

Precursors_cci+

ESA Climate Change Initiative (CCI)



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Executive Summary

This note contains the second release of the Precursors_cci+ Climate Research Data Package (CRDP, deliverable D3.2). This short document describes the status of the data production at the term of the second cycle of User requirements, Algorithm development and Data production. It covers tropospheric NO₂, HCHO, SO₂, CHOCHO, CO and NH₃ data products that were used as an input for the second round of validation activities. It also addresses efforts being undertaken to upload the CDR datasets on the CCI Open Data Portal.

1. Purpose and scope

1.1. Purpose and scope

This document describes the Precursors_cci+ Climate Research Data Package (CRDP), i.e. the ECV data products that were generated as part of WP4 Data Processing. This first version of the CRDP contains description of the L2 and L3 data sets generated at the end of the second cycle of algorithm development and data processing. This data package is used as an input for the Product Validation and Intercomparison Report (PVIR) version 2.

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

1.3. Reference documents

- [RD-1] Precursors CCI+ Product User Guide, deliverable 4.2, Precursors_cci+_D4.2_PUG_01_00, draft version.
- [RD-2] van Geffen, J.; Eskes, H.; Compernelle, S.; Pinardi, G.; Verhoelst, T.; Lambert, J.-C.; Sneep, M.; ter Linden, M.; Ludewig, A.; Boersma, K. F. & Veefkind, J. P. Sentinel-5P TROPOMI NO₂ retrieval: impact of version v2.2 improvements and comparisons with OMI and ground-based data Atmos. Meas. Tech., 2022, 15, 2037-2060
- [RD-3] S5P Nitrogen Dioxide v02.03.01 intermediate reprocessing on the S5P-PAL system: Readme file, issue 1.0, by Henk Eskes, Jos van Geffen, Maarten Sneep, Pepijn Veefkind, Sander Niemeijer, Claus Zehner, 15 December 2021
- [RD-4] *Product Specification Document for the QA4ECV NO₂ ECV precursor product* by F. Boersma et al., in 'Product User Guide for Land ECVs and Product Specification Document for Atmosphere ECV precursors' (D4.6), QA4ECV EC FP7 project deliverable 4.6, March 2017.
- [RD-5] Boersma, K. F.; Eskes, H. J.; Richter, A.; De Smedt, I.; Lorente, A.; Beirle, S.; van Geffen, J. H. G. M.; Zara, M.; Peters, E.; Van Roozendaal, M.; Wagner, T.; Maasakkers, J. D.; van der A, R. J.; Nightingale, J.; De Rudder, A.; Irie, H.; Pinardi, G.; Lambert, J.-C. & Compernelle, S. C. Improving algorithms and uncertainty estimates for satellite NO₂ retrievals: results from the quality assurance for the essential climate variables (QA4ECV) project Atmos. Meas. Tech., 2018, 11, 6651-6678, <https://doi.org/10.5194/amt-11-6651-2018>



