

Precursors_cci+

ESA Climate Change Initiative (CCI)



D4.2 Product User Guide (PUG)

Version 2

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DOCUMENT CHANGE RECORD

Issue	Revision	Date	Modified items	Observations
0	0	15/05/2023	Initial template	Creation of document
1	0	24/01/2024	First version	Some sections still incomplete
1	1	15/05/2024	Various minor changes + changes related to RID	
2	0	02/10/2025	Initial version 2	
2	1	21/01/2026	Revised second version	Update: Added data links (some are previews) and the DOIs



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1. Purpose and scope

The Precursors_CCI+ project (<https://climate.esa.int/en/projects/precursors-for-aerosols-and-ozone/>) aims to develop long-term climate data records of precursor species of aerosol and ozone. The species include the short-lived atmospheric trace gases: nitrogen dioxide (NO₂), sulphur dioxide (SO₂), carbon monoxide (CO), formaldehyde (HCHO), ammonia (NH₃) and glyoxal (CHOCHO). The data records originate from measurements from the satellite sounders IASI A/B/C, MOPITT, TROPOMI, OMI, GOME, GOME2 A/B/C and SCIAMACHY.

This product user guide serves as the primary reference for users seeking information to successfully employ the products in their work. The next section provides an overview of the different products. The remaining sections then provide detailed information on the products related to the each of the different species, including a short description of the input data and algorithms used, the file parameters, data access, format and reading examples, usage recommendation, preliminary evaluation/validation and finally contacts and citation.

2. Overview of the Precursors_CCI+ products

2.1. Overview

All satellite products, summarized in Table 2-1 constitute gridded data sets (L3), on daily or monthly basis and with varying spatial resolutions depending on the species. In addition to datasets from individual satellite sounders, also certain merged datasets are available (tagged as MRG in the product identifier). All data sets are reported in NetCDF -4 CF format following CCI and GCOS standards, and are freely available on the Precursors_CCI+ web site <https://climate.esa.int/en/projects/precursors-for-aerosols-and-ozone/>.

Table 2-1: List of the Precursors_cci+ datasets and associated characteristics.

Species	Product identifier	Source	Time period	Spatial res.	Temp. res.	L2 or L3 version
NH ₃	NH3_L3_IASI_A/B/C	ULB-LATMOS	200701-202506	0.2°	Monthly	ANNI v4.0.0R
	NH3_L3_IASI_MRG	ULB-LATMOS	200701-202506	0.2°	Monthly	ANNI v4.0.0R
CO	CO_L3_MRG	LATMOS-ULB	2007-2024	1°	Monthly	IASI L3 multiplatform v1.2 MOPITT L3 v9T
NO ₂	NO2_L3_S5P_TROPOMI	KNMI	2018-2021	2.0°x2.5°/1.0°/0.5°/0.2°	Daily/Monthly	v2.3.1
	NO2_L3_EOS-AURA_OMI	KNMI	2004-2021	2.0°x2.5°/1.0°/0.5°/0.2°	Daily/Monthly	QA4ECV v1.1
	NO2_L3_METOP_GOME2_A/B/C	DLR/EUMETSAT	2007-2023	0.2°	Monthly	AC-SAF prototype DLR
	NO2_L3_ENVISAT_SCIAMACHY	DLR/KNMI/QA4 ECV	2002-2012	0.2°	Monthly	QA4ECV v1.1



	NO2_L3_ERS2_GOME	DLR/KNMI/QA4 ECV	1995-2003	0.2°	Monthly	QA4ECV v1.1
HCHO	HCHO_L3_S5P_TROPOMI	BIRA-IASB/DLR/ESA	2018-2024	0.25°/0.125°	Daily/Monthly	OFFL v0.3_02/CCI+p v2.0
	HCHO_L3_S5P_OMI	BIRA-IASB/QA4ECV	2005-2023	0.25°/0.125°	Daily/Monthly	QA4ECV v1.2/CCI+p v2.0
	HCHO_L3_METOP_GOME2_A/B/C	DLR/BIRA-IASB/EUMETSAT	2007-2023	0.25°	Monthly	AC SAF prototype/CCI+p v2.0
	HCHO_L3_ENVISAT_SCIAMACHY	BIRA-IASB/QA4ECV	2003-2012	1°	Monthly	QA4ECV v1.2/CCI+p v2.0.
	HCHO_L3_ERS2_GOME	BIRA-IASB/QA4ECV	1996-2002	1°	Monthly	QA4ECV v1.2/CCI+p v2.0.
SO ₂	SO2_L3_S5P_TROPOMI	BIRA-IASB/DLR/ESA	2018-2024	0.25°/0.125°	Daily/Monthly	OFFL v0.3_02/CCI+p v1.0
	SO2_L3_S5P_OMI	BIRA-IASB	2005-2022	0.25°/0.125°	Daily/Monthly	CCI+p v1.0
	SO2_L3_ENVISAT_SCIAMACHY	BIRA-IASB	2003-2012	0.25°	Monthly	TBD
	SO2_L3_ERS2_GOME	BIRA-IASB	1996-2002	0.25°	Monthly	CCI+p v1.0
CHOCHO	CHOCHO_L3_S5P_TROPOMI	BIRA-IASB/ESA	2018-2024	0.25° / 0.125°	Daily/Monthly	S5P_PAL v01.00.02 / CCI+p v1.0
	CHOCHO_L3_AURA_OMI	BIRA-IASB	2005-2023	0.25° / 0.125°	Daily/Monthly	CCI+p v1.0
	CHOCHO_L3_METOP_GOME2_A/B/C	BIRA-IASB	2007-2023	0.25°	Monthly	CCI+p v1.0

2.2. Terms and conditions for use of Precursors_CCI+ data

The Precursors_CCI+ datasets may be used by any user for any purpose, with the following terms and conditions:

- (1) Users of the CCI data are required to acknowledge the ESA Climate Change Initiative and Precursors_CCI+ together with the individual data providers if the data are used in a presentation or publication. Please also cite any relevant dataset DOIs (see contacts and citation information in the respective sections).
- (2) Users of the CCI data are encouraged to interact with the CCI programme on use of the products, and to provide a copy of all reports and publications using the dataset. A co-authorship offer should be considered if CCI data constitute a significant part of a scientific publication.
- (3) Intellectual property rights (IPR) in the CCI data lie with the researchers and organisations producing the data.





- (4) Liability: No warranty is given as to the quality or the accuracy of the CCI data or its suitability for any use. All implied conditions relating to the quality or suitability of the information, and all liabilities arising from the supply of the information (including any liability arising in negligence) are excluded to the fullest extent permitted by law.

3. NH₃ L3 from IASI

3.1. Input data and algorithm

The IASI instrument is a Fourier transform spectrometer that measures the thermal infrared emission of the Earth-atmosphere system between 645 and 2760 cm⁻¹ with a spectral resolution of 0.5 cm⁻¹ and sampling of 0.25 cm⁻¹. IASI provides global coverage of the Earth twice a day (at 9:30 and 21:30 mean local solar time) thanks to the combination of a wide swath width of 2 times 1100 km and a set of four simultaneous footprints of 12 km diameter at nadir.

The IASI NH₃ L2 product has been generated at ULB using the ANNI (Artificial Neural Network for IASI) v4 code. ANNI implements a two-step retrieval consisting of the calculation of a NH₃ hyperspectral range index, followed by the conversion of the index to a total column product using a neural network. This last step also includes calculation of diagnostic variables (averaging kernels, uncertainties). The input data for the retrieval algorithm consists of L1C spectra, parameters related to the geolocation (time, latitude, longitude) and observation (zenith angle), meteorological data (cloud and surface temperature, pressure, temperature, and humidity profiles). Clouds and surface temperature are derived from the L1C spectra using dedicated neural networks. Other meteorological data originates from ECMWF ERA5 reanalysis. All the data was postfiltered using the recommended L2 postfilter and keeping data with a cloud fraction below 10%.

The monthly L3 products are directly derived from the L2 by means of oversampled averaging on a 0.2° x 0.2°, where the exact IASI footprint on ground is taken into account. The L3 product consists of NH₃ total columns and associated random and systematic uncertainties for the morning and evening overpass separately. L3 data are available for each instrument separately.

The merged product is formally identical to the NH₃ L3 product, but for each point in time 200701-202506 uses one IASI instrument only, thereby guaranteeing a consistent L3 product that uses approximately the same number of measurements for each month throughout. This L3 NH₃ CDR is generated based on observations from IASI/Metop-A (2008-2013), IASI/Metop-B, (2014-2019), IASI/Metop-C (2020-...) data. An alternative L3 merged product would consist of averaging multiple IASI datasets, but that would result in an uneven number of measurements (e.g. L3 that is based on less measurements before 2013 then after), and for this reason this alternative was not implemented.

The reader is invited to refer to the NH₃ ATBD available at <https://climate.esa.int/en/projects/precursors-for-aerosols-and-ozone/> and to Clarisse et al. (2023) for a full description of the L2 and L3 algorithm.



3.2. File parameters

Tables 3.1 describe the variables contained in the L3 NH₃ NetCDF files. The fill value is NaN for all.

Table 3.1: Variables in the L3 NH₃ NetCDF files. N_{lat} (900) and N_{lon} (1800) are the number of grid cells corresponding to the latitude and longitude respectively.

Parameter	Unit	Dimension	Description
time	days	Time=1	Number of days since 1970-01-01
latitude	degrees	lat	latitude
longitude	degrees	lon	longitude
nh3_total_column_ampm	mol.m ⁻²	time,lat,lon	L3 (AM+PM) NH ₃ total column
nh3_total_column_am	mol.m ⁻²	time,lat,lon	L3 (AM) NH ₃ total column
nh3_total_column_pm	mol.m ⁻²	time,lat,lon	L3 (PM) NH ₃ total column
number_of_observations_ampm	1	time,lat,lon	number of observations used for calculating the L3 (AM+PM)
number_of_observations_am	1	time,lat,lon	number of observations used for calculating the L3 (AM)
number_of_observations_pm	1	time,lat,lon	number of observations used for calculating the L3 (PM)
nh3_total_column_random_uncertainty_ampm	mol.m ⁻²	time,lat,lon	random total uncertainty on the NH ₃ total column (AM+PM)
nh3_total_column_random_uncertainty_am	mol.m ⁻²	time,lat,lon	random total uncertainty on the NH ₃ total column (AM)
nh3_total_column_random_uncertainty_pm	mol.m ⁻²	time,lat,lon	random total uncertainty on the NH ₃ total column (PM)
nh3_total_column_systematic_uncertainty_ampm	mol.m ⁻²	time,lat,lon	systematic total uncertainty on the NH ₃ total column (AM+PM)
nh3_total_column_systematic_uncertainty_am	mol.m ⁻²	time,lat,lon	systematic total uncertainty on the NH ₃ total column (AM)
nh3_total_column_systematic_uncertainty_pm	mol.m ⁻²	time,lat,lon	systematic total uncertainty on the NH ₃ total column (PM)
surface_altitude_ampm	m	time,lat,lon	surface altitude (AM+PM)
surface_altitude_am	m	time,lat,lon	surface altitude (AM)
surface_altitude_pm	m	time,lat,lon	surface altitude (PM)
surface_air_pressure_ampm	Pa	time,lat,lon	surface air pressure (AM+PM)
surface_air_pressure_am	Pa	time,lat,lon	surface air pressure (AM)
surface_air_pressure_pm	Pa	time,lat,lon	surface air pressure (PM)
eff_fract_day_am	1	time,lat,lon	effective fractional day in local solar time. UTC = local_solar_time - longitude/360
eff_fract_day_pm	1	time,lat,lon	effective fractional day in local solar time. UTC = local_solar_time - longitude/360



float eff_date_ampm	days	time,lat,lon	effective date of observation in days since the start of the month (1-31)
float eff_date_am	days	time,lat,lon	effective date of observation in days since the start of the month (1-31)
float eff_date_pm	days	time,lat,lon	effective date of observation in days since the start of the month (1-31)

3.3. DOI, data access and volume

The DOI is: 10.5285/463862326d574951bea52527f9df397d [NOT LIVED YET]

The L3 product can be accessed from:

- <https://catalogue.ceda.ac.uk/uuid/c152a24620504209b59e07c6f97f26e0/> [PREVIEW NOT PUBLISHED YET] (L3 Metop-A)
- <https://catalogue.ceda.ac.uk/uuid/559901afef54425f8e755f9305d0af3a/> [PREVIEW NOT PUBLISHED YET] (L3 Metop-B)
- <https://catalogue.ceda.ac.uk/uuid/c1cee19b22ae4c6187605ada036477e4/> [PREVIEW NOT PUBLISHED YET] (L3 Metop-C)
- <https://catalogue.ceda.ac.uk/uuid/2ec5b1fb653445bdbbd0dcd69dd223da/> [PREVIEW NOT PUBLISHED YET] (L3 MERGED)

The CCI filename convention is as follows:

ESACCI-PREC-{L3type} -{gas} -{platform} _{instrument} _{institute} -{spat.resolution in no of pixels}_ {duration}-{date}-fvx.x.nc

Example file name for one monthly IASI file:

ESACCI-PREC-L3C-NH3-METOPB_IASI_ULB-LATMOS_0900x1800_1M-201405-fv4.0.1R.nc

The content of the NetCDF files is listed in Tables 3.1.

Data volume is as follows:

- One file one sensor: 80-90 MB
- One year one sensor: 1.1 GB
- IASI-A 200710-202110: 15 GB
- IASI-B 201303-202506: 14 GB
- IASI-C 201909-202506: 6.5 GB
- Merged product 200710-202506: 19 GB

Note that the L2 source product (not described here) can be downloaded from AERIS (<https://iasi.aeris-data.fr/>) (one file per day).

3.4. Data reading examples

Examples on how to read the NetCDF files are provided below, for Matlab or Python.





Matlab code

```
% Filename of the NetCDF file
fn = 'IASI_METOPB_L3_NH3_202304_ULB-LATMOS_V4.0.0R.nc';

% Retrieve information about the file
fileinfo = ncinfo(fn);

% Read in all variables from the file
for i = 1:length(fileinfo.Variables)
    NH3.(fileinfo.Variables(i).Name) = ncread(fn, fileinfo.Variables(i).Name);
end

% Read in conversion factor from molesConversion to molecules/cm^2
conversion = fileinfo.Variables(3).Attributes(4).Value;

% Create a figure
figure;
imagesc(NH3.longitude, NH3.latitude, NH3.nh3_total_column_am' * conversion, [0 5e16]);
set(gca, 'ydir', 'normal');
colorbar;

% Load and display coastlines
load coastlines;
geoshow(coastlat, coastlon, 'DisplayType', 'line', 'Color', 'k');

% Set the title of the figure
title(fn, 'Interpreter', 'none');
```

Python code

```
import os
import netCDF4 as nc
import matplotlib.pyplot as plt
import cartopy.crs as ccrs

# Full file path of the NetCDF file
file_path = 'IASI_METOPB_L3_NH3_202304_ULB-LATMOS_V4.0.0R.nc'

# Extract file name and directory path
file_name = os.path.basename(file_path)
directory_path = os.path.dirname(file_path)

# Open the NetCDF file
dataset = nc.Dataset(file_path)

# Create a dictionary to hold the data
NH3 = {}

# Read in all variables from the file
for variable in dataset.variables:
    NH3[variable] = dataset.variables[variable][:]

# Read NH3 total column data and conversion factor
conversion = dataset.variables['nh3_total_column_am'].getncattr('multiplication_factor_to_convert_to_molecules_per_cm2')

# Get longitude and latitude data
longitude = NH3['longitude'][:,:]
latitude = NH3['latitude'][:,:]

# Create a figure with specific size based on the grid's aspect ratio
fig = plt.figure(figsize=(14, 10 * (latitude.max() - latitude.min()) / (longitude.max() - longitude.min())))
ax = fig.add_subplot(1, 1, 1, projection=ccrs.PlateCarree())

# Display the data
image = plt.imshow(NH3['nh3_total_column_am'] * conversion, extent=[longitude.min(), longitude.max(), latitude.min(), latitude.max()], origin='lower', cmap='viridis')
plt.colorbar(image, label='NH3 Total Column (molec/cm²)')
plt.clim(0, 2e+16)

# Plot coastlines
ax.coastlines()

# Set the title of the figure using just the file name
plt.title(file_name)

# Show the plot
plt.show()
```

3.5. Usage recommendations and known limitations

- Users interested in long-term trends should use the merged L3 dataset. Users interested in short time periods are advised to use the L3 from the three instruments, taking caution that IASI-A started to drift from 2018 onwards, with gradually earlier overpass times as shown in Figure 3.1.



- Higher uncertainties are expected during the evening overpass over land (PM) at high latitude (>60° N or <60° S) and in absence of thermal contrast, which occurs mainly in the colder months (surface temperature below 10°C).
- Over land, it is recommended to use primarily the morning (AM) data, as the PM data is more noisy, and has known biases (some monthly L3 are substantially negative). Over ocean, both AM, PM and AM+PM L3 are recommended for use.
- When averaging the L3 data to larger time periods, to reduce the influence of months with very few measurements, it is recommended to disregard cells with fewer than 0.25 observations (using the appropriate number_of_observations variables).
- Mean random (σ_r) and systematic (σ_s) uncertainties are available for each grid cell. If a total uncertainty is desired, this can be obtained from the square root of the sum of squares of the different terms:

$$\sigma^2 = \sigma_r^2 + \sigma_s^2$$
- When averaging L3 data over larger temporal or spatial scales, an averaged uncertainty can be obtained from combine the different random (σ_{ri}) and systematic (σ_{si}) uncertainties as

$$\sigma^2 = \sum_{i=1}^n \left(\frac{\sigma_{ri}}{n} \right)^2 + \left(\sum_{i=1}^n \frac{\sigma_{si}}{n} \right)^2$$

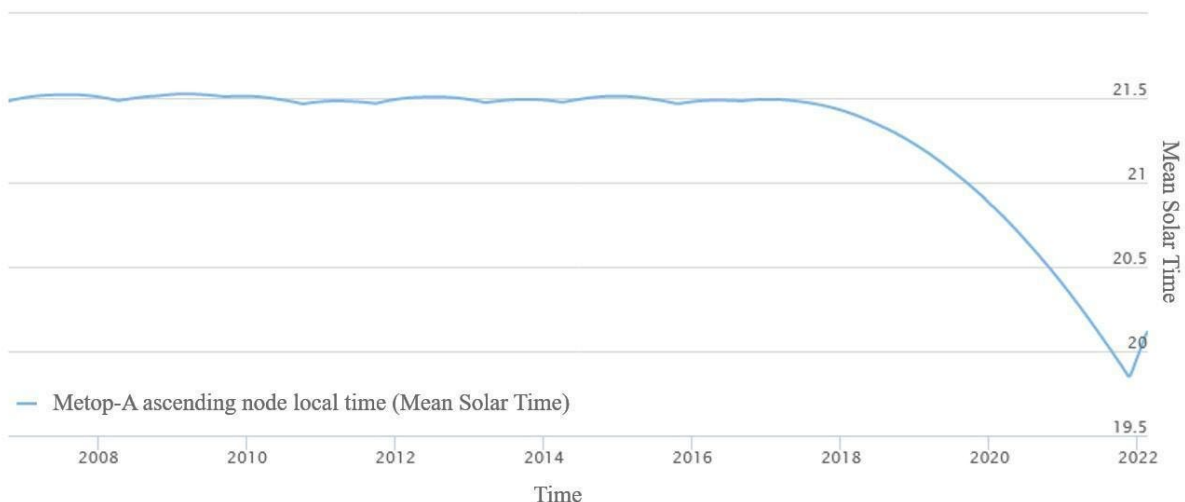


Figure 3.1 Mean Solar Time of Metop-A as a function of time, showing the drift after 2018. Source: <https://climserv.ipsl.polytechnique.fr/ixion/>

3.6. Preliminary evaluation

A preliminary evaluation of the product's consistency between the three IASI instruments is provided in Figure 3.2. The figure shows NH₃ monthly average values over selected regions for the three IASI instruments separately. These are seen to agree well, with no obvious large biases.



Full validation results are provided for each sensor dataset in the Product Validation and Intercomparison Report (PVIR) available at <https://climate.esa.int/en/projects/precursors-for-aerosols-and-ozone/>.

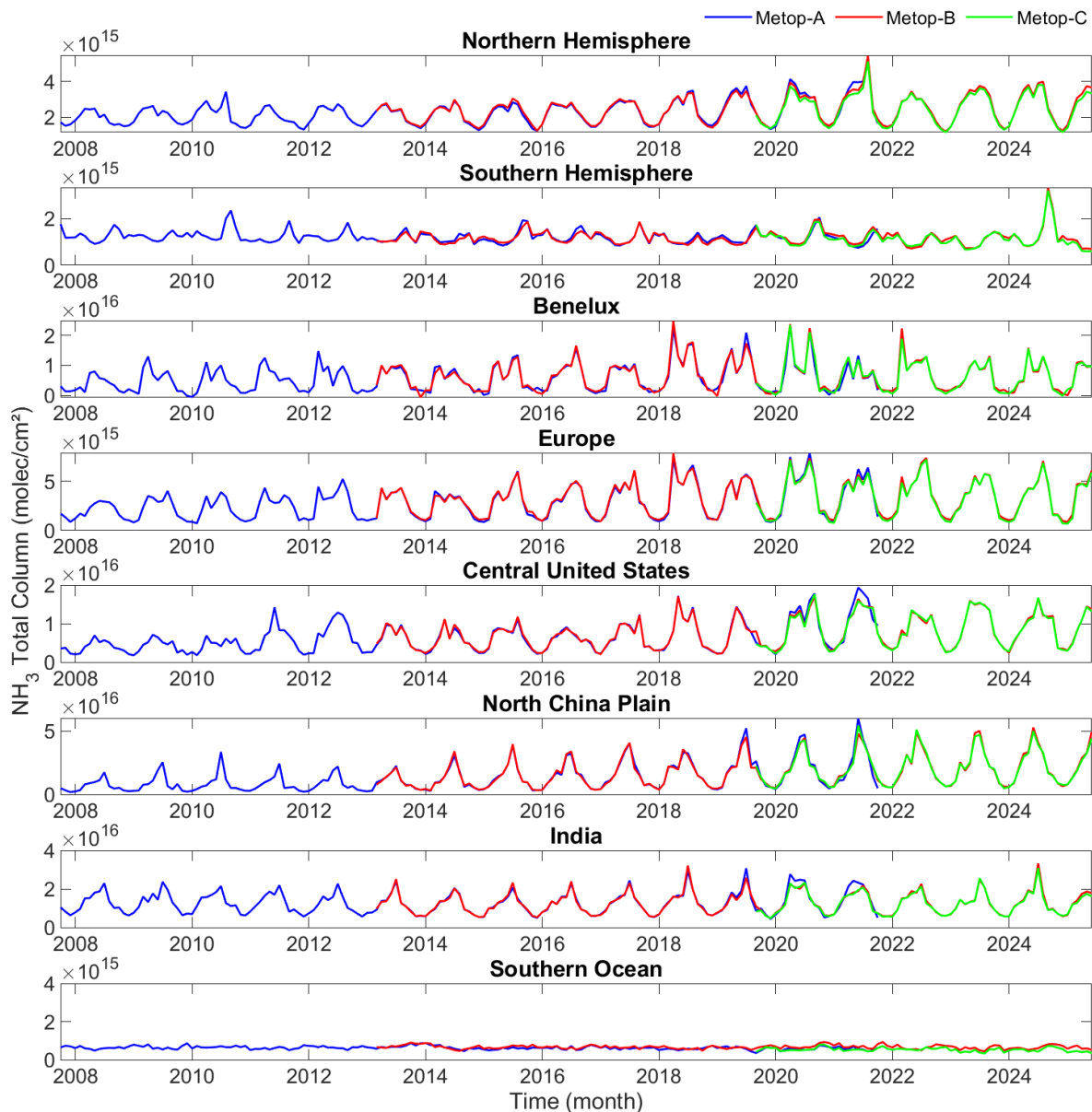


Figure 3.2 Monthly NH_3 columns for selected regions for the three IASI instruments onboard Metop A, B and C.

3.7. Contacts and citation

Contacts:

- Lieven Clarisse: Lieven.Clarisse@ulb.be
- Martin Van Damme: Martin.Van.Damme@ulb.be
- Pierre-François Coheur: Pierre.Coheur@ulb.be





Dataset citation:

- Clarisse, L., Van Damme M., Coheur P. (2024), IASI L3 NH₃ ANNI v4 Climate Data Record, ESA Precursors CCI+. <https://doi.org/10.5285/463862326d574951bea52527f9df397d> [NOT LIVED YET]

Paper citation:

- Clarisse, L., Franco, B., Van Damme, M., Di Gioacchino, T., Hadji-Lazaro, J., Whitburn, S., Noppen, L., Hurtmans, D., Clerbaux, C., and Coheur, P.: The IASI NH₃ version 4 product: averaging kernels and improved consistency, Atmos. Meas. Tech., 16, 5009–5028, <https://doi.org/10.5194/amt-16-5009-2023>, 2023.



4. CO L3 product from IASI and MOPITT

4.1. Input data and algorithm

We generate a monthly Climate Data Record (CDR) Level 3 Carbon Monoxide (CO) product from IASI and MOPITT monthly L3 datasets. It consists in monthly grids for daytime and nighttime measurements. The objective is to produce a harmonized dataset that combines the strengths of both instruments while minimizing uncertainties.

The merged product incorporates data from a IASI non-public intermediate multiplatform dataset as well as MOPITT V9T data, processed with a weighted averaging approach. We first generated the IASI non-public intermediate multiplatform dataset averaging cloud free data from Metop-A, Metop-B, and Metop-C. MOPITT data consist in the latest version available: v9T.

The merged dataset spans from January 2008 to December 2024 and consist in 1°x1° monthly grids.

The different steps are summarised in Figure 4.1.

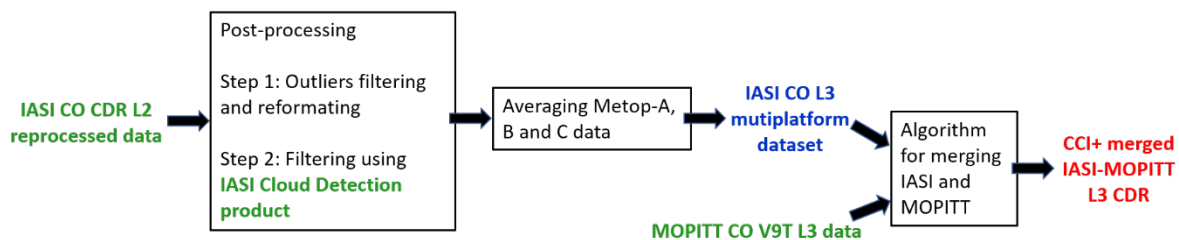


Figure 4.1: Graphic representation of the processing steps of the generation of the CCI+ IASI-MOPITT CO L3 merged product.

We refer to the Algorithm Theoretical Basis Document for the description of the weighted averaging of the CO total columns as well as the uncertainty grids calculation (See Algorithm Theoretical Basis Document (ATBD) v2 on <https://climate.esa.int/en/projects/precursors-for-aerosols-and-ozone/>) (See the “Key Documents” tab).

4.2. File parameters

Table 4.1 describes the variables to be contained in the L3 CO IASI MOPITT MERGED NetCDF files. The fill value is NaN for all the grids except for the flag grids where it is -999.

Table 4.1: Variables to be in the L3 CO IASI MOPITT MERGED NetCDF files. The dimensions Nlat (180) and Nlon (360) are the number of grid cells corresponding to the latitude and longitude respectively.



Parameter	Unit	Dimension	Description
latitude	degrees	N_{lat}	latitude
longitude	degrees	N_{lon}	longitude
co_total_column_day	molecules cm^{-2}	$N_{lat} \times N_{lon}$	monthly merged IASI MOPITT total carbon monoxide columns for daytime observations
co_total_column_night	molecules cm^{-2}	$N_{lat} \times N_{lon}$	monthly merged IASI MOPITT total carbon monoxide columns for nighttime observations
co_total_column_uncertainty_day	molecules cm^{-2}	$N_{lat} \times N_{lon}$	Uncertainty in monthly merged IASI MOPITT total carbon monoxide columns for daytime observations
co_total_column_uncertainty_night	molecules cm^{-2}	$N_{lat} \times N_{lon}$	Uncertainty in monthly merged IASI MOPITT total carbon monoxide columns for nighttime observations
flag_day	unitless	$N_{lat} \times N_{lon}$	flag for instruments used in the weighted average, for daytime observations: 3 for IASI and MOPITT, 2 for IASI only, 1 for MOPITT only and 0 when no data
flag_night	unitless	$N_{lat} \times N_{lon}$	flag for instruments used in the weighted average, for nighttime observations: 3 for IASI and MOPITT, 2 for IASI only, 1 for MOPITT only and 0 when no data
surface_altitude_day	m	$N_{lat} \times N_{lon}$	altitude of the surface for IASI daytime observations
surface_altitude_night	m	$N_{lat} \times N_{lon}$	altitude of the surface for IASI nighttime observations

4.3. DOI, data access and volume

The DOI is: 10.5285/6242532d87d442a3acf0171d35c02e56

The CO L3 product can be accessed from <https://catalogue.ceda.ac.uk/uuid/6242532d87d442a3acf0171d35c02e56/> under the "Download" tab.

The CCI filename convention is as follows:

ESACCI-PREC-L3S-CO-IASI_MOPITT_MERGED_LATMOS-180x360_1M-YYYYMM-fv1.0.nc
where YYYYMM is the date. The content of the NetCDF files is listed in Tables 4.1.

Data volume is estimated as follows:

- One monthly file: 2,1 MB
- One year (12 files): 25,2 MB
- 2008-2024 period (17 years x 12 files = 204 files): 428,4 MB

4.4. Data reading examples





Here is an example of a python code to read one NetCDF file and plot one CO monthly grid.

```
#!/usr/bin/env python3
# -*- coding: utf-8 -*-

import xarray as xr
import matplotlib.pyplot as plt
import cartopy.crs as ccrs
import cartopy.feature as cfeature

# -----
# Parameters: year and month
# -----
year = 2009
month = 10 # Month between 1 and 12
month_str = f"{month:02d}"

# -----
# Generate file path
# -----
file_path = f'ESACCI-PREC-L3S-CO-IASI_MOPITT_MERGED_LATMOS-180x360_1M-{year}{month_str}-fv1.0.nc'

# -----
# Load and visualize
# -----
# Load the NetCDF file
dataset = xr.open_dataset(file_path)

# Extract variable and coordinates
co_total_column_day = dataset['co_total_column_day']
latitudes = dataset['latitude']
longitudes = dataset['longitude']

# Create the figure with projection
fig = plt.figure(figsize=(10, 6))
ax = plt.axes(projection=ccrs.PlateCarree())
ax.set_extent([-180, 180, -90, 90], crs=ccrs.PlateCarree())

# Plot the CO variable
mesh = ax.pcolormesh(longitudes, latitudes, co_total_column_day,
                    cmap='jet', transform=ccrs.PlateCarree(),
                    vmin=0.5e18, vmax=6e18)

# Add colorbar
cbar = plt.colorbar(mesh, ax=ax, orientation='vertical',
                    label='CO Total Column (molecules/cm²)', shrink=0.7)

# Add coastlines, borders, and grid
ax.add_feature(cfeature.COASTLINE)
ax.add_feature(cfeature.BORDERS, linestyle=':')
gl = ax.gridlines(draw_labels=True, dms=True, x_inline=False, y_inline=False)
gl.top_labels = False
gl.right_labels = False

# Dynamic title based on selected month and year
plt.title(f'IASI MOPITT Merged CO Total Column Day ({month_str} {year})', fontsize=15)

# Show plot
plt.show()

# Close the dataset
dataset.close()
```

4.5. Usage recommendations and known limitations

- Users interested in long-term CO trends should use the IASI-MOPITT merged Level 3 dataset.





- The main variables are "co_total_column_day" and "co_total_column_night", which represent monthly merged IASI-MOPITT total column carbon monoxide data for daytime and nighttime observations, respectively, on a 1°x1° grid.
- Associated uncertainty grids are "co_total_column_uncertainty_day" and "co_total_column_uncertainty_night".
- There are no quality flags; the grids can be used as provided.
- The "flag_day" and "flag_night" grids indicate which sensors contributed to the weighted average:
 - 3: both IASI and MOPITT
 - 2: IASI only
 - 1: MOPITT only
 - 0: no data available (neither MOPITT nor IASI)

4.6. Preliminary evaluation

This new product has been validated against NDACC measurements by BIRA. We refer to the Product Validation and Intercomparison Report (See Product Validation and Intercomparison Report (PVIR) on <https://climate.esa.int/en/projects/precursors-for-aerosols-and-ozone/>). The validation methodology is based on a nearest-pixel (1°x1°) co-location criterion. All ground-based measurements within each month have been averaged to enable direct comparison with the IASI-MOPITT MERGED product.

No smoothing has been applied, as no averaging kernel information is provided. IASI surface altitude grids, available in the NetCDF files, allow for altitude correction of the station column. This correction is performed by scaling the column using the ratio of the prior partial column between the two surface altitudes (merged and station) to the total prior column.

Considering all ground-based stations, the following statistics are obtained:

- Median mean bias: 3.93%
- Median Absolute Deviation: 1E+17
- Correlation coefficient: 0.96
- 1/2IP68: 7.4%

4.7. Contacts and citation

Contact:

- Maya George: maya.george@latmos.ipsl.fr
- Cathy Clerbaux: cathy.clerbaux@latmos.ipsl.fr

Dataset citation:

- George M., Clerbaux C. (2026), L3 CO IASI MOPITT MERGED LATMOS, ESA Precursors CCI+, <https://doi.org/10.5285/6242532d87d442a3acf0171d35c02e56>



5. NO₂ L3 from GOME, SCIAMACHY, GOME2-A/B/C, OMI and TROPOMI

5.1. Input data and algorithm

NO₂ can be retrieved from a series of nadir UV-VIS sensors. We focus on the following sensors: GOME, SCIAMACHY, GOME2-A/B/C, OMI, TROPOMI.

The NO₂ retrieval procedure consists of a procedure with three steps, and is performed for each level-1 spectrum:

- (1) Retrieval of the total NO₂ slant column density (N_s) from the level-1 radiance and irradiance spectra measured by the sensor with the Differential Optical Absorption Spectroscopy (DOAS) method,
- (2) Separation of the N_s into a stratospheric (N_s^{strat}) and tropospheric part ($N_s^{trop} = N_s - N_s^{strat}$) based on information from a system incorporating slant columns and modelled or climatological information on tropospheric contributions,
- (3) Conversion of the tropospheric slant column density into a vertical column density (N_v^{trop}) via a tropospheric air mass factor (M^{trop}).

The central retrieval equation can thus be written as:

$$N_v^{trop} = \frac{N_s - N_s^{strat}}{M^{trop}} \quad 5-1$$

In Eq. 5-1 the factor M^{trop} quantifies how the tropospheric slant column has been influenced by scattering, absorption, and reflection in the troposphere or by the Earth's surface. M^{trop} depends on the satellite viewing geometry, the presence of clouds or aerosols, surface properties, and the vertical distribution of NO₂ in the troposphere. The retrieval procedure therefore requires accurate, pixel-specific information on these geophysical parameters, and the NO₂ level-2 algorithms obtain this from the satellite measurements themselves, or from well-tested ancillary datasets.

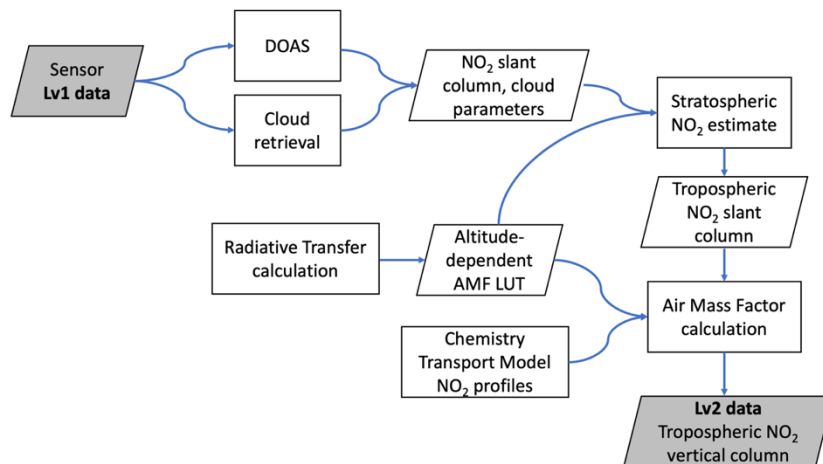


Figure 5-1: General overview of the processing chain for the retrieval of the level-2 tropospheric NO₂ columns.

The L2 versions used to produce the L3 CDR are summarized in Table 2-1. The GOME-2-A, B, C data are directly taken from the AC SAF prototype product, developed in parallel of this project. For the other sensors, the slant columns are directly taken from the operational product (TROPOMI; van Geffen et al. (2022)), or from the QA4ECV products (OMI, SCIAMACHY, GOME; Boersma et al., 2018). The air mass factors, and stratospheric correction are calculated with consistent and updated settings. For further details on the L2 algorithm settings selected for this project, the reader is invited to refer to the NO₂ ATBD available at <https://climate.esa.int/en/projects/precursors-for-aerosols-and-ozone/>.

The L3 products are directly derived from the L2 products. The L3 product consists of NO₂ tropospheric columns and associated uncertainties, detailed results, and input data. L3 are available for each instrument separately.

Two merged CDRs will also be provided, separately for morning and afternoon observations.

- Morning sensors: GOME/ERS-2, SCIAMACHY/ENVISAT, GOME2/METOP-A, B, C
- Afternoon sensors: OMI/AURA, TROPOMI/S5P

Since the spatial resolution and signal-to-noise ratio of the sensors are different, and significantly better for the afternoon sensors, different spatial resolutions are used. This is motivated by different user needs and applications, and various spatial resolutions can be generated. Table 5-1 provides the spatial and temporal resolution (preliminary) chosen for the morning and afternoon CDRs.

Table 5-1: spatial resolution of the L3 NO₂ products for morning and afternoon sensors, at daily and monthly time resolution.

Spatial resolution	Daily L3	Monthly L3
Morning CDR		0.5°/0.2°
Afternoon CDR	In progress	2.0°x2.5°/1.0°/0.5°/0.2°

The spatial resolution for daily L3 files needs to be coarser than for the monthly data, so that spatial averaging and gridding does not introduce major issues of spatial misallocation. KNMI (superobservations) and DLR (HARP) use similar tools for L3 gridding and averaging, but there are differences with respect to L3 uncertainty propagation and temporal weighting of daily (gridded) satellite data that make up the monthly mean (Rijsdijk et al. [2024]; D2.2 E3UB[2025]).

5.2. File parameters

Table 5-2 describes the variables contained in the L3 NO₂ NetCDF files. The fill value is NaN for all.

Table 5-2: Variables in the L3 NO₂ NetCDF files.

Parameter	Unit	Dimension	Description
time	days	time=1	start date of monthly mean



latitude	degrees	lat	latitude
longitude	degrees	lon	longitude
latitude_bounds	degrees	lat, independent_2	grid latitude bounds
longitude_bounds	degrees	lon, independent_2	grid longitude bounds
eff_date	days	time=1	effective date of observation (number between 1-31)
eff_frac_day	1	time, lat, lon	effective fractional day (number between 0-1)
vertical	1	vertical	vertical dimension index
tm5_sigma_a	hPa	vertical, independent_2	pressure = tm5_sigma_a + surface_pressure * tm5_sigma_b
tm5_sigma_b	1		
surface_pressure	hPa	time, lat, lon	surface pressure
surface_albedo	1	time, lat, lon	surface LER (440 nm)
land_water_mask	1	time, lat, lon	0: water, 1: land, 2: land water transition
qa_L3	1	time, lat, lon	gridded data quality assurance value (0: not valid, 1: valid)
tropospheric_NO2_column_number_density	molec.c m ⁻²	time, lat, lon	NO ₂ tropospheric vertical column number density
tropospheric_NO2_column_number_density_temporal_std	molec.c m ⁻²	time, lat, lon	Temporal standard deviation in the NO ₂ tropospheric vertical column.
tropospheric_NO2_column_number_density_total_uncertainty	molec.c m ⁻²	time, lat, lon	Total uncertainty on the NO ₂ tropospheric vertical column number density associated with time-averaged propagated uncertainty of L2 input data and temporal representativity
tropospheric_NO2_column_number_density_total_uncertainty_kernel	molec.c m ⁻²	time, lat, lon	Total uncertainty on the NO ₂ tropospheric vertical column number density associated with time-averaged propagated uncertainty of L2 input data and temporal representativity, without the profile uncertainty contribution
tropospheric_NO2_column_number_density_count	1	time, lat, lon	Effective number of observations per cell / fractional coverage (coverage divided by number of days) .
NO2_slant_column_number_density	molec.c m ⁻²	time, lat, lon	NO ₂ slant column number density
NO2_slant_column_number_density_uncertainty	molec.c m ⁻²	time, lat, lon	NO ₂ slant column number density uncertainty component of the tropospheric column uncertainty
NO2_slant_column_number_density_troposphere	molec.c m ⁻²	time, lat, lon	Tropospheric NO ₂ slant column number density





stratospheric_NO2_column_number_density	molec.c m ⁻²	time, lat, lon	Stratospheric NO2 vertical column number density
tropospheric_NO2_column_number_density_amf	1	time, lat, lon	tropospheric air mass factor
total_NO2_column_number_density_amf	1	time, lat, lon	total air mass factor
tropopause_layer_index	1	time, lat, lon	TM5 tropopause layer index
cloud_fraction	1	time, lat, lon	effective cloud fraction
cloud_pressure	hPa	time, lat, lon	cloud pressure at optical centroid
NO2_averaging_kernel	1	time, lat, lon, layer	NO2 full column averaging kernel

5.3. DOI, data access and volume

The DOIs are:

For OMI L3: <https://doi.org/10.21944/cci-no2-omi-l3>

For TROPOMI L3: <https://doi.org/10.21944/cci-no2-tropomi-l3>

The L3 product can be accessed from:

- <https://catalogue.ceda.ac.uk/uuid/a2ac22ae97a34b51a81c8f53d414ec6b> [PREVIEW NOT PUBLISHED YET] (L3 TROPOMI)

The L3 product is following the CCI filename convention:

ESACCI-PREC-{L3type} -{gas} -{platform} _{instrument} _{institute} -{spat.resolution in no of pixels}_ {duration}-{date}-fvx.x.nc

Example of file name for one TROPOMI monthly L3 file:

ESACCI-PREC-L3C-NO2-S5P_TROPOMI_KNMI-0900x1800_1M-201805-fv1.0.nc

The content of the NetCDF files is listed in Table 5-2.

Data volume is as follows:

Table 5-3: Size of one L3 file for morning and afternoon sensors, at daily and monthly time resolution.

Spatial resolution	Daily L3	Monthly L3
Morning CDR		100MB
Afternoon CDR	In progress	450MB (max)

5.4. Data reading examples

```
import numpy as np
import netCDF4 as nc
```





```

import matplotlib.pyplot as plt
import cartopy.crs as ccrs
import cartopy

#Read File

path='...' #file location path

filename='ESACCI-PREC-L3C-NO2-S5P_TROPOMI_KNMI-0900x1800_1M-201805-fv1.0.nc'

ds=nc.Dataset(f'{path}'+f'{filename}','r')

# Read Variables

no2=np.array(ds.variables['tropospheric_NO2_column_number_density'])[0,:,:]
qa=np.array(ds.variables['qa_L3'])[0,:,:]
lat=np.array(ds.variables['latitude'])
lon=np.array(ds.variables['longitude'])

no2[qa==0]=np.nan # Quality Assurance (QA) value of the L3 data

# Plot NO2 Map

fig1 = plt.figure(figsize = (12,7))
plt.rcParams.update({'font.size': 14})
ax1 = plt.subplot(111, projection=ccrs.Robinson())
ax1.add_feature(cartopy.feature.COASTLINE, linewidth=0.6)
ax1.add_feature(cartopy.feature.BORDERS, linestyle='-', linewidth=.2)
h=ax1.pcolormesh(lon, lat,no2/1e15, cmap='magma_r', vmin=0, vmax=10,transform=ccrs.PlateCarree())
plt.title('OMI NO2 2$ Monthly Mean of Tropospheric VCD on May 2018', fontsize = 18)
ax1.set_extent([-179,179,-90,90])
cb=plt.colorbar(h, fraction=0.02, extend='both')
cb.set_label('10 $^{15}$ molecules/cm$^{2}$')

plt.show()

```

5.5. Usage recommendations and known limitations

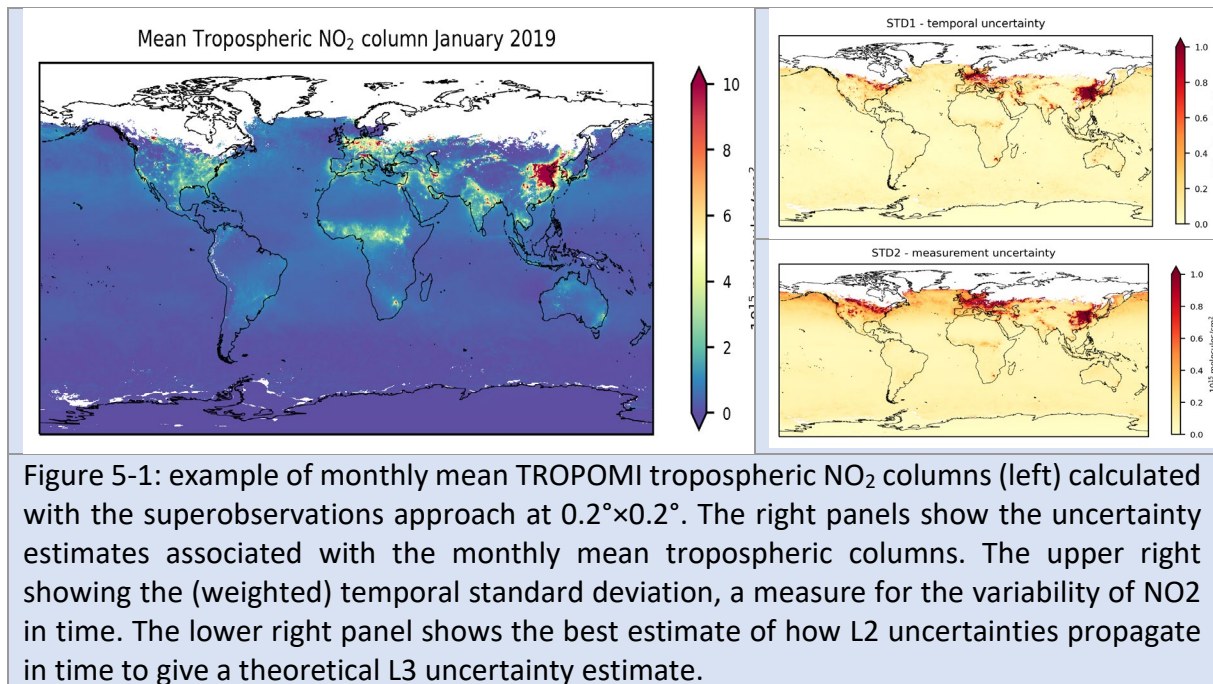
- The main product is the “**tropospheric_NO2_column_number_density**”.
- A quality flag is provided for the L3 file, with the aim to filter cells containing not enough observations. The criterion for sufficient coverage is that the fractional coverage of a grid cell should exceed 0.1, which is equivalent to more than 3 days (10% of 30 or 31 days) with a fully covered grid cell to calculate a monthly mean. In coding, if tropospheric_NO2_column_number_density_count > 0.1, then qa_L3=1. If tropospheric_NO2_column_number_density_count < 0.1, then qa_L3=0. Users are advised to use only qa_L3=1.
- Various uncertainty estimates for NO₂ monthly mean L3 data are available for each grid cell. The first uncertainty estimate (σ_1) represents the temporal standard deviation of the gridded L2 data within the cell and is a measure of the temporal variability of NO₂. The total L3 uncertainty represents time-averaged propagated uncertainty of L2 input data in the cell, and explicitly accounts for random and systematic contributions to the total uncertainty. The total uncertainty kernel is the time-averaged propagated uncertainty of L2 input data excluding the contributions of the a priori profile uncertainty to the total L3 uncertainty.
- When averaging L3 data over larger temporal or spatial scales, an averaged uncertainty can be obtained from combining the different random (σ_{ri}) and systematic (σ_{si}) uncertainties as

$$\sigma^2 = \sum_{i=1}^n \left(\frac{\sigma_{ri}}{n} \right)^2 + \left(\sum_{i=1}^n \frac{\sigma_{si}}{n} \right)^2$$
- Mean averaging kernels are provided for each grid cell. This is only an approximation of these quantities with a vertical dimension. L2 data should preferably be used for an accurate exploitation of the averaging kernels.

5.6. Preliminary evaluation

Figure 5-1 below shows the monthly mean tropospheric NO₂ column at a resolution of 0.2° for January 2019. A complete L3 dataset for monthly mean tropospheric NO₂ columns has been generated for the entire period covered by TROPOMI v2.2 data, i.e. from May 2018 – December 2021.





5.7. Contacts and citation

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- Folkert Boersma: folkert.boersma@knmi.nl
- Henk Eskes: henk.eskes@knmi.nl

Dataset citation:

- Glissenaar, I. A., Anglou, I., Boersma, K. F., & Eskes, H. (2024). ESA CCI+ TROPOMI L3 monthly mean NO₂ columns [Data set]. Royal Netherlands Meteorological Institute (KNMI). <https://doi.org/10.21944/CCI-NO2-TROPOMI-L3>
- Anglou, I., Glissenaar, I. A., Boersma, K. F., & Eskes, H. (2024). ESA CCI+ OMI L3 monthly mean NO₂ columns [Data set]. Royal Netherlands Meteorological Institute (KNMI). <https://doi.org/10.21944/cci-no2-omi-l3>

Dataset availability:

- <https://www.temis.nl/airpollution/no2col/cci-no2-tropomi.php>
- <https://www.temis.nl/airpollution/no2col/cci-no2-omi.php>

Paper citations:

- TROPOMI NO₂

van Geffen, J., Eskes, H., Compernelle, S., Pinardi, G., Verhoelst, T., Lambert, J.-C., Sneep, M., ter Linden, M., Ludewig, A., Boersma, K. F., and 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.*, 15, 2037–2060, <https://doi.org/10.5194/amt-15-2037-2022>, 2022.



- OMI, SCIAMACHY, and GOME NO₂

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., and 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., 11, 6651–6678, <https://doi.org/10.5194/amt-11-6651-2018>, 2018.

- L3 TROPOMI NO₂

Glissenaar, I., Boersma, K. F., Angloul, I., Rijdsdijk, P., Verhoelst, T., Compernelle, S., Pinardi, G., Lambert, J.-C., Van Roozendaal, M., and Eskes, H.: TROPOMI Level 3 tropospheric NO₂ Dataset with Advanced Uncertainty Analysis from the ESA CCI+ ECV Precursor Project, Earth System Science Data Discussions, 2025, 1–36, 2025.

6. HCHO L3 from TROPOMI, OMI, GOME2, SCIAMACHY and GOME

6.1. Input data and algorithm

HCHO can be retrieved from a series of nadir UV-VIS sensors. We focus more particularly on the ESA and ESA Third Party Mission (ESA-TPM) sensors: GOME, SCIAMACHY, GOME-2, OMI, TROPOMI.

Figure 6-1 shows the flow diagram of the L2 HCHO DOAS retrieval algorithm, common to all UV-VIS sensors. The HCHO slant column (N_s) fit is performed in the UV. Subsequently, to convert the slant column to a vertical column (N_v), an air mass factor that accounts for the average light path through the atmosphere is calculated. For this purpose, several auxiliary data are read from external sources: cloud cover data, topographic information, surface albedo, and the a priori shape of the vertical HCHO profile in the atmosphere. Two types of air mass factors are calculated, including a correction for the cloud altitude, or not (M or M_{clear}). Additional background normalization is required in the case of weak absorbers such as formaldehyde to compensate for unknown offsets ($N_{s,0}$). Finally, a background vertical column derived from a CTM is added ($N_{v,0}$). The HCHO vertical column (N_v or $N_{v,clear}$) is obtained using the following equation:

$$N_v = \frac{N_s - N_{s,0}}{M} + N_{v,0} \quad 6-1$$

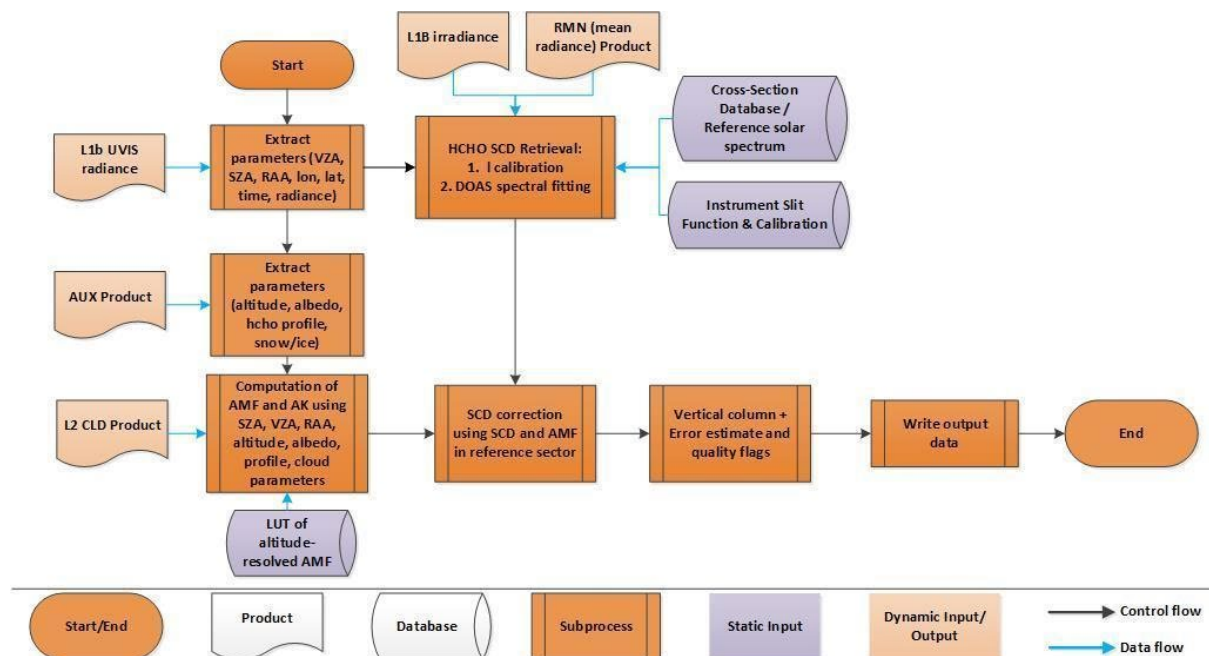


Figure 6-1: Flow Diagram of the DOAS retrieval algorithm for HCHO.

The L2 versions used to produce the L3 CDR are summarized in Table 2-1. The GOME-2-A, B, C data have been reprocessed to generate the AC SAF prototype product, developed in parallel



of this project. For the other sensors, the slant columns are directly taken from the operational product (TROPOMI), or from the QA4ECV products (OMI, SCIAMACHY, GOME). The air mass factors and background correction are re-calculated with consistent and updated settings. For further details on the L2 algorithm settings selected for this project, the reader is invited to refer to the HCHO ATBD available at <https://climate.esa.int/en/projects/precursors-for-aerosols-and-ozone/>.

The L3 products are derived from the L2 products. The L2 versions used to produce the L3 CDR, and the corresponding L3 versions, are summarized in Table 6 1. The L3 product consists of HCHO tropospheric columns and associated random and systematic uncertainties, detailed results, and input data. L3 are available for each instrument separately.

- Morning sensors: GOME/ERS-2, SCIAMACHY/ENVISAT, GOME2/METOP-A, B, C
- Afternoon sensors: OMI/AURA, TROPOMI/S5P

Since the spatial resolution and signal-to-noise ratio of the sensors are different, and significantly better for the afternoon sensors, daily and monthly L3 files are provided for the afternoon sensors, while only monthly L3 files are provided for the morning sensors.

Table 6-1: List of CCI+p HCHO datasets (L3) and associated characteristics.

Product identifier	Time period	Temp. res.	Spatial res.	L2 version (doi)	L3 version (doi)	L3 Data Download
HCHO_L3_S5P_TROPOMI	2018-2024	Day/Month	0.2°/0.2°	RPRO+OFFL v03.02 (10.5270/S5P-tjlxfd2)	CCIp L3 v1.0 (10.18758/2imqez32)	https://distributions.aeronome.be/32d1492e-3a37-4ca6-9b1e-762e09e4bb
			0.25°/0.125°	CCIp L2 v1.0 (internal product)	CCIp L3 v2.0 (https://doi.org/10.18758/y591kda5)	https://distributions.aeronome.be/32ddd2e-3a37-4ca6-9b1e-762e09e4bb
HCHO_L3_S5P_OMI	2005-2023	Day/Month	0.2°/0.2°	QA4ECV (10.18758/71021031)	CCIp L3 v1.0 (10.18758/h2v1uo6x)	https://distributions.aeronome.be/d9868f2a-e17a-4ce2-acbf-e0e3a61a5f3f
			0.25°/0.125°	CCIp L2 v1.0 (internal product)	CCIp L3 v2.0 (https://doi.org/10.18758/bf145884)	https://distributions.aeronome.be/d9868f2a-e17a-4ce2-acbf-e0e3a61a5f3f
HCHO_L3_METOP_GOME2_A/B/C	2007-2023	Month	0.25°	GDP4.8/4.9 (?)		
				AC SAF prototype (internal product)	https://doi.org/10.18758/e9z1tqb2	https://distributions.aeronome.be/22d149ff-cc22-4ca6-9b1e-762e09e4bb
HCHO_L3_ENVISAT_SCIAMACHY	2003-2012	Month	0.25°	QA4ECV v1.2 (10.18758/71021033)	CCI+p v1.0 (https://doi.org/10.18758/jasyj4lx)	https://distributions.aeronome.be/bbd1492e-3a37-4ca6-9b1e-762e09e4bb
				CCIp L2 v1.0 (internal product)	CCIp L3 v2.0 (https://doi.org/10.18758/4yaeg97o)	https://distributions.aeronome.be/bbd1492e-3a37-4ca6-9b1e-762e09e4bb
HCHO_L3_ERS2_GOME	1996-2002	Month	0.25°	QA4ECV v1.2 (internal product)	CCI+p v1.0 (https://doi.org/10.18758/yxnj72yv)	https://distributions.aeronome.be/11d1492e-4a11-4ca6-9b1e-762e09e4bb
				CCIp L2 v1.0 (internal product)	CCIp L3 v2.0 (https://doi.org/10.18758/saabns5o)	https://distributions.aeronome.be/11d1492e-4a11-4ca6-9b1e-762e09e4bb





6.2. File parameters

Table 6-2 describes the variables contained in the L3 HCHO NetCDF files. The fill value is NaN for all.

Table 6-2: Variables in the L3 HCHO NetCDF files.

Parameter	Unit	Dimension	Description
latitude	degrees	lat	grid latitude centres
longitude	degrees	lon	grid longitude centres
latitude_bounds	degrees	lat, independent_2	grid latitude bounds
longitude_bounds	degrees	lon, independent_2	grid longitude bounds
time	days	time=1	number of days since 1995-01-01
layer	1	layer	layer dimension index
ctm_sigma_a	hPa	layer	pressure = ctm_sigma_a + surface_pressure * ctm_sigma_b
ctm_sigma_b	1		
surface_pressure	hPa	time, lat, lon	surface pressure
surface_albedo	1	time, lat, lon	surface LER (340 nm)
land_water_mask	1	time, lat, lon	0: water, 1: land, 2: land water transition
eff_fract_day	1	time, lat, lon	effective fractional day in local solar time (between 0 and 1)
eff_date	days	time, lat, lon	effective day-of-month (number between 1-31)
solar_zenith_angle	degree	time, lat, lon	solar zenith angle, averaged in each grid cell
sensor_zenith_angle	degree	time, lat, lon	viewing zenith angle, averaged in each grid cell
cloud_fraction	1	time, lat, lon	effective cloud fraction
cloud_pressure	hPa	time, lat, lon	cloud top pressure
intensity_weighted_cloud_fra ction	1	time, lat, lon	intensity-weighted cloud radiance fraction (340 nm)
tropospheric_HCHO_column_ number_density_clear	molec.cm ⁻²	time, lat, lon	HCHO tropospheric vertical column number density, no cloud correction (amf_clear, ak_clear)
tropospheric_HCHO_column_ number_density	molec.cm ⁻²	time, lat, lon	HCHO tropospheric vertical column number density, cloud correction (amf, ak)
tropospheric_HCHO_column_ number_density_uncertainty_ random	molec.cm ⁻²	time, lat, lon	Random uncertainty on the HCHO tropospheric vertical column number density



tropospheric_HCHO_column_number_density_uncertainty_systematic	molec.cm ⁻²	time, lat, lon	Systematic uncertainty on the HCHO tropospheric vertical column number density
tropospheric_HCHO_column_number_density_uncertainty_systematic_kernel	molec.cm ⁻²	time, lat, lon	Systematic uncertainty on the HCHO tropospheric vertical column number density, without the profile uncertainty contribution
tropospheric_HCHO_column_number_density_clear_std	molec.cm ⁻²	time, lat, lon	Standard deviation of HCHO tropospheric vertical column number density without cloud correction, within the cell
tropospheric_HCHO_column_number_density_std	molec.cm ⁻²	time, lat, lon	Standard deviation of HCHO tropospheric vertical column number density within the cell
tropospheric_HCHO_column_number_density_count	1	time, lat, lon	Effective number of observations per cell
HCHO_slant_column_number_density_rms	1	time, lat, lon	DOAS rms
HCHO_slant_column_number_density	molec.cm ⁻²	time, lat, lon	HCHO slant column number density
HCHO_slant_column_number_density_uncertainty	molec.cm ⁻²	time, lat, lon	HCHO slant column number density uncertainty
HCHO_slant_column_number_density_corrected	molec.cm ⁻²	time, lat, lon	Background-corrected HCHO slant column number density uncertainty
tropospheric_HCHO_column_number_density_background_correction	molec.cm ⁻²	time, lat, lon	a priori HCHO vertical column density number density in the Pacific reference sector
tropospheric_HCHO_column_number_density_amf	1	time, lat, lon	tropospheric air mass factor
tropospheric_HCHO_column_number_density_amf_clear	1	time, lat, lon	tropospheric air mass factor, no cloud correction
tropospheric_HCHO_column_number_density_apriori	molec.cm ⁻²	time, lat, lon	a priori HCHO vertical column number density (integrated profile)
HCHO_volume_mixing_ratio_dry_air_apriori	ppv	time, lat, lon, layer	a priori HCHO vertical profile
HCHO_averaging_kernel	1	time, lat, lon, layer	Column averaging kernel with cloud correction (amf)
HCHO_averaging_kernel_clear	1	time, lat, lon, layer	Column averaging kernel, no cloud correction (amf_clear)
qa_L3	1	time, lat, lon	gridded data quality assurance value (0: not valid, 1: valid)





6.3. DOI, data access and volume

The L3 products can be accessed from <https://distributions.aeronomie.be>. The DOIs are provided in Table 6-2, as well as the data volume.

Example of file name for one TROPOMI monthly L3 file:

ESACCI-PREC-L3-HCHO_TC-TROPOMI_S5P_v0301-BIRA-20230701_20230731-fv0200.nc

At the end of the project, the data will be available from <https://climate.esa.int/en/data/>.

Table 6-2: Size of one L3 file for morning and afternoon sensors, at daily and monthly time resolution. The DOIs of each L3 dataset are provided.

Sensor	Data volume Monthly L3 (Daily L3)	doi
OMI	1.5Gb (300Mb)	https://doi.org/10.18758/bf145884
TROPOMI	1.5Gb (300Mb)	https://doi.org/10.18758/y591kda5
GOME	25Mb	https://doi.org/10.18758/saabns5o
SCIAMACHY	25Mb	https://doi.org/10.18758/4yaeg97o
GOME-2A	300Mb	https://doi.org/10.18758/e9z1tqb2
GOME-2B	300Mb	https://doi.org/10.18758/e9z1tqb2
GOME-2C	300Mb	https://doi.org/10.18758/e9z1tqb2

6.4. Data reading examples

```
import numpy as np
from netCDF4 import Dataset
from mpl_toolkits.basemap import Basemap
import matplotlib.pyplot as plt
from matplotlib import cm
from mpl_toolkits.axes_grid1 import make_axes_locatable

# Full file path of the NetCDF file
filename='MPC-L3-HCHO_TC-TROPOMI_S5P_OFFL_v0302-BIRA-202310-fv0200.nc'

# Map settings
proj_name='cyl'
Mspace=40
Pspace=30
parallels = np.arange(-90,90,Pspace)
meridians = np.arange(-180,180,Mspace)
LW=0.4
size_label=10

# Colorbar settings
ncolor=100
colormap = 'turbo'
scFactor=1e15
minScale = 0
maxScale = 20

# Variable to map and title
var2plot = "tropospheric_HCHO_column_number_density_clear"
title_txt="Oct. 2023"

# Read the NetCDF file
with Dataset(filename, "r") as fid:
    HCHO2Map = fid[var2plot][:]
    HCHO2Map = HCHO2Map/scFactor
    varunit = fid[var2plot].units
    scaletitle='TROPOMI {} [{} {}]''.format(fid[var2plot].long_name,format(scFactor,'1.0e'),varunit)
    qa_Map = fid["qa_L3"][:]
    HCHO2Map[qa_Map<1]=np.nan

# Create the map
plt.figure(1,figsize=(12,12))
plt.title(scaletitle, loc='left',fontname="Times New Roman",fontweight="bold")
plt.annotate("ESA CCI+ ozone and aerosol precursors", xy=(0.01,0.015), xycoords='axes fraction',size=10,fontname="Times New Roman",fontweight="bold")
```





```
plt.title(title_txt, fontdict=None, loc='right', fontname="Times New Roman", fontweight="bold")

map = Basemap(projection=proj_name, llcrnrlon=-180, llcrnrlat=-90, urcrnrlon=180,
urcrnrlat=90, resolution='l', lat_0=0, lon_0=0)
map.drawcoastlines(linewidth=LW, color='grey')
map.drawcountries(linewidth=LW, color='whitesmoke')
map.fillcontinents(color='lightgrey', zorder=0)
map.drawmeridians(meridians, color='black', linewidth=LW/2)
map.drawparallels(parallels, color='black', linewidth=LW/2)

im = map.imshow(HCHO2Map[0,:,:], cmap=cm.get_cmap(colormap, ncolor), interpolation='none')
plt.colorbar(im, orientation="horizontal")
plt.clim(minScale, maxScale)

plt.show()
```

6.5. Usage recommendations and known limitations

- The main product is the “tropospheric_HCHO_column_number_density_clear”.
- Users interested in long-term trends should use the variable “tropospheric_HCHO_column_number_density_clear” in each dataset in order to minimize bias related to different cloud products.
- A quality flag is provided for the L3 file, with the aim to filter cells containing not enough observations. It is advised to use only $qa_L3==1$. The qa_L3 flag is based on the effective number of observations within the cell (tropospheric_HCHO_column_number_density_count), after applying the L2 quality filtering. If the tropospheric_HCHO_column_number_density_count is lower than the 5th percentile of the cell counts for the day/month, the qa_L3 is set to 0.
- Mean random (σ_r) and systematic (σ_s) uncertainties are available for each grid cell. If a total uncertainty is desired, this can be obtained from the square root of the sum of squares of the different terms:
$$\sigma^2 = \sigma_r^2 + \sigma_s^2$$
- When averaging L3 data over larger temporal or spatial scales, an averaged uncertainty can be obtained from combining the different random (σ_{ri}) and systematic (σ_{si}) uncertainties as
$$\sigma^2 = \sum_{i=1}^n \left(\frac{\sigma_{ri}}{n} \right)^2 + \left(\sum_{i=1}^n \frac{\sigma_{si}}{n} \right)^2$$
- Mean averaging kernels and a priori vertical profiles are provided for each grid cell. This is only an approximation of these quantities with a vertical dimension. L2 data should preferably be used for an accurate exploitation of the averaging kernels.
- The example python script below uses the L3 AKs and ap Profiles to recalculate the AMFs, and compare the results with the provided L3 AMFs.

```
import numpy as np
from netCDF4 import Dataset
import matplotlib.pyplot as plt

# Initialisation
dryair = 28.9644;          #g/mole
ra = 6.0221367e23;        #molec/mole
g = 9.80665;              #m/s

# Full file path of the NetCDF file
filename='MPC-L3-HCHO_TC-TROPOMI_S5P_OFFL_v0302-BIRA_1D-20231031-fv0200.nc'

# Read the NetCDF file
with Dataset(filename, "r") as fid:
    sigma_a_Layer= fid["ctm_sigma_a"][:].flatten()
    sigma_b_Layer= fid["ctm_sigma_b"][:].flatten()
    nlayers = np.shape(sigma_a_Layer)[0]
    profile_Map = fid["HCHO_volume_mixing_ratio_dry_air_apriori"][0,...].flatten()
    profile_Map = np.reshape(profile_Map, [-1,nlayers])
    ak_Map = fid["HCHO_averaging_kernel"][0,...].flatten()
    ak_Map = np.reshape(ak_Map, [-1,nlayers])
    xa_Map = fid["tropospheric_HCHO_column_number_density_apriori"][0,...].flatten()
    sp_Map = fid["surface_pressure"][0,...].flatten()
    amf_Map = fid["tropospheric_HCHO_column_number_density_amf"][0,...].flatten()
    qa_Map = fid["qa_L3"][0,...].flatten()

total_size = np.shape(sp_Map)[0]

# Calculate the pressure at layer centers
pressure_Map = np.full((total_size,nlayers), np.nan, dtype = np.dtype('f4')) # pressure at layer center [hPa]
for l in range(0,nlayers):
    pressure_Map[:,l] = (sigma_a_Layer[l] + sp_Map[:,sigma_b_Layer[l]]) # [hPa]

pi = np.full((total_size,nlayers+1), np.nan, dtype = np.dtype('f4')) # pressure at layer borders [hPa]
pi[:,0]=sp_Map[:,0] # surface pressure [hPa]
for l in range(0,nlayers-1):
    pi[:,l+1] = np.exp(np.log(pressure_Map[:,l])-(np.log(pressure_Map[:,l])-np.log(pressure_Map[:,l+1]))/2)
```





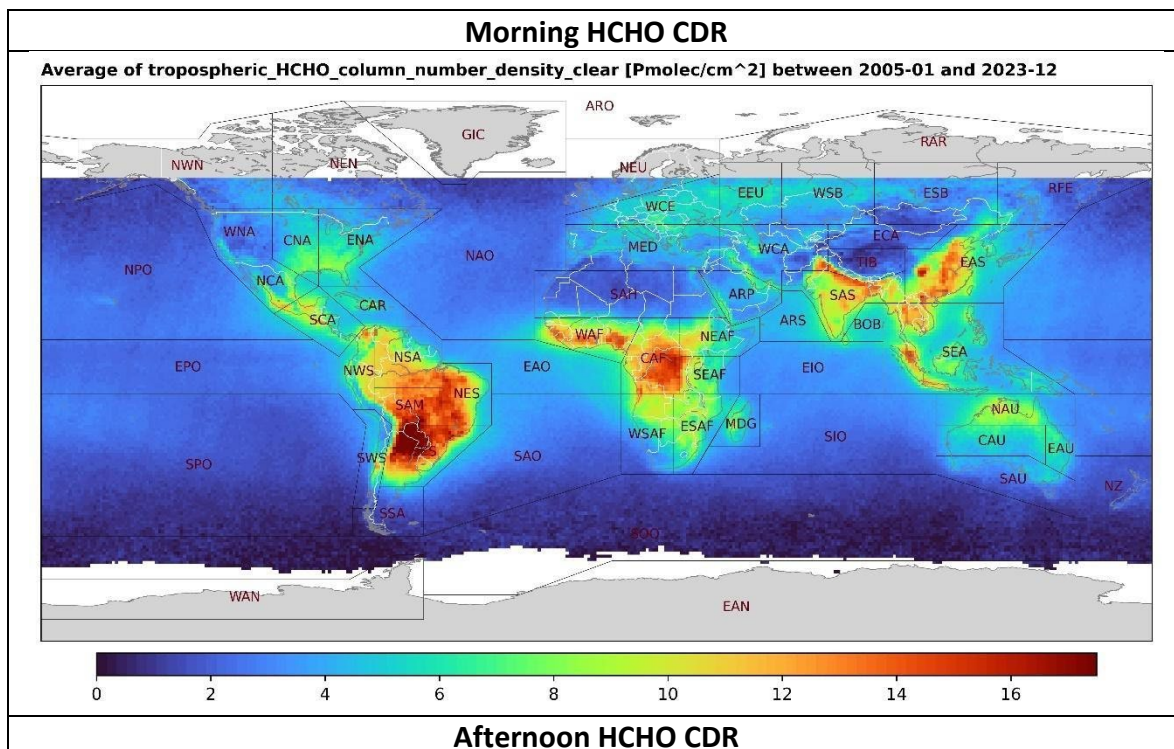
```
pi[:,nlayers]=np.exp( np.log(pi[:,nlayers-1])-2*( np.log(pi[:,nlayers-1])-np.log(pressure_Map[:,nlayers-1]) ) )
# Re-calculate the AMF using the a priori profile and the averaging kernel
dp = np.full((total_size,nlayers),np.nan,dtype = np.dtype('f4')) # delta pressure per layer [hPa]
m_check = np.full((total_size,nlayers),np.nan,dtype = np.dtype('f4')) # recalculate AMF
vodal = np.full((total_size,nlayers),np.nan,dtype = np.dtype('f4')) # a priori partial columns per layer [molec./cm2]
for l in range(0,nlayers):
    dp[:,l] = pi[:,l] - pi[:,l+1]
    vodal[:,l] = 10*ra*np.multiply(profile_Map[:,l],dp[:,l])/(g*dryair)
    %% Check AMF
    m_check[:,l] = ra*10*amf_Map[:,l]*np.multiply(ak_Map[:,l],np.multiply(profile_Map[:,l],dp[:,l]))/(g*dryair)
VCDa = np.nansum(vodal,axis=1)
amf_check = np.nansum(m_check,axis=1)/VCDa

kok = (qa_Map>0)

# Plot the re-calculated AMF versus the L3 AMF
fig, ax =plt.subplots(1,1,figsize=(12,6))
plt.plot(amf_Map[kok],amf_check[kok], '.',c='black',markersize=0.2,fillstyle='full',linestyle='')
plt.grid(True)
plt.ylabel("Recalculated AMF using AK and ap Profile", fontsize=12, fontweight='bold', color='k')
plt.xlabel("L3 AMF", fontsize=12, fontweight='bold', color='k')
plt.title(filename, fontsize=10, fontweight='bold', color='k')
plt.xlim([0,3.5])
plt.ylim([0,3.5])
plt.show()
```

6.6. Preliminary evaluation

Figure 6-2 below shows multi-year averages of tropospheric HCHO columns between 2005 and 2023, from the morning and afternoon HCHO datasets. The full time-series for morning and afternoon HCHO datasets are illustrated in Figure 6-3 for two selected regions. Validation results are provided for each sensor dataset in the Product Validation and Intercomparison Report available at <https://climate.esa.int/en/projects/precursors-for-aerosols-and-ozone/>.



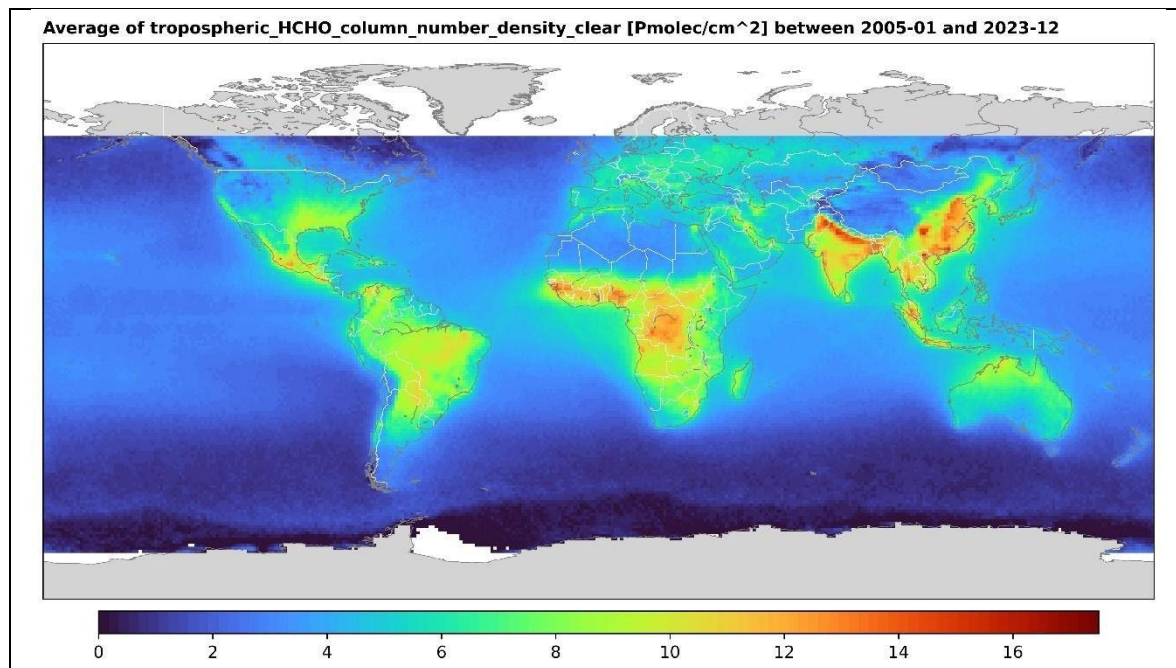


Figure 6-2: Global Maps of HCHO VCD clear between 2005 and 2023, for morning and afternoon overpass times. The morning CDR combines data from SCIAMACHY and GOME2-A/B/C, while the afternoon CDR combines data from OMI and TROPOMI.

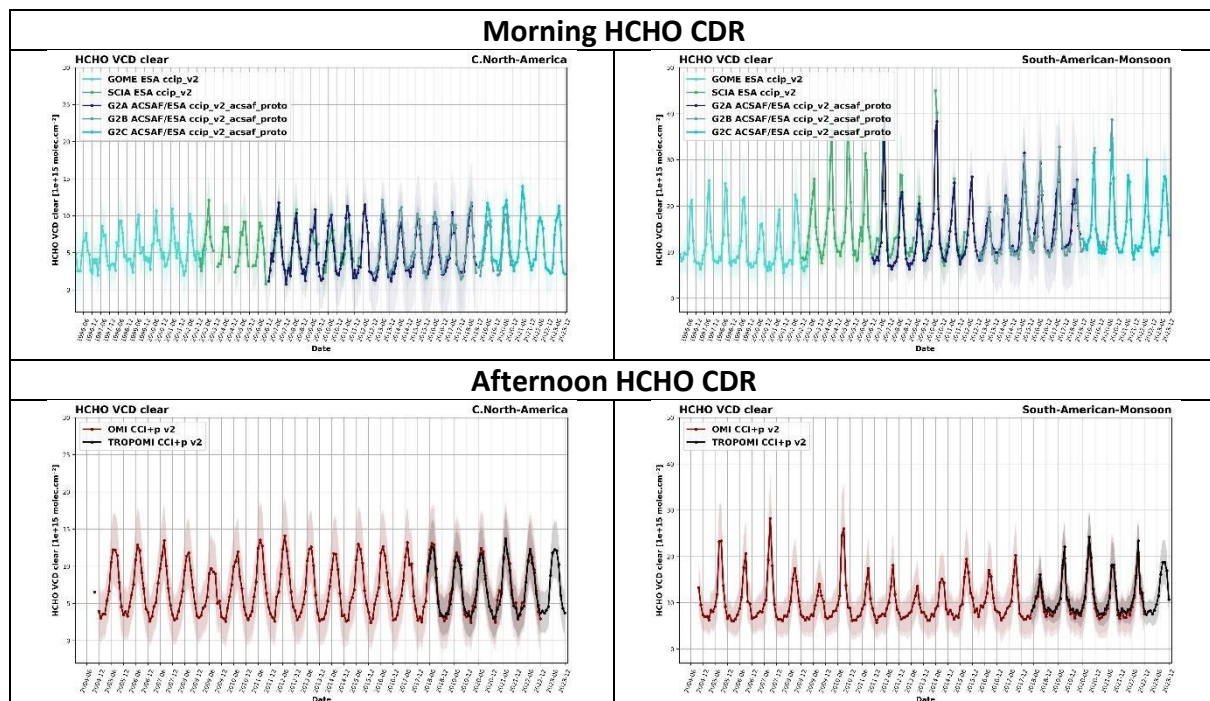


Figure 6-3: Time series of HCHO VCD clear for morning and afternoon HCHO CDRs averaged over two selected regions: Central North America and South American Monsoon, illustrated in the first map of Figure 6-2 (CAN and SAM).



6.7. Contacts and citation

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Dataset citation:

- De Smedt, I., Vlietinck, J., YU, H., Theys, N., Danckaert, T., & Van Roozendaal, M. (2025). CCI+P HCHO tropospheric column L3 data from TROPOMI, v2 (Version 2) [Data set]. Royal Belgian Institute for Space Aeronomy. <https://doi.org/10.18758/Y591KDA5>
- De Smedt, I., Vlietinck, J., YU, H., Theys, N., Danckaert, T., & Van Roozendaal, M. (2025). CCI+P HCHO tropospheric column L3 data from OMI, v2 (Version 2) [Data set]. Royal Belgian Institute for Space Aeronomy. <https://doi.org/10.18758/BF145884>
- De Smedt, I., Vlietinck, J., Yu, H., Theys, N., Danckaert, T., & Van Roozendaal, M. (2025). CCI+P HCHO tropospheric column L3 data from GOME, v2 (Version 2) [Data set]. Royal Belgian Institute for Space Aeronomy. <https://doi.org/10.18758/SAABNS50>
- De Smedt, I., Vlietinck, J., Yu, H., Theys, N., Danckaert, T., & Van Roozendaal, M. (2025). CCI+P HCHO tropospheric column L3 data from SCIAMACHY, v2 (Version 2) [Data set]. Royal Belgian Institute for Space Aeronomy. <https://doi.org/10.18758/4YAE970>
- De Smedt, I., Vlietinck, J., Yu, H., Theys, N., Danckaert, T., Van Roozendaal, M., & Heue, K.-P. (2025). CCI+P HCHO tropospheric column L3 data from GOME-2, v2 (Version 2) [Data set]. Royal Belgian Institute for Space Aeronomy. <https://doi.org/10.18758/E9Z1TQB2>

Dataset availability:

<https://distributions.aeronomie.be>

Paper citations:

- TROPOMI HCHO (Operational version)

De Smedt, I., Pinardi, G., Vigouroux, C., Compernelle, S., Bais, A., Benavent, N., Boersma, F., Chan, K.-L., Donner, S., Eichmann, K.-U., Hedelt, P., Hendrick, F., Irie, H., Kumar, V., Lambert, J.-C., Langerock, B., Lerot, C., Liu, C., Loyola, D., PETERS, A., Richter, A., Rivera Cárdenas, C., Romahn, F., Ryan, R. G., Sinha, V., Theys, N., Vlietinck, J., Wagner, T., Wang, T., Yu, H., and Van Roozendaal, M.: Comparative assessment of TROPOMI and OMI formaldehyde observations and validation against MAX-DOAS network column measurements, *Atmos. Chem. Phys.*, 21, 12561–12593, <https://doi.org/10.5194/acp-21-12561-2021>, 2021.

- OMI HCHO (QA4ECV version)

De Smedt, I., Theys, N., Yu, H., Danckaert, T., Lerot, C., Compernelle, S., Van Roozendaal, M., Richter, A., Hilboll, A., Peters, E., Pedernana, M., Loyola, D., Beirle, S., Wagner, T., Eskes, H., van Geffen, J., Boersma, K. F., and Veefkind, P.: Algorithm theoretical baseline for formaldehyde retrievals from S5P TROPOMI and from the QA4ECV project, *Atmos. Meas. Tech.*, 11, 2395–2426, <https://doi.org/10.5194/amt-11-2395-2018>, 2018.

7. SO₂ L3 from TROPOMI, OMI, SCIAMACHY and GOME

7.1. Input data and algorithm

SO₂ can be retrieved from a series of nadir UV-VIS sensors. We focus more particularly on the following sensors: GOME, SCIAMACHY, OMI, TROPOMI.

Figure 7-1 shows the flow diagram of the L2 SO₂ COBRA vertical column retrieval algorithm, common to all UV-VIS sensors. First, the measured top-of-atmosphere radiances in the UV are analyzed and yield the slant columns (SCD). The SO₂ fit is performed using COBRA in multiple fitting windows, characterized by different SO₂ absorption strengths. Depending on the retrieved column amounts in the different fitting windows, a selection of the final SCD is performed. Subsequently, to convert the slant column to a vertical column ($VCD = SCD / AMF$), an air mass factor (AMF) that accounts for the average light path through the atmosphere is calculated. For this purpose, several auxiliary data are read from external sources: cloud cover data, topographic information, surface albedo, and the a priori shape of the vertical SO₂ profile in the atmosphere. Two types of air mass factors are calculated, one for an SO₂ profile from a chemical transport model and another one for box profiles with prescribed SO₂ plume heights, representative of volcanic scenarios. The AMF module also includes calculation of errors and column averaging kernels.

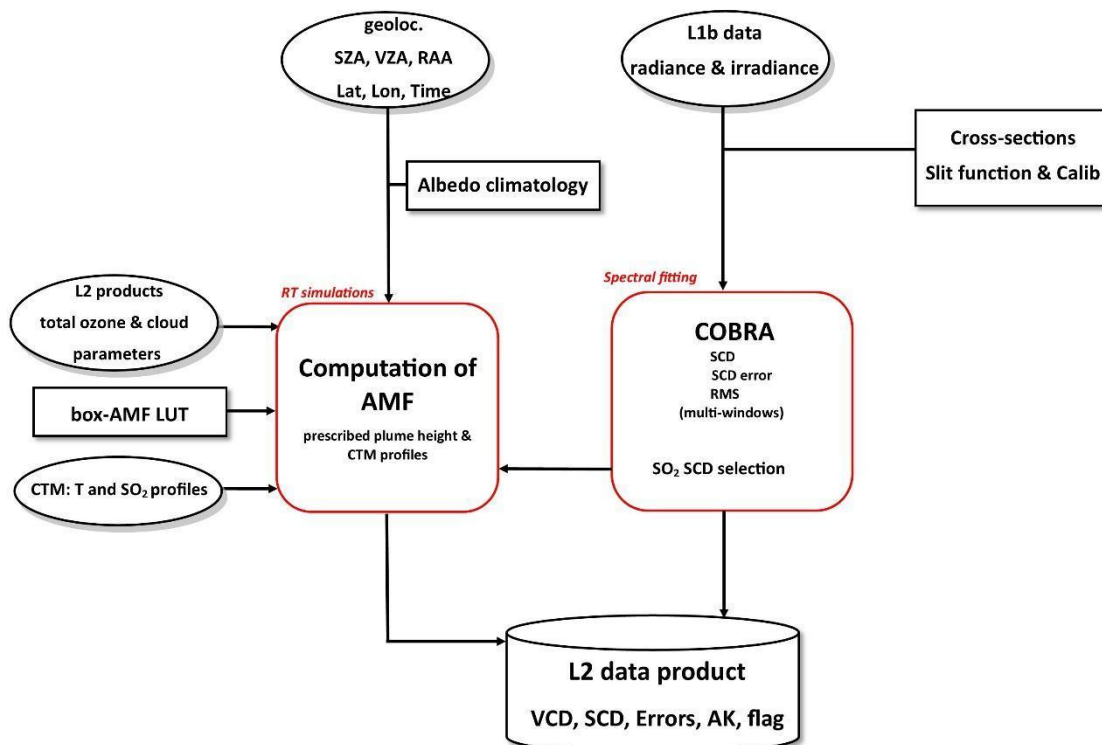


Figure 7-1: Flow diagram of the SO₂ column retrieval algorithm.



For further details on the L2 algorithm settings selected for this project, the reader is referred to the SO₂ ATBD available at <https://climate.esa.int/en/projects/precursors-for-aerosols-and-ozone/>.

The L3 products are directly derived from the L2 products. The L3 product consists of SO₂ total columns for CTM and box profiles, and associated random and systematic uncertainties, detailed results, and input data. L3 are available for each instrument separately.

7.2. File parameters

Table 7-1 describes the variables contained in the L3 SO₂ NetCDF files. The fill value is NaN for variables with a float or double as datatype.

Table 7-1: Variables in the L3 SO₂ NetCDF files.

Parameter	Unit	Dimension	Description
latitude	degrees	lat	latitude
longitude	degrees	lon	longitude
latitude_bounds	degrees	lat, independent_2	grid latitude bounds
longitude_bounds	degrees	lon, independent_2	grid longitude bounds
time	days	time=1	number of days since 1995-01-01
eff_date	days	time, lat, lon	effective day-of-month (number between 1-31)
eff_fract_day	1	time, lat, lon	effective fractional day in local solar time. UTC = local_solar_time - longitude/180
ctm_sigma_a	hPa	layer	pressure = ctm_sigma_a + surface_pressure * ctm_sigma_b
ctm_sigma_b	1		
surface_pressure	hPa	time, lat, lon	surface pressure
surface_albedo	1	time, lat, lon	surface LER (340 nm)
land_water_mask	1	time, lat, lon	0: water, 1: land, 2: land water transition
qa_L3	1	time, lat, lon	gridded data quality assurance value (0: not valid, 1: valid)
total_SO2_column_number_density_clear	1	time, lat, lon	SO2 total vertical column number density, no cloud correction
total_SO2_column_number_density	1	time, lat, lon	SO2 total vertical column number density
total_SO2_column_number_density_uncertainty_random	molec.c m ⁻²	time, lat, lon	Random uncertainty on the SO2 total vertical column number density
total_SO2_column_number_density_uncertainty_systematic	molec.c m ⁻²	time, lat, lon	Systematic uncertainty on the SO2 total vertical column number density
total_SO2_column_number_density_uncertainty_systematic_kernel	molec.c m ⁻²	time, lat, lon	Systematic uncertainty on the SO2 total vertical column number density, without the profile uncertainty contribution



total_SO2_column_number_density_clear_std	molec.c m ⁻²	time, lat, lon	Standard deviation of the SO2 total vertical column number density without cloud correction, within the cell
total_SO2_column_number_density_std	molec.c m ⁻²	time, lat, lon	Standard deviation of the SO2 total vertical column number density within the cell
total_SO2_column_number_density_count	1	time, lat, lon	Effective number of observations per cell
SO2_slant_column_number_density_rms	1	time, lat, lon	COBRA rms
SO2_slant_column_number_density	molec.c m ⁻²	time, lat, lon	SO2 slant column number density
SO2_slant_column_number_density_uncertainty	molec.c m ⁻²	time, lat, lon	SO2 slant column number density uncertainty
total_SO2_column_number_density_amf	1	time, lat, lon	tropospheric air mass factor
total_SO2_column_number_density_amf_clear	1	time, lat, lon	tropospheric air mass factor, no cloud correction
cloud_fraction	1	time, lat, lon	effective cloud fraction
cloud_pressure	hPa	time, lat, lon	cloud top pressure
total_SO2_column_number_density_apriori	molec.c m ⁻²	time, lat, lon	a priori SO2 vertical column number density (integrated profile)
SO2_volume_mixing_ratio_dry_air_apriori	ppv	time, lat, lon, layer	a priori SO2 vertical profile
SO2_averaging_kernel	1	time, lat, lon, layer	Column averaging kernel
total_SO2_column_number_density_box	1	time, lat, lon, 3	SO2 total vertical column number density, for box profiles at 1, 7, 15 km

7.3. DOI, data access and volume

DOI: in progress (in contact with Emily Anderson STFC)

The L3 product will soon be accessible from <https://climate.esa.int/en/data/> following the CCI filename convention:

ESACCI-PREC-L3C-SO2-<instrument>_<platform>_BIRA-<nlat>x<nlon>_<period>-<date>-fv<file version>.nc,

where

- instrument is one of 'GOME', 'OMI' or 'TROPOMI',
- platform is one of 'ERS2', 'AURA' or 'S5P',
- nlat x nlon is the number of latitude/longitude grid cells,
- period is '1D' for daily grids, and '1M' for monthly grids,
- the date is formatted as 'yyyymmdd' for daily grids, and 'yyyymm' for monthly grids.
- File version is a two digit number.

Example of a filename for a TROPOMI monthly L3 file:





ESACCI-PREC-L3C-SO2-TROPOMI_S5P_BIRA-1440x2880_1M-202106-fv10.nc

The content of the NetCDF files is listed in Table 7.1.

Data volume is as follows:

Table 7-2: Size of one L3 file, at daily and monthly time resolution.

Sensor	Data volume Monthly L3 (Daily L3)
OMI	1.2Gb (240Mb)
TROPOMI	1.2Gb (240Mb)
GOME	18Mb
SCIAMACHY	NA

7.4. Data reading examples

```
import numpy as np
from netCDF4 import Dataset
from mpl_toolkits.basemap import Basemap
import matplotlib.pyplot as plt
from matplotlib import cm
from mpl_toolkits.axes_grid1 import make_axes_locatable

# Full file path of the NetCDF file
filename= 'MPC-L3-SO2_TC-TROPOMI_S5P_OFFL_v0302-BIRA-202310-fv0200.nc'

# Map settings
proj_name='cyl'
Mspace=40
Pspace=30
parallels = np.arange(-90,90,Pspace)
meridians = np.arange(-180,180,Mspace)
LW=0.4
size_label=10

# Colorbar settings
ncolor=100
colormap= 'turbo'
scFactor=1e15
minScale = 0
maxScale = 20

# Variable to map and title
var2plot = "total_SO2_column_number_density "
title_txt="Oct. 2023"

# Read the NetCDF file
with Dataset(filename, "r") as fid:
    SO22Map = fid[var2plot][:]
    SO22Map = SO22Map/scFactor
    varunit = fid[var2plot].units
    scaletitle='TROPOMI {} [{} {}]' .format(fid[var2plot].long_name,format(scFactor,'1.0e'),varunit)
    qa_Map = fid["qa_L3"][:]
    SO22Map[qa_Map<1]=np.nan

# Create the map
plt.figure(1,figsize=(12,12))
plt.title(scaletitle, loc='left',fontname="Times New Roman",fontweight="bold")
plt.annotate("ESA CCI+ ozone and aerosol precursors", xy=(0.01,0.015), xycoords='axes fraction',size=10,fontname="Times New Roman",fontweight="bold")
plt.title(title_txt, fontdict=None, loc='right',fontname="Times New Roman",fontweight="bold")

map = Basemap(projection=proj_name, llcrnrlon=-180, llcrnrlat=-90, urcrnrlon=180, urcrnrlat=90,resolution='l',lat_0=0,lon_0=0)
map.drawcoastlines(linewidth=LW,color='grey')
map.drawcountries(linewidth=LW,color='whitesmoke')
map.fillcontinents(color='lightgrey',zorder=0)
map.drawmeridians(meridians,color='black',linewidth=LW/2)
map.drawparallels(parallels,color='black',linewidth=LW/2)

im = map.imshow(SO22Map[0,:,:], cmap=cm.get_cmap(colormap, ncolor),interpolation='none')
plt.colorbar(im, orientation="horizontal")
plt.clim(minScale, maxScale)

plt.show()
```





7.5. Usage recommendations and known limitations

- The main product is the **"total_SO2_column_number_density"**. Users interested in long-term trends should use the variable **"total_SO2_column_number_density_clear"** in each dataset in order to minimize bias related to different cloud products.
- For volcanic applications, the product to be used is the **"total_SO2_column_number_density_box"**.
- A quality flag for the main product **"total_SO2_column_number_density"** is provided for the L3 file, with the aim to filter cells containing not enough observations. It is advised to use only qa_L3==1. The qa_L3 flag is based on the effective number of observations within the cell (total_SO2_column_number_density_count), after applying the L2 quality filtering. If the total_SO2_column_number_density_count is lower than the 5th percentile of the cell counts for the day/month, the qa_L3 is set to 0.
- Mean random (σ_r) and systematic (σ_s) uncertainties are available for each grid cell. If a total uncertainty is desired, this can be obtained from the square root of the sum of squares of the different terms:

$$\sigma^2 = \sigma_r^2 + \sigma_s^2$$

- When averaging L3 data over larger temporal or spatial scales, an averaged uncertainty can be obtained from combining the different random (σ_{ri}) and systematic (σ_{si}) uncertainties as

$$\sigma^2 = \sum_{i=1}^n \left(\frac{\sigma_{ri}}{n} \right)^2 + \left(\sum_{i=1}^n \frac{\sigma_{si}}{n} \right)^2$$

- Mean averaging kernels and a priori vertical profiles are provided for each grid cell. This applies only to the main product **"total_SO2_column_number_density"**. This is only an approximation of these quantities with a vertical dimension. L2 data should preferably be used for an accurate exploitation of the averaging kernels.
- The example python script below uses the L3 AKs and ap Profiles to recalculate the AMFs, and compare the results with the provided L3 AMFs.

```
import numpy as np
from netCDF4 import Dataset
import matplotlib.pyplot as plt

# Initialisation
dryair = 28.9644;          #g/mole
ra = 6.0221367e23;        #molec/mole
g = 9.80665;              #m/s

# Full file path of the NetCDF file
filename = 'MPC-L3-SO2_TC-TROPOMI_S5P_OFFL_v0302-BIRA-202310-fv0200.nc'

# Read the NetCDF file
with Dataset(filename, "r") as fid:
    sigma_a_Layer = fid["ctm_sigma_a"][:,].flatten()
    sigma_b_Layer = fid["ctm_sigma_b"][:,].flatten()
    nlayers = np.shape(sigma_a_Layer)[0]
    profile_Map = fid["SO2_volume_mixing_ratio_dry_air_apriori"][0,...].flatten()
    profile_Map = np.reshape(profile_Map, [-1, nlayers])
    ak_Map = fid["SO2_averaging_kernel"][0,...].flatten()
    ak_Map = np.reshape(ak_Map, [-1, nlayers])
    xa_Map = fid["total_SO2_column_number_density_apriori"][0,...].flatten()
    sp_Map = fid["surface_pressure"][0,...].flatten()
    amf_Map = fid["total_SO2_column_number_density_amf"][0,...].flatten()
    qa_Map = fid["qa_L3"][0,...].flatten()

total_size = np.shape(sp_Map)[0]

# Calculate the pressure at layer centers
pressure_Map = np.full((total_size, nlayers), np.nan, dtype = np.dtype('f4')) # pressure at layer center [hPa]
for l in range(0, nlayers):
    pressure_Map[:, l] = (sigma_a_Layer[l] + sp_Map[:, :]*sigma_b_Layer[l]) # [hPa]

pi = np.full((total_size, nlayers+1), np.nan, dtype = np.dtype('f4')) # pressure at layer borders [hPa]
pi[:, 0] = sp_Map[:, :] # surface pressure [hPa]
for l in range(0, nlayers-1):
    pi[:, l+1] = np.exp(np.log(pressure_Map[:, l]) - (np.log(pressure_Map[:, l]) - np.log(pressure_Map[:, l+1]))/2)
pi[:, nlayers] = np.exp( np.log(pi[:, nlayers-1]) - 2*( np.log(pi[:, nlayers-1]) - np.log(pressure_Map[:, nlayers-1]) ) )

# Re-calculate the AMF using the a priori profile and the averaging kernel
dp = np.full((total_size, nlayers), np.nan, dtype = np.dtype('f4')) # delta pressure per layer [hPa]
m_check = np.full((total_size, nlayers), np.nan, dtype = np.dtype('f4')) # recalculate AMF
vcdal = np.full((total_size, nlayers), np.nan, dtype = np.dtype('f4')) # a priori partial columns per layer [molec./cm2]
```





```
for l in range(0,nlayers):
    dp[:,l] = pi[:,l] - pi[:,l+1]
    vcdal[:,l] = 10*ra*np.multiply(profile_Map[:,l],dp[:,l])/(g*dryair)
    %% Check AMF
    m_check[:,l] = ra*10*amf_Map[:,l]*np.multiply(ak_Map[:,l],np.multiply(profile_Map[:,l],dp[:,l]))/(g*dryair)
VCDa = np.nansum(vcdal,axis=1)
amf_check = np.nansum(m_check,axis=1)/VCDa

kok = (qa_Map>0)

# Plot the re-calculated AMF versus the L3 AMF
fig, ax =plt.subplots(1,1,figsize=(12,6))
plt.plot(amf_Map[kok],amf_check[kok], '.',c='black',markersize=0.2,fillstyle='full',linestyle='')
plt.grid(True)
plt.ylabel("Recalculated AMF using AK and ap Profile", fontsize=12, fontweight='bold', color='k')
plt.xlabel("L3 AMF", fontsize=12, fontweight='bold', color='k')
plt.title(filename, fontsize=10, fontweight='bold', color='k')
plt.xlim([0,3.5])
plt.ylim([0,3.5])
plt.show()
```

7.6. Preliminary evaluation

Validation results are provided for OMI and TROPOMI in the Product Validation and Intercomparison Report available at <https://climate.esa.int/en/projects/precursors-for-aerosols-and-ozone/>.

7.7. Contacts and citation

Contact:

- Nicolas Theys: theys@aeronomie.be

Dataset citation:

- TBD

Paper citation:

- 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., and Van Roozendaal, M.: A sulfur dioxide Covariance-Based Retrieval Algorithm (COBRA): application to TROPOMI reveals new emission sources, Atmos. Chem. Phys., 21, 16727–16744, <https://doi.org/10.5194/acp-21-16727-2021>, 2021.



8. CHOCHO L3 from TROPOMI, OMI and GOME2

8.1. Input data and algorithm

CHOCHO can be retrieved from a series of nadir UV-VIS sensors. We focus on the following sensors: GOME2, OMI and TROPOMI.

Figure 8-1 shows the flow diagram of the L2 DOAS retrieval algorithm for CHOCHO, which is common to all UV-VIS sensors. First, we fit a CHOCHO slant column N_s , based on VIS radiance measurements in the 435-460nm window. Next, we compute an air mass factor M which accounts for the average light path through the atmosphere for the wavelengths in the fitting window, which we use to convert the slant column into a vertical column N_v . To compute the air mass factor, we rely on auxiliary data from a number of external sources: cloud cover data, topographic information, surface albedo, and the a priori shape of the CHOCHO vertical profile in the atmosphere. The effect of clouds is not modelled in the L2 air mass factor computation. Instead, pixels with significant cloud cover (cloud fraction > 20%) are excluded from the L3 product. Finally, a background normalization Δ_{bg} is performed to correct for detector row or viewing angle biases in the retrieved slant columns. We then obtain the CHOCHO vertical column from the equation

$$N_v = \frac{N_s - \Delta_{bg}}{M}.$$

8-1

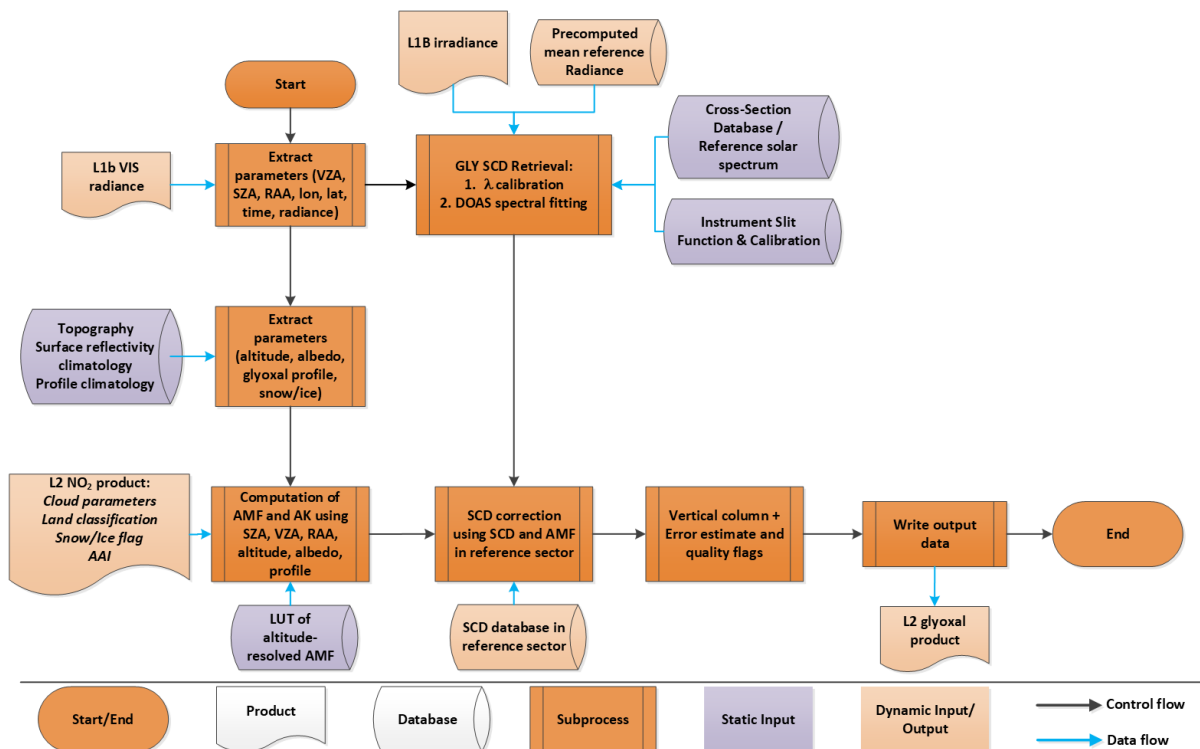


Figure 8-1 Flow diagram of the CHOCHO DOAS retrieval algorithm.





For TROPOMI, the L3 CDR are produced using the slant column fitting results from the S5P-PAL L2 data. For the GOME-2 and OMI sensors, level 1 data have fully reprocessed. Air mass factors and background correction values have been recalculated using consistent settings for all sensors. More details on the L2 algorithm settings can be found in the CHOCHO ATBD available at <https://climate.esa.int/en/projects/precursors-for-aerosols-and-ozone/>.

The L3 products are directly derived from the L2 products. L2 values are binned into regular longitude/latitude grids, where each L3 grid cell is assigned the area-weighted mean of all overlapping L2 pixels. The L3 product consists of CHOCHO tropospheric columns and associated random and systematic uncertainties, detailed results, and input data. L3 data are available for each instrument separately.

Since the afternoon sensors have a significantly higher signal-to-noise ratio and spatial resolution, we provide daily and monthly grids for the afternoon sensors, while only monthly grids are available for the GOME-2 sensors.

8.2. File parameters

Table 8-1 describes the content of the L3 CHOCHO NetCDF files. The fill values are NaN for real-valued fields.

Table 8-1: Variable content of L3 CHOCHO NetCDF files.

Parameter	Unit	Dimension	Description
latitude	degrees	lat	latitude
longitude	degrees	lon	longitude
latitude_bounds	degrees	lat, independent_2	grid latitude bounds
longitude_bounds	degrees	lon, independent_2	grid longitude bounds
time	days	time=1	number of days since 1995-01-01
delta_time	seconds	time, lat, lon	seconds since time
ctm_sigma_a	hPa	layer	pressure = ctm_sigma_a + surface_pressure * ctm_sigma_b
ctm_sigma_b	1		
surface_pressure	hPa	time, lat, lon	surface pressure
surface_albedo	1	time, lat, lon	surface DLER (448 nm)
land_water_mask	1	time, lat, lon	0: water, 1: land, 2: land water transition
qa_L3	1	time, lat, lon	gridded data quality assurance value (0: not valid, 1: valid)
tropospheric_C2H2O2_column_number_density	1	time, lat, lon	Background-corrected glyoxal tropospheric vertical column number density
tropospheric_C2H2O2_column_number_density_uncertainty_random	molec.c m ⁻²	time, lat, lon	Random uncertainty on the background-corrected glyoxal tropospheric vertical column number density
tropospheric_C2H2O2_column_number_density_uncertainty_systematic	molec.c m ⁻²	time, lat, lon	Systematic uncertainty on the background-corrected glyoxal tropospheric vertical column number density





tropospheric_C2H2O2_column_number_density_uncertainty_systematic_kernel	molec.c m ⁻²	time, lat, lon	Systematic uncertainty on the background-corrected glyoxal tropospheric vertical column number density, without the profile uncertainty contribution
tropospheric_C2H2O2_column_number_density_std	molec.c m ⁻²	time, lat, lon	Standard deviation of the background-corrected glyoxal tropospheric vertical column number density within the cell
tropospheric_C2H2O2_column_number_density_count	1	time, lat, lon	Effective number of observations per cell
C2H2O2_slant_column_number_density_rms	1	time, lat, lon	DOAS rms
C2H2O2_slant_column_number_density	molec.c m ⁻²	time, lat, lon	glyoxal slant column number density
C2H2O2_slant_column_number_density_uncertainty	molec.c m ⁻²	time, lat, lon	glyoxal slant column number density uncertainty
C2H2O2_slant_column_number_density_corrected	molec.c m ⁻²	time, lat, lon	Background-corrected glyoxal slant column number density uncertainty
tropospheric_C2H2O2_column_number_density_background_correction	molec.c m ⁻²	time, lat, lon	a priori glyoxal vertical column density number density in the Pacific reference sector
tropospheric_C2H2O2_column_number_density_amf	1	time, lat, lon	tropospheric air mass factor
cloud_fraction	1	time, lat, lon	effective cloud fraction
tropospheric_C2H2O2_column_number_density_apriori	molec.c m ⁻²	time, lat, lon	a priori glyoxal vertical column number density (integrated profile)
C2H2O2_volume_mixing_ratio_dry_air_apriori	ppv	time, lat, lon, layer	a priori glyoxal vertical profile
C2H2O2_averaging_kernel	1	time, lat, lon, layer	Column averaging kernel

8.3. DOI, data access and volume

The DOIs are listed in section 8.7.

The L3 product is available in NetCDF format, and will soon be accessed from <https://climate.esa.int/en/data/> following the CCI filename convention:

ESACCI-PREC-L3C-CHOCHO-<instrument>_<platform>_BIRA-<nlat>x<nlon>_<period>-<date>-fv01.nc,

where

- instrument is one of 'GOME2', 'OMI' or 'TROPOMI',
- platform is one of 'METOPA', 'METOPB', 'METOPC', 'AURA' or 'S5P',
- nlat x nlon is the number of latitude/longitude grid cells,
- period is '1D' for daily grids, and '1M' for monthly grids,
- the date is formatted as 'yyyymmdd' for daily grids, and 'yyyymm' for monthly grids.

Example file name for a June 2022 TROPOMI monthly L3 file:





ESACCI-PREC-L3C-CHOCHO-TROPOMI_S5P_BIRA-1440x2880_1M-202206-fv01.nc.

The content of the NetCDF files is listed in Table 8-1.

8.4. Data reading examples

```
import numpy as np
from netCDF4 import Dataset
from mpl_toolkits.basemap import Basemap
import matplotlib.pyplot as plt
from matplotlib import cm
from mpl_toolkits.axes_grid1 import make_axes_locatable

# Full file path of the NetCDF file
filename='ESACCI-PREC-L3C-CHOCHO-TROPOMI_S5P_BIRA-1440x2880_1M-202206-fv01.nc'

# Map settings
proj_name='cyl'
Mspace=40
Pspace=30
parallels = np.arange(-90,90,Pspace)
meridians = np.arange(-180,180,Mspace)
LW=0.4
size_label=10

# Colorbar settings
ncolor=100
colormap = 'turbo'
scFactor=1e15
minScale = 0
maxScale = 20

# Variable to map and title
var2plot = "tropospheric_C2H2O2_column_number_density"
title_txt="June 2022"

# Read the NetCDF file
with Dataset(filename, "r") as fid:
    CHOCHO2Map = fid[var2plot][:]
    CHOCHO2Map = CHOCHO2Map/scFactor
    varunit = fid[var2plot].units
    scaletitle='TROPOMI {} [{} {}]' .format(fid[var2plot].long_name,format(scFactor,'1.0e'),varunit)
    qa_Map = fid["qa_L3"][:]
    CHOCHO2Map[qa_Map<1]=np.nan

# Create the map
plt.figure(1,figsize=(12,12))
plt.title(scaletitle, loc='left',fontname="Times New Roman",fontweight="bold")
plt.annotate("ESA CCI+ ozone and aerosol precursors", xy=(0.01,0.015), xycoords='axes fraction',size=10,fontname="Times New Roman",fontweight="bold")
plt.title(title_txt, fontdict=None, loc='right',fontname="Times New Roman",fontweight="bold")

map = Basemap(projection=proj_name, llcrnrlon=-180, llcrnrlat=-90, urcrnrlon=180,
urcrnrlat=90,resolution='l',lat_0=0,lon_0=0)
map.drawcoastlines(linewidth=LW,color='grey')
map.drawcountries(linewidth=LW,color='whitesmoke')
map.fillcontinents(color='lightgrey',zorder=0)
map.drawmeridians(meridians,color='black',linewidth=LW/2)
map.drawparallels(parallels,color='black',linewidth=LW/2)

im = map.imshow(CHOCHO2Map[0,:,:], cmap=cm.get_cmap(colormap, ncolor),interpolation='none')
plt.colorbar(im, orientation="horizontal")
plt.clim(minScale, maxScale)

plt.show()
```

8.5. Usage recommendations and known limitations

- The main product is the **"tropospheric_C2H2O2_column_number_density"**.
- A quality flag is provided for the L3 file, with the aim to filter cells which do not contain enough observations. It is advised to use only qa_L3==1. The qa_L3 flag is based on the effective number of observations within the cell (tropospheric_C2H2O2_column_number_density_pixelcount_weight), after applying the L2 quality filtering. If the tropospheric_C2H2O2_column_number_density_pixelcount_weight is lower than the 5th percentile of the cell counts for the day/month, the qa_L3 is set to 0.
- Mean random (σ_r) and systematic (σ_s) uncertainties are available for each grid cell. If a total uncertainty is desired, this can be obtained from the square root of the sum of squares of the different terms:

$$\sigma^2 = \sigma_r^2 + \sigma_s^2$$





- When averaging L3 data over larger temporal or spatial scales, the uncertainty on the average can be obtained by combining the different random (σ_{ri}) and systematic (σ_{si}) uncertainties as

$$\sigma^2 = \sum_{i=1}^n \left(\frac{\sigma_{ri}}{n} \right)^2 + \left(\sum_{i=1}^n \frac{\sigma_{si}}{n} \right)^2$$

- Mean averaging kernels and a priori vertical profiles are provided for each grid cell. This is only an approximation of these quantities with a vertical dimension. L2 data should preferably be used for an accurate exploitation of the averaging kernels.
- The example python script below uses the L3 AKs and ap Profiles to recalculate the AMFs, and compare the results with the provided L3 AMFs.

```
import numpy as np
from netCDF4 import Dataset
import matplotlib.pyplot as plt

# Initialisation
dryair = 28.9644;          #g/mole
ra = 6.0221367e23;        #molec/mole
g = 9.80665;              #m/s

# Full file path of the NetCDF file
filename='ESACCI-PREC-L3C-CHOCHO-TROPOMI_S5P_BIRA-0720x1440_1D-20231031-fv01.nc'

# Read the NetCDF file
with Dataset(filename, "r") as fid:
    sigma_a_Layer= fid["ctm_sigma_a"][:].flatten()
    sigma_b_Layer= fid["ctm_sigma_b"][:].flatten()
    nlayers = np.shape(sigma_a_Layer)[0]
    profile_Map = fid["C2H2O2_volume_mixing_ratio_dry_air_apriori"][0,...].flatten()
    profile_Map = np.reshape(profile_Map, [-1, nlayers])
    ak_Map = fid["C2H2O2_averaging_kernel"][0,...].flatten()
    ak_Map = np.reshape(ak_Map, [-1, nlayers])
    xa_Map = fid["tropospheric_C2H2O2_column_number_density_apriori"][0,...].flatten()
    sp_Map = fid["surface_pressure"][0,...].flatten()
    amf_Map = fid["tropospheric_C2H2O2_column_number_density_amf"][0,...].flatten()
    qa_Map = fid["qa_L3"][0,...].flatten()

total_size = np.shape(sp_Map)[0]

# Calculate the pressure at layer centers
pressure_Map = np.full((total_size, nlayers), np.nan, dtype = np.dtype('f4')) # pressure at layer center [hPa]
for l in range(0, nlayers):
    pressure_Map[:, l] = (sigma_a_Layer[l] + sp_Map[:, l]*sigma_b_Layer[l]) # [hPa]

pi = np.full((total_size, nlayers+1), np.nan, dtype = np.dtype('f4')) # pressure at layer borders [hPa]
pi[:, 0]=sp_Map[:, 0] # surface pressure [hPa]
for l in range(0, nlayers-1):
    pi[:, l+1] = np.exp(np.log(pressure_Map[:, l]) - (np.log(pressure_Map[:, l]) - np.log(pressure_Map[:, l+1]))/2)
pi[:, nlayers]=np.exp( np.log(pi[:, nlayers-1]) - 2*( np.log(pi[:, nlayers-1]) - np.log(pressure_Map[:, nlayers-1]) ) )

# Re-calculate the AMF using the a priori profile and the averaging kernel
dp = np.full((total_size, nlayers), np.nan, dtype = np.dtype('f4')) # delta pressure per layer [hPa]
m_check = np.full((total_size, nlayers), np.nan, dtype = np.dtype('f4')) # recalculate AMF
vcdal = np.full((total_size, nlayers), np.nan, dtype = np.dtype('f4')) # a priori partial columns per layer [molec./cm2]
for l in range(0, nlayers):
    dp[:, l] = pi[:, l] - pi[:, l+1]
    vcdal[:, l] = 10*ra*np.multiply(profile_Map[:, l], dp[:, l])/(g*dryair)
    # Check AMF
    m_check[:, l] = ra*10*amf_Map[:, l]*np.multiply(np.multiply(ak_Map[:, l], np.multiply(profile_Map[:, l], dp[:, l]))/(g*dryair)
VCDa = np.nansum(vcdal, axis=1)
amf_check = np.nansum(m_check, axis=1)/VCDa

kok = (qa_Map>0)

# Plot the re-calculated AMF versus the L3 AMF
fig, ax =plt.subplots(1,1,figsize=(12,6))
plt.plot(amf_Map[kok], amf_check[kok], '.', c='black', markersize=0.2, fillstyle='full', linestyle='')
plt.grid(True)
plt.ylabel("Recalculated AMF using AK and ap Profile", fontsize=12, fontweight='bold', color='k')
plt.xlabel("L3 AMF", fontsize=12, fontweight='bold', color='k')
plt.title(filename, fontsize=10, fontweight='bold', color='k')
plt.xlim([0, 3.5])
plt.ylim([0, 3.5])
plt.show()
```





8.6. Preliminary evaluation

L3 datasets have been generated, covering each sensor's mission period until the end of the year 2023 (2024 for TROPOMI). In the Product Validation and Intercomparison Report (PVIR), the Precursors CCI+ TROPOMI glyoxal data was validated against limited ground-based measurements, as well as the heritage S5P-PAL TROPOMI glyoxal data and the IUP Bremen TROPOMI glyoxal product. Based on these comparisons, the Precursors CCI+ TROPOMI glyoxal data was found to meet the goal requirements stated in the User Requirements Document. We refer to the PVIR for more details.

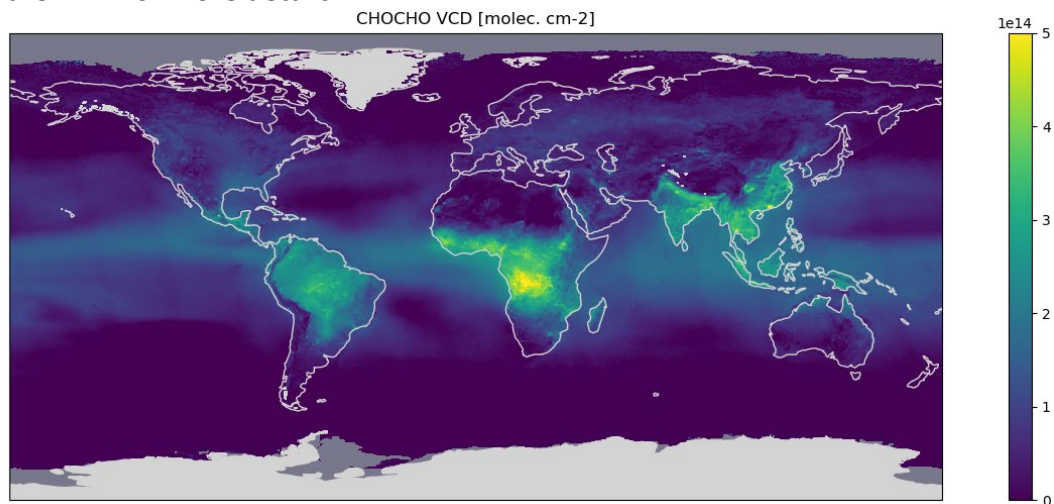


Figure 8-1: Mean TROPOMI/S5P glyoxal vertical column density, May 2018-December 2023

8.7. Contacts and citation

Contact:

- Thomas Danckaert (thomas.danckaert@aeronomie.be)
- Jonas Vlietinck (jonas.vlietinck@aeronomie.be)

Dataset citation:

- Danckaert, T., & Lerot, C. (2025). *CCI+P Glyoxal tropospheric column L3 data from TROPOMI* (Version 1) [Dataset]. Royal Belgian Institute for Space Aeronomy. <https://doi.org/10.18758/CDYUBELO>
- Danckaert, T., & Lerot, C. (2025). *CCI+P Glyoxal tropospheric column L3 data from OMI* (Version 1) [Dataset]. Royal Belgian Institute for Space Aeronomy. <https://doi.org/10.18758/RKEJIUW2>
- Danckaert, T., & Lerot, C. (2025). *CCI+P Glyoxal tropospheric column L2 data from GOME-2A* (Version 1) [Dataset]. Royal Belgian Institute for Space Aeronomy. <https://doi.org/10.18758/fnrftm2ui>
- Danckaert, T., & Lerot, C. (2025). *CCI+P Glyoxal tropospheric column L2 data from GOME-2B* (Version 1) [Dataset]. Royal Belgian Institute for Space Aeronomy. <https://doi.org/10.18758/daeknlqj>
- Danckaert, T., & Lerot, C. (2025). *CCI+P Glyoxal tropospheric column L3 data from GOME-2C* (Version 1) [Dataset]. Royal Belgian Institute for Space Aeronomy. <https://doi.org/10.18758/l29fjyd3>

Paper citation:



- Lerot, C., Hendrick, F., Van Roozendaal, M., Alvarado, L. M. A., Richter, A., De Smedt, I., Theys, N., Vlietinck, J., Yu, H., Van Gent, J., Stavrakou, T., Müller, J.-F., Valks, P., Loyola, D., Irie, H., Kumar, V., Wagner, T., Schreier, S. F., Sinha, V., Wang, T., Wang, P., and Retscher, C.: Glyoxal tropospheric column retrievals from TROPOMI – multi-satellite intercomparison and ground-based validation, Atmos. Meas. Tech., 14, 7775–7807, <https://doi.org/10.5194/amt-14-7775-2021>, 2021.





9. ESA Reference documents

Available from <https://climate.esa.int/en/projects/precursors-for-aerosols-and-ozone/> (See the “Key Documents” tab).

- Algorithm Theoretical Basis Document: Precursors_cci+_D2.1_ATBD_02_02
- End to End ECV Uncertainty Budget: Precursