOME-2 A / B / C</b> <ul style="list-style-type: none"><li>• Name of the program (versioning)</li><li>• Version</li><li>• Language</li><li>• Responsibility</li></ul> | chocho_l3 (git)<br><br>1.10<br>Python<br>BIRA-IASB  | HARP<br><br>1.23<br>C / Python<br>S&T |
| <b>OMI</b> <ul style="list-style-type: none"><li>• Name of the program (versioning)</li><li>• Version</li><li>• Language</li><li>• Responsibility</li></ul>              | chocho_l3 (git)<br><br>1.0.5<br>Python<br>BIRA-IASB | HARP<br><br>1.23<br>C / Python<br>S&T |
| <b>TROPOMI</b> <ul style="list-style-type: none"><li>• Name of the program (versioning)</li><li>• Version</li></ul>                                                      | chocho_l3 (git)<br><br>1.0.4.                       | HARP<br><br>1.23                      |





|                  |           |            |
|------------------|-----------|------------|
| • Language       | Python    | C / Python |
| • Responsibility | BIRA-IASB | S&T        |

### 3.5. CO processing

The objective of the project is to generate a merged CO L3 product from existing IASI and MOPITT CO products. These input products are processed at EUMETSAT and NCAR facilities respectively (external processors, not described here).

Within the CCI+ project, the first step was to generate an intermediate L3 product : IASI monthly grids averaged from IASI-A, B and C, after filtering outliers, reformatting the data and applying an additional cloud flag. We call it “multi-platform product”. This intermediate product is not intended to be publicly released. In a second step, these IASI multi-platform data were combined with MOPITT V9T L3 data using a weighted averaging approach. Weights were determined based on the MOPITT CO total column to prior ratio.

The merged dataset includes CO total column monthly  $1^\circ \times 1^\circ$  resolution grids as well as uncertainty grids, for both daytime and nighttime from January 2008 to December 2024. Surface altitude grids as well as data source flags grids are also provided.

Figure 5 provides an overview of the ECV processing chain for the production of the CO L3 merged product.

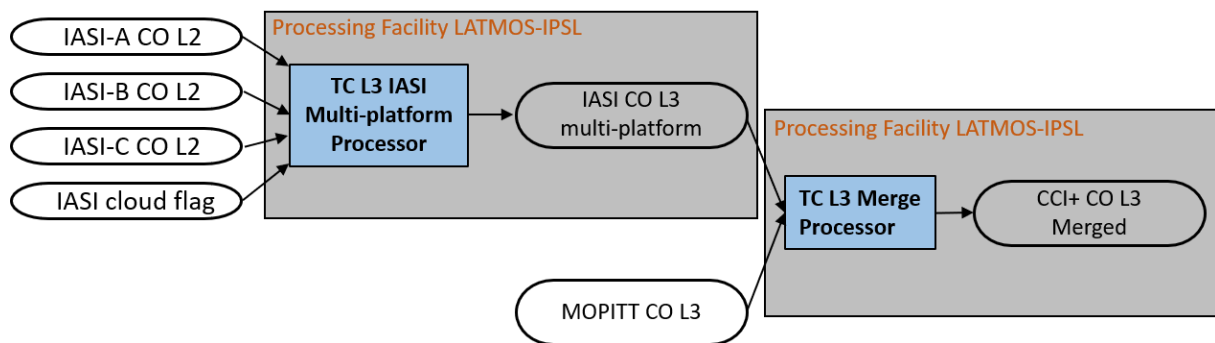


**Figure 5: ECV production scenario for CO columns**

The L3 processing facility located at LATMOS-IPSL provides:

- Generation of the CO\_L3\_IASI\_multi-platform product from CO\_L2\_IASIA, CO\_L2\_IASIB, IASI\_L2\_IASIC and IASI\_L2\_cloud\_flag products.

The L3 Merge processing facility located at LATMOS-IPSL provides:

- Generation of the CO\_L3\_Merge product from CO\_L3\_IASI\_multi-platform and CO\_L3\_MOPITT\_v9T products.

Further information on L3 processing is given in Table 11 and Table 12.

**Table 9: Information on CO L3 processing.**

| Sensor                             | L3 framework                      |
|------------------------------------|-----------------------------------|
| IASI                               |                                   |
| • Name of the program (versioning) | make_iasimulti_from_A_B_C_v1.2.py |
| • Version                          | v1.2                              |
| • Language                         | Python3                           |
| • Responsibility                   | LATMOS-IPSL                       |

**Table 10: Information on CO L3 merged processing.**

| CDR                                |                                      |
|------------------------------------|--------------------------------------|
| • Name of the program (versioning) | merging_iasimulti_mopitt9T_v2.6.2.py |
| • Version                          | v2.6.2                               |
| • Language                         | Python3                              |
| • Responsibility                   | LATMOS-IPSL                          |

### 3.6. NH<sub>3</sub> processing

The algorithm to produce NH<sub>3</sub> column ECV parameters is described in detail in the CCI+ precursor ATBD (D2.1 Algorithm Theoretical Basis Document). Figure 6 provides an overview of the processing chain.

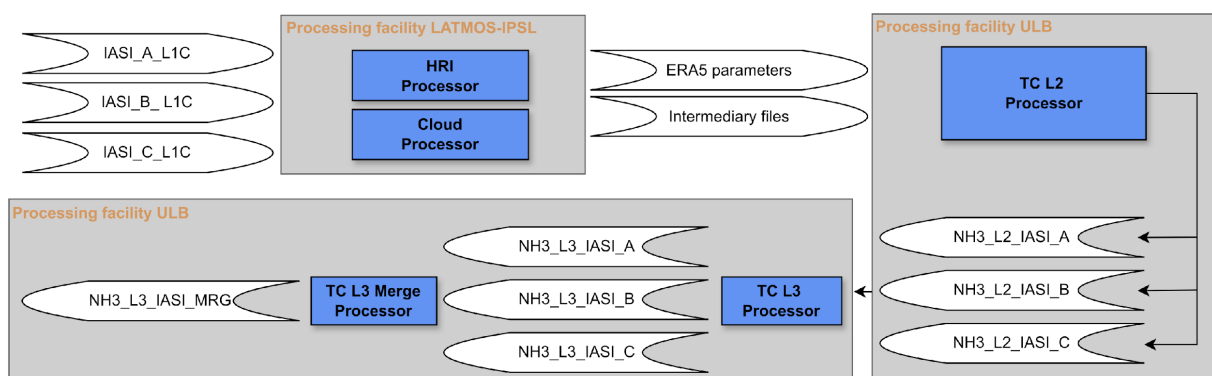


**Figure 6: ECV production scenario for NH<sub>3</sub> columns.**

The pre-processing facility located at LATMOS-IPSL provides the following functions:

- Calculation, on a per pixel basis, of NH<sub>3</sub> HRI values and a cloud-flag from IASI L1C data. Extraction of latitude, longitude and time information.

The L2 processing facility located at ULB provides the following functions:

- Generation of NH3\_L2\_IASI\_A/B/C products from the intermediary files from the pre-processing facility and collocated ERA5 parameters.

The L2 processing facility located at ULB provides the following functions:

- Generation of NH3\_L3\_IASI\_A/B/C products from the NH3\_L2\_IASI\_A/B/C products.

The L3 merge processing facility located at ULB provides the following functions:

- Generation of NH3\_L3\_IASI\_MRG product from the NH3\_L3\_IASI\_A/B/C products.



Detailed information (program name, version, implementation language) about the processing facilities is provided in Tables 11 to 14.

**Table 11: Information on NH<sub>3</sub> pre-processing.**

|                     |                                                 |
|---------------------|-------------------------------------------------|
| Name of the program | L1Call_v6.cpp                                   |
| Purpose             | HRI and geolocation extraction                  |
| Version             | v6                                              |
| Language            | C++                                             |
| Responsability      | LATMOS-IPSL/ULB                                 |
| Name of the program | cloud_detection_from_IASI_L1C_0_10_25pc.m (HRI) |
| Version             | v1                                              |
| Language            | Matlab                                          |
| Responsability      | LATMOS-IPSL/ULB                                 |

**Table 12: Information on the NH<sub>3</sub> L2 processing.**

|                                  |                              |
|----------------------------------|------------------------------|
| Name of the program (versioning) | NN_retrieval_allspecies_v4.m |
| Version                          | v4                           |
| Language                         | Matlab                       |
| Responsability                   | ULB                          |

**Table 13: Information on the NH<sub>3</sub> L3 processing.**

|                     |             |
|---------------------|-------------|
| Name of the program | makeL3_v4.m |
| Version             | v4          |
| Language            | Matlab      |
| Responsability      | ULB         |

**Table 14: Information on the NH<sub>3</sub> L3 merged processing.**

|                     |              |
|---------------------|--------------|
| Name of the program | mergeL3_v4.m |
| Version             | v4           |
| Language            | Matlab       |
| Responsability      | ULB          |



## 4. Processing facilities

This section describes the processing facilities available at the different institutes for generation of the ECV products. It is a general technical description of the relevant infrastructure in place, with an indication of its lifetime and sustainability.

### 4.1. Processing facility at BIRA

The processing facilities available at BIRA are as follows:

- x86\_64 linux compute cluster with 11 nodes and a total of 300+ cores.
- Between 20 and 52 cores/node
- Between 384GB and 1.5TB RAM/node
- GPU enabled nodes based on Nvidia A30 accelerators
- SGI, 112 compute nodes with each 2 Xeon E5-2680V3 processors running 24 cores (total of 2688 cores), 12Tb Ram, 200 Tb dedicated data storage
- Hitachi, 4 PB (2 fully redundant HDS HNAS 4080 clusters)

### 4.2. Processing facility at KNMI

KNMI computing will occur at local workstations (for testing) and at ECMWF facilities, where massive processing can take place, as was done in the QA4ECV-project for NO<sub>2</sub>. KNMI, a registered user of ECMWF services, is granted access to computing capability on the ecgate server, to ECMWF's meteorological archive (relevant for TM5-MP modelling), and a tape archive. ecgate holds 12 compute nodes, each with 2 Intel Xeon E5-2680 (16 cores) and 2 x 900 GB SAS HDD. ECMWF facilities work with a job scheduler, allowing users to request and use resources of the cluster efficiently and effectively. For more information: <http://www.ecmwf.int/en/computing/our-facilities/ecgate>.

### 4.3. Processing facility at DLR

DLR is equipped with a local cloud environment (GeoService) for processing large amounts of satellite data and it host the long-term archives for the operational level-1 and level-2 products from the ESA missions GOME, SCIAMACHY, TROPOMI and the AC-SAF missions GOME-2A, GOME-2B, and GOME-2C.

Additionally, The HPDA (High Performance Data Analytics) terrabyte compute infrastructure provides two clusters hosted at the Leibniz Supercomputing Centre. These are described in Table 15.

Table 15: HPDA clusters hosted at the Leibniz Supercomputing Centre

|                         | CPU cluster          | GPU cluster          |
|-------------------------|----------------------|----------------------|
| Number of nodes         | 262                  | 47                   |
| Number of CPUs per node | 2                    | 2                    |
| Number of cores per CPU | 40 (80 Hyperthreads) | 24 (48 Hyperthreads) |
| Number of GPUs per Node | 0                    | 4                    |



|                                             |                                             |                                          |
|---------------------------------------------|---------------------------------------------|------------------------------------------|
| <b>CPU Type</b>                             | Intel Xeon Platinum 8380 40C<br>270W 2.3GHz | Intel Xeon Gold 6336Y 24C<br>185W 2.4GHz |
| <b>GPU Type</b>                             | N/A                                         | NVIDIA HGX A100 80GB 500W                |
| <b>RAM per node</b>                         | 1024 GByte                                  | (1024 + 320) GByte                       |
| <b>Bandwidth to Infiniband HDR per node</b> | 200 GBit/s                                  | 200 GBit/s                               |
| <b>LINPACK computing power per node</b>     | 4,5 TFlop/s                                 | 68,5 TFlop/s                             |
| <b>Memory bandwidth per node</b>            | 409,6 GByte/s                               | (409,6 + 8156) GByte/s                   |

#### 4.4. Processing facility at ULB

The processing facility used for the NH<sub>3</sub> processing at ULB is as follows:

- Intel® Core™ i9-7940X CPU @ 3.1Ghz, 14 Cores, 28 Logical processors
- 8 x 16 GB of 2400 MHz RAM
- 100 TB data storage
- NVIDIA GeForce GT 730
- TUF X299 Mark 2 system

#### 4.5. Processing facility at LATMOS

The processing facilities available at LATMOS are the ones from IPSL. The characteristics of the Spirit cluster are the following:

Number of cores is without HyperThreading (This is real core)

2 nodes type:

- zen4: 64 cores 256GB 4GB/core (2 AMD EPYC 7452 32-Core)
  - 240GB max allocatable for job and 4000M (not 4096) per core
  - there are also 4 nodes with 96 cores and 256GB (2 AMD EPYC 7552 48-Core)
- zen16: 32 cores 512GB 16GB/core (2 AMD EPYC 7302 16-Core)
  - 496GB max allocatable for job and 16000M (not 16384) per core

20 Computing nodes = 12 zen4 + 8 zen16

Linux distribution is Ubuntu 20.04.6 LTS (GNU/Linux 5.4.0-170-generic x86\_64).

### 5. Data flow for ECV production

This section consists of a set of overview tables describing for each molecule, the data flow for each sensor. The table indicates the amount of data being processed in Gbyte, Gbyte/year and number of years covered by the processing. For each sensor, it specifies the amount of processed data for L1, L2 and L3 products.



**Table 16: NO<sub>2</sub> processing**

| L1 products   |         |            | Ancillary data |            |       | Intermediate L2 products |       | Sensor L3 products |       |
|---------------|---------|------------|----------------|------------|-------|--------------------------|-------|--------------------|-------|
|               | # years | Gbyte/Year | Gbyte          | Gbyte/Year | Gbyte | Gbyte/Year               | Gbyte | Gbyte/Year         | Gbyte |
| GOME          | 9       | 220        | 1980           | 46         | 414   | 7                        | 63    | 0.3                | 2.7   |
| SCIAMACHY     | 10      | 640        | 6400           | 58         | 580   | 15                       | 150   | 0.3                | 3     |
| GOME2A        | 15      | 2000       | 30000          | 120        | 1800  | 55                       | 825   | 6                  | 90    |
| GOME2B        | 12      | 2000       | 24000          | 120        | 1440  | 55                       | 660   | 6                  | 72    |
| GOME2C        | 6       | 2000       | 12000          | 120        | 720   | 55                       | 330   | 6                  | 36    |
| OMI           | 20      | 1000       | 20000          | 164        | 3280  | 200                      | 4000  | 100                | 2000  |
| TROPOMI       | 6       | 10500      | 63000          | 2444       | 14664 | 3500                     | 21000 | 100                | 600   |
|               |         |            |                |            |       |                          |       |                    |       |
| morning CDR   | 28      |            |                |            |       |                          |       | 5                  | 140   |
| afternoon CDR | 20      |            |                |            |       |                          |       | 100                | 2000  |

- Morning CDR: monthly files, 0.2°x0.2°
- Afternoon CDR: monthly files, 0.05°x0.05°+ daily files, 0.2°x0.2°

**Table 17: HCHO processing**

| L1 products   |         |            | Ancillary data |            |       | Intermediate L2 products |       | Sensor L3 products |       |
|---------------|---------|------------|----------------|------------|-------|--------------------------|-------|--------------------|-------|
|               | # years | Gbyte/Year | Gbyte          | Gbyte/Year | Gbyte | Gbyte/Year               | Gbyte | Gbyte/Year         | Gbyte |
| GOME          | 9       | 220        | 1980           | 46         | 414   | 7                        | 63    | 5                  | 45    |
| SCIAMACHY     | 10      | 640        | 6400           | 58         | 580   | 15                       | 150   | 5                  | 50    |
| GOME2A        | 15      | 2000       | 30000          | 121        | 1815  | 55                       | 825   | 5                  | 75    |
| GOME2B        | 12      | 2000       | 24000          | 120        | 1440  | 55                       | 660   | 5                  | 60    |
| GOME2C        | 6       | 2000       | 12000          | 114        | 684   | 55                       | 330   | 5                  | 30    |
| OMI           | 20      | 1000       | 20000          | 164        | 3280  | 200                      | 4000  | 100                | 2000  |
| TROPOMI       | 6       | 10500      | 63000          | 2444       | 14664 | 3500                     | 21000 | 100                | 600   |
| Total         |         | 18360      | 157380         | 5147       | 64477 | 3887                     | 27028 | 225                | 2860  |
|               |         |            |                |            |       |                          |       |                    |       |
| morning CDR   | 28      |            |                |            |       |                          |       | 5                  | 140   |
| afternoon CDR | 20      |            |                |            |       |                          |       | 100                | 2000  |

- Morning CDR: monthly files, 0.2°x0.2°
- Afternoon CDR: monthly files, 0.05°x0.05°+ daily files, 0.2°x0.2°



**Table 18: SO<sub>2</sub> processing**

| L1 products |         |            | Ancillary data |            | Intermediate L2 products |            | Sensor L3 products |            |       |
|-------------|---------|------------|----------------|------------|--------------------------|------------|--------------------|------------|-------|
|             | # years | Gbyte/Year | Gbyte          | Gbyte/Year | Gbyte                    | Gbyte/Year | Gbyte              | Gbyte/Year | Gbyte |
| GOME        | 9       | 220        | 1980           | 46         | 414                      | 15         | 135                | 5          | 45    |
| SCIAMACHY   | 10      | 640        | 6400           | 58         | 580                      | 25         | 250                | 5          | 50    |
| OMI         | 18      | 1000       | 18000          | 215        | 3870                     | 300        | 5400               | 100        | 1800  |
| TROPOMI     | 6       | 10500      | 63000          | 2444       | 14664                    | 5000       | 30000              | 100        | 600   |
|             |         |            |                |            |                          |            |                    |            |       |
| Merged CDR  | 20      |            |                |            |                          |            |                    | 100        | 2000  |

- Merged CDR: monthly files, 0.05°x0.05° + daily files, 0.2°x0.2°

**Table 19: CHOCHO processing**

| Table 15: CHRS-0 processing |         |            |                |            |                          |            |                    |            |       |
|-----------------------------|---------|------------|----------------|------------|--------------------------|------------|--------------------|------------|-------|
| L1/L2 products              |         |            | Ancillary data |            | Intermediate L2 products |            | Sensor L3 products |            |       |
|                             | # years | Gbyte/Year | Gbyte          | Gbyte/Year | Gbyte                    | Gbyte/Year | Gbyte              | Gbyte/Year | Gbyte |
| GOME2A                      | 15      | 2000       | 30000          | 75         | 1125                     | 30         | 450                | 5          | 75    |
| GOME2B                      | 12      | 2000       | 24000          | 75         | 900                      | 30         | 360                | 5          | 60    |
| GOME2C                      | 6       | 2000       | 12000          | 75         | 450                      | 30         | 180                | 5          | 30    |
| OMI                         | 20      | 1000       | 20000          | 117        | 2340                     | 168        | 3360               | 100        | 2000  |
| TROPOMI                     | 6       | 2880       | 17280          | 2208       | 13248                    | 2880       | 17280              | 100        | 600   |
| Total                       |         | 20380      | 103280         | 2550       | 18063                    | 3138       | 21630              | 225        | 2860  |
|                             |         |            |                |            |                          |            |                    |            |       |
| morning CDR                 | 28      |            |                |            |                          |            |                    | 5          | 140   |
| afternoon CDR               | 20      |            |                |            |                          |            |                    | 100        | 2000  |

- Morning CDR: monthly files, 0.2°x0.2°
- Afternoon CDR: monthly files, 0.05°x0.05° + daily files, 0.2°x0.2°

**Table 20: CO processing**

| Table 20: CO processing |         |            |                  |            |                         |            |                         |            |       |
|-------------------------|---------|------------|------------------|------------|-------------------------|------------|-------------------------|------------|-------|
| L2 input products       |         |            | L3 input product |            | Intermediate L3 product |            | L3 final merged product |            |       |
|                         | # years | Gbyte/Year | Gbyte            | Gbyte/Year | Gbyte                   | Gbyte/Year | Gbyte                   | Gbyte/Year | Gbyte |
| IASIA CO                | 14      | 670        | 9380             | NA         | NA                      | NA         | NA                      | NA         | NA    |
| IASIB CO                | 10      | 670        | 6700             | NA         | NA                      | NA         | NA                      | NA         | NA    |
| IASIC CO                | 3,25    | 810        | 2630             | NA         | NA                      | NA         | NA                      | NA         | NA    |
| IASI Cloud IASI         | 15      | 18         | 270              | NA         | NA                      | NA         | NA                      | NA         | NA    |





|                        |    |      |       |     |      |       |       |        |        |
|------------------------|----|------|-------|-----|------|-------|-------|--------|--------|
| IASI CO multi-platform | 15 | NA   | NA    | NA  | NA   | 0,025 | 0,375 | NA     | NA     |
| MOPITT CO              | 15 | NA   | NA    | 1,7 | 25,5 | NA    | NA    | NA     | NA     |
| Merged Product         |    | NA   | NA    | NA  | NA   |       |       | 0,0252 | 0,4284 |
| Total                  |    | 2168 | 18980 | 1,7 | 25,5 | 0,025 | 0,375 | 0,0252 | 0,4284 |

**Table 21: NH<sub>3</sub> processing**

|                         |         | L1 products |       | Ancillary and intermediate data |       | L2 products |       | L3 products |       |
|-------------------------|---------|-------------|-------|---------------------------------|-------|-------------|-------|-------------|-------|
|                         | # years | Tbyte/Year  | Tbyte | Gbyte/Year                      | Gbyte | Gbyte/Year  | Gbyte | Gbyte/Year  | Gbyte |
| IASI-A NH3              | 14      | 5.2         | 72.5  | 62                              | 868   | 43          | 585   | 1.8         | 26.2  |
| IASI-B NH3              | 11      | 5.2         | 57.1  | 62                              | 682   | 43          | 499   | 1.8         | 21.2  |
| IASI-C NH3              | 5       | 5.2         | 25.2  | 62                              | 310   | 43          | 205   | 1.8         | 8.7   |
| IASI NH3 multi-platform | 30      | 5160        | 154.8 | 62                              | 1860  | 43          | 1289  | 1.8         | 56    |
| Merged CDR              | 20      | NA          | NA    | NA                              | NA    | NA          | NA    | 1.8         | 36    |