- [RD-6] De Smedt, I.; Theys, N.; Yu, H.; Danckaert, T.; Lerot, C.; Compernelle, S.; Van Roozendael, M.; Richter, A.; Hilboll, A.; Peters, E.; Pedernana, M.; Loyola, D.; Beirle, S.; Wagner, T.; Eskes, H.; van Geffen, J.; Boersma, K. F. & Veefkind, P. Algorithm theoretical baseline for formaldehyde retrievals from S5P TROPOMI and from the QA4ECV project Atmos. Meas. Tech., 2018, 11, 2395-2426, <https://doi.org/10.5194/amt-11-2395-2018>
- [RD-7] S5P MPC Product Readme Formaldehyde V02.05.00, issue 2.6, by I. De Smedt, F. Romahn, K.-U. Eichmann, 20 July 2023.
- [RD-8] *Product Specification Document for the QA4ECV HCHO ECV precursor product* by I. De Smedt et al., in 'Product User Guide for Land ECVs and Product Specification Document for Atmosphere ECV precursors' (D4.6), QA4ECV EC FP7 project deliverable 4.6, March 2017.
- [RD-9] Product User Manual for GOME Total Column Products of Ozone, NO₂, BrO, HCHO, SO₂, H₂O, OCIO and Cloud Properties, GDP 4.8, SAF/AC/DLR/PUM/01, Iss. 3/C, Rev. 1, by Valks, P., et al., (2023). Oct, 2023
- [RD-10] Theys, N.; Fioletov, V.; Li, C.; De Smedt, I.; Lerot, C.; McLinden, C.; Krotkov, N.; Griffin, D.; Clarisse, L.; Hedelt, P.; Loyola, D.; Wagner, T.; Kumar, V.; Innes, A.; Ribas, R.; Hendrick, F.; Vlietinck, J.; Brenot, H. & Van Roozendael, M. A sulfur dioxide Covariance-Based Retrieval Algorithm (COBRA): application to TROPOMI reveals new emission sources Atmos. Chem. Phys., 2021, 21, 16727-16744, <https://doi.org/10.5194/acp-21-16727-2021>
- [RD-11] Algorithm Theoretical Basis Document of "Fast Optimal Retrieval on Layers for IASI (FORLI), IASI Reprocessed CO L2 CDR (O3M-517) Metop-A&B", by Daniel Hurtmans (ULB), Pierre Coheur (ULB), Rosa Astoreca (ULB), Juliette Hadji-Lazaro (LATMOS), Camille Viatte (LATMOS), Cathy Clerbaux (LATMOS), SAF/AC/ULB/ATBD/003, Issue 1.2, 9 March 2023, https://acsaf.org/docs/atbd/Algorithm_Theoretical_Basis_Document_IASI_CO_Mar_2023.pdf.
- [RD-12] Deeter, M.; Francis, G.; Gille, J.; Mao, D.; Martinez-Alonso, S.; Worden, H.; Ziskin, D.; Drummond, J.; Commane, R.; Diskin, G. & McKain, K. The MOPITT Version 9 CO product: sampling enhancements and validation Atmos. Meas. Tech., 2022, 15, 2325-2344, <https://doi.org/10.5194/amt-15-2325-2022>
- [RD-13] Clarisse, L.; Franco, B.; Van Damme, M.; Di Gioacchino, T.; Hadji-Lazaro, J.; Whitburn, S.; Noppen, L.; Hurtmans, D.; Clerbaux, C. & Coheur, P. The IASI NH₃ version 4 product: averaging kernels and improved consistency Atmos. Meas. Tech., 2023, 16, 5009-5028, <https://doi.org/10.5194/amt-16-5009-2023>
- [RD-14] Precursors CCI+ Product Validation and Algorithm Selection Report (PVASR), deliverable 2.3, issue 1, Precursors_cci+_D2.3_PVASR_01_00, draft, 29 Feb 2024.



- [RD-15] Quarterly Validation Report of the Copernicus Sentinel-5 Precursor Operational Data Products #21: April 2018 – November 2023. Lambert, J.-C., A. Keppens, S. Compernelle, K.-U. Eichmann, M. de Graaf, D. Hubert, B. Langerock, A. Ludewig, M.K. Sha, T. Verhoelst, T. Wagner, C. Ahn, A. Argyrouli, D. Balis, K.L. Chan, M. Coldewey-Egbers, I. De Smedt, H. Eskes, A.M. Fjæraa, K. Garane, J.F. Gleason, F. Goutail, J. Granville, P. Hedelt, K.-P. Heue, G. Jaross, Q. Kleipool, M.L. Koukouli, R. Lutz, M.C Martinez Velarte, K. Michailidis, S. Nanda, S. Niemeijer, A. Pazmiño, G. Pinardi, A. Richter, N. Rozemeijer, M. Sneep, D. Stein Zweers, N. Theys, G. Tilstra, O. Torres, P. Valks, J. van Geffen, C. Vigouroux, P. Wang, and M. Weber. S5P MPC Routine Operations Consolidated Validation Report series, Issue #21, Version 21.01.00, 194 pp., 18 December 2023.
- [RD-16] Gaia Pinardi, Isabelle De Smedt, Klaus-Peter Heue, Pieter Valks, AC SAF Validation Report of Reprocessed L2 Total HCHO, GOME-2/MetopA&MetopB, doc ref: SAF/AC/IASB/VR/HCHO, October 2023. Draft.
- [RD-17] Müller, J.-F.; Stavrakou, T.; Oomen, G.-M.; Opacka, B.; De Smedt, I.; Guenther, A.; Vigouroux, C.; Langerock, B.; Aquino, C. A. B.; Grutter, M.; Hannigan, J.; Hase, F.; Kivi, R.; Lutsch, E.; Mahieu, E.; Makarova, M.; Metzger, J.-M.; Morino, I.; Murata, I.; Nagahama, T.; Notholt, J.; Ortega, I.; Palm, M.; Röhling, A.; Stremme, W.; Strong, K.; Sussmann, R.; Té, Y. & Fried, A. Bias correction of OMI HCHO columns based on FTIR and aircraft measurements and impact on top-down emission estimates Atmos. Chem. Phys., 2024, 24, 2207-2237, <https://doi.org/10.5194/acp-24-2207-2024>
- [RD-18] AC SAF FORLI CO validation report, by B. Langerock et al. Submitted.



2. Climate Research Data Package

2.1. NO₂ column data sets

Table 1 presents an overview of data products input to or produced within the CCI+precursors project. The QA4ECV L2 products and the S5P PAL L2 product have been publicly released. The GOME-2A AC SAF L2 product is a demonstrational product developed within the EUMETSAT AC SAF.

Table 1: NO₂ column data sets input to, or produced within, the CCI+precursors project. In analogy to [RD-1], product ID is given as {species}_{processing level}_{platform}_{sensor}.

Product ID	Processor	Provider	Time range
<i>L2 data sets</i>			
NO2_L2_ERS2_GOME1	QA4ECV v1.1 ¹	QA4ECV/KNMI	1995-2003
NO2_L2_ENVISAT_SCIAMACHY	QA4ECV v1.1 ¹	QA4ECV/KNMI	2002-2012
NO2_L2_METOP_GOME2_A	AC SAF proto ²	AC SAF/DLR	2007-2020
NO2_L2_METOP_GOME2_B	AC SAF proto ²	AC SAF/DLR	2013-2024
NO2_L2_METOP_GOME2_C	AC SAF proto ²	AC SAF/DLR	2019-2024
NO2_L2_AURA_OMI	QA4ECV v1.1/ L1v4 ³	QA4ECV/KNMI	2004-2021
NO2_L2_S5P_TROPOMI	PAL RPRO v2.3.1 ¹	EU/ESA/KNMI	2018-2021
<i>L3 data sets:</i>			
NO2_L3_ERS2_GOME1	QA4ECV v1.1, L3: fv0200	QA4ECV/KNMI/DLR	1995-2003
NO2_L3_ENVISAT_SCIAMACHY	QA4ECV v1.1, L3: fv0200	QA4ECV/KNMI/DLR	2002-2012
NO2_L3_METOP_GOME2_A	AC SAF proto, L3: fv1.0	AC SAF/DLR	2007-2020
NO2_L3_METOP_GOME2_B	AC SAF proto, L3: fv1.0	AC SAF/DLR	2013-2024
NO2_L3_METOP_GOME2_C	AC SAF proto, L3: fv1.0	AC SAF/DLR	2019-2024
NO2_L3_AURA_OMI	QA4ECV v1.1, L3: fv1.0	QA4ECV/KNMI	2004-2021
NO2_L3_S5P_TROPOMI	PAL RPRO v2.3.1, L3: fv1.0	EU/ESA/KNMI	2018-2021

¹: publicly available product, input to this project. ²: intermediate non-public product. ³: Reprocessed OMI/EOS Aura data (based on L1 v4) were not yet available at the time of this analysis.

2.2. HCHO column data sets

Table 2 presents an overview of L2 and L3 data products input to or produced within the Precursors_cci+ project. The L2 version 1 products consist of the S5P and QA4ECV products and AC SAF GOME2 product which are publicly available products and were input to the L3 v1 products, which were prototype products. The version 2 L2 and L3 products are significant upgrades entirely generated within this project.

Table 2: HCHO column data sets input to, or produced within, the CCI+precursors project. In analogy to [RD-1], product ID is given as {species}_{processing level}_{platform}_{sensor}.

Product ID	L2 Processor {L3 processor}	Provider	Time range
<i>L2 data sets</i>			
HCHO_L2_ERS2_GOME1	v1: QA4ECV v1.2 ¹ v2 ⁵	QA4ECV/ BIRA-IASB	1995-2003
HCHO_L2_ENVISAT_SCIAMACHY	v1: QA4ECV v1.2 ¹ v2 ⁵	QA4ECV/ BIRA-IASB	2003-2012 ⁴
HCHO_L2_GOME2_A	v1: GDP 4.8/4.9 RPRO ¹ v2 ⁵	AC SAF/DLR	2007-2018
HCHO_L2_GOME2_B	v1: GDP 4.8/4.9 RPRO ¹ v2 ⁵	AC SAF/DLR	2013-now
HCHO_L2_GOME2_C	v1: GDP 4.8/4.9 RPRO ¹ v2 ⁵	AC SAF/DLR	2018-now
HCHO_L2_AURA_OMI	v1: QA4ECV v1.2 ¹ v2	QA4ECV/ BIRA-IASB	2004-2021
HCHO_L2_S5P_TROPOMI	v1: Operational ¹ , collection 3, ≥v2.4 v2	EU/ESA/BIRA- IASB/DLR	2018-now
<i>L3 data sets²</i>			
HCHO_L3_ERS2_GOME1 Monthly	v2: cci+p v1.0	BIRA-IASB	1996-2002 ³
HCHO_L3_ENVISAT_SCIAMACHY Monthly	v2: cci+p v1.0	BIRA-IASB	2003-2012 ⁴
HCHO_L3_METOP_GOME2_A Monthly	v2: AC SAF prototype	BIRA- IASB/DLR/EUMETSAT	2007-2018
HCHO_L3_METOP_GOME2_B Monthly	v2: AC SAF prototype	BIRA- IASB/DLR/EUMETSAT	2013-2020
HCHO_L3_METOP_GOME2_C Monthly	v2: AC SAF prototype	BIRA- IASB/DLR/EUMETSAT	2019-2023
HCHO_L3_AURA_OMI Daily, monthly	v2: cci+p v1.0	BIRA-IASB	2005-2022
HCHO_L3_S5P_TROPOMI Daily, monthly	v2: cci+p v1.0	BIRA-IASB/DLR/ESA	2018-2023

1: publicly available product, input to this project. 2: intermediate non-public product. 3: Although GOME did still observations in 2003, global coverage of GOME ends in early 2003, after which only Europe is covered, therefore



background correction can no longer be performed. 4: Although there are SCIAMACHY observations from 08/2002, QA4ECV processing only starts in 2003.

2.3. SO₂ column data sets

The SO₂ L2 and L3 data products were produced during the CCI+precursors project. The retrieval is based on the COBRA algorithm. In the current document, validation results for L2 and L3 daily OMI & TROPOMI are presented. The L3 daily products have a spatial grid of 0.25°x0.25°. The GOME product is not validated because of lack of FRM data within the temporal range. The SCIAMACHY product was not yet available at the time of creating the current document.

The L2 products are currently not scheduled for release.

Table 3: SO₂ column data sets (to be) produced within, the CCI+precursors project. In analogy to [RD-1], product ID is given as {species}_{processing level}_{platform}_{sensor}.

Product ID	Processor	Provider	Time range
<i>L2 data sets</i>			
SO2_L2_ERS2_GOME1	CCI+p v1.0	BIRA-IASB	1996-2003
SO2_L2_ENVISAT_SCIAMACHY	CCI+p v1.0	BIRA-IASB	2003-2012 (planned)
SO2_L2_AURA_OMI	CCI+p v1.0	BIRA-IASB	2004-2022
SO2_L2_S5P_TROPOMI	OFFL v0.3_02/ CCI+p v1.0	BIRA-IASB	2018-2023
<i>L3 data sets</i>			
SO2_L3_ERS2_GOME1	CCI+p v1.0	BIRA-IASB	1996-2003
SO2_L3_ENVISAT_SCIAMACHY	CCI+p v1.0	BIRA-IASB	2003-2012 (planned)
SO2_L3_AURA_OMI	CCI+p v1.0	BIRA-IASB	2004-2022
SO2_L3_S5P_TROPOMI	OFFL v0.3_02/ CCI+p v1.0	BIRA-IASB	2018-2023

2.4. CO column data sets

The L3 CO IASI multi-platform product is a non-public intermediate product, based on IASI L2 FORLI CO data reprocessed by EUMETSAT in 2021. The L2 CO total columns from IASI A, B and C are filtered with an a posteriori cloud product and averaged into monthly 1°x1° grids. This process resulted in a new product, generated during Cycle 1 of the project, referred to as the L3 CO IASI multi-platform product.

This IASI multi-platform product was then combined with MOPITT/Terra V9T L3 data using a weighted averaging approach, where weights were determined based on the MOPITT CO total column-to-prior ratio.

The final outcome is a Level 3 merged CO product that combines the IASI and MOPITT L3 CO data.

Table 4: CO column data sets produced within the CCI+precursors project. In analogy to [RD-1], product ID is given as {species}_{processing level}_{platform}_{sensor}.



Product ID	Processor	Provider	Time range
<i>L3 data sets</i>			
CO_L3_IASI_A/B/C ¹	V2	LATMOS-ULB	2008-2024
CO_L3_MRG (IASI-MOPITT)	V2	LATMOS-ULB	2008-2024

¹. IASI multi-platform product. Intermediate product provided to BIRA, not for end users.

2.5. NH₃ column data sets

The L3 NH₃ IASI data validated here (see Table 5) is based on the L2 ANNI v4.0.0 product, described in [RD-13].

Table 5: NH₃ column data sets produced within the CCI+precursors project. In analogy to [RD-1], product ID is given as {species}_{processing level}_{platform}_{sensor}.

Product ID	Processor	Provider	Time range
<i>L3 data sets</i>			
NH3_L3_IASI_A/B/C	ANNI v4.0.0	ULB-LATMOS	2007-2022
NH3_L3_MRG	ANNI v4.0.0	ULB-LATMOS	2007-2022

2.6. CHOCHO column data sets

The CHOCHO L3 data products are generated within the CCI+precursors project. The retrieval is based on the GLYRETRO glyoxal product available through the PAL system, but it includes several improvements. Two variants are available: a daily product at 0.25°x0.25° spatial resolution, and a monthly product at 0.125°x0.125° resolution.

Table 6: CHOCHO column data sets produced within the CCI+precursors project. In analogy to [RD-1], product ID is given as {species}_{processing level}_{platform}_{sensor}.

Product ID	Processor	Provider	Time range
<i>L3 data sets</i>			
CHOCHO_L3_S5P_TROPOMI Daily and monthly	S5P_PAL v1.0.2 / CCI+p v1.0	BIRA-IASB	2018 - 2023



3. Distribution of L3 data products to the CCI Open Data Portal

KNMI, BIRA-IASB and LATMOS have been in contact with Emily Anderson and Alison Waterfall (STFC UKRI) representatives of the CCI Open Data Portal, since January 2025 (first contact by KNMI), regarding the provision of the TROPOMI L3 NO₂, IASI-MOPITT L3 CO datasets as well as other Precursors_cci+ L3 datasets. The NO₂ and CO datasets have been submitted to the Centre for Environmental Data Analysis (CEDA) archive in October and September 2025, respectively.

Issues discussed:

- Checking whether sample files adhered to the CCI data format¹ (they did, apart from minor discrepancies such as the omission of some global attributes, e.g., 'spatial resolution'. LATMOS also had to add a 'time' dimension.
- Testing the data on CF-compliance² (passed successfully, no errors were found, only a warning regarding units in the boundary variables of latitude and longitude, which were included for HARP-compliance)
- Clarification on whether a L3 dataset already has an assigned DOI (in which case it remains) or whether the CCI Open Data Portal provides one (as for the IASI-MOPITT CO dataset).
- Instructions for creating catalogue records.

To upload the datasets, KNMI and LATMOS followed the procedure described on the CEDA archive website³.

KNMI submitted the TROPOMI L3 NO₂ dataset to the archive and created a catalogue for the ESA CCI ECV Precursor project as a whole and one for the TROPOMI NO₂ data record in particular. The total data size is 21 Gb. KNMI is currently uploading the OMI L3 NO₂ dataset to the CEDA archive (120 Gb).

LATMOS also submitted the IASI-MOPITT L3 CO dataset. A 'time' dimension and several missing global attributes were added. The DOI, generated by ESA, was included in the file attributes (it will not be active until CEDA has archived the data). The dataset size is 417 M.

	Catalogue record at CEDA
ECV Precursors project	https://catalogue.ceda.ac.uk/uuid/3a41ada4bcc24208a0b7f860ad69e29e/
TROPOMI L3 NO ₂	https://catalogue.ceda.ac.uk/uuid/a2ac22ae97a34b51a81c8f53d414ec6b/
OMI L3 NO ₂	

¹ https://climate.esa.int/media/documents/CCI_DataStandards_v2-3.pdf

² <https://cfchecker.ncas.ac.uk/>

³ <https://help.ceda.ac.uk/article/4660-depositing-data-at-ceda-a-step-by-step-guide>



IASI-MOPITT L3 CO	https://catalogue.ceda.ac.uk/uuid/6242532d87d442a3acf0171d35c02e56/
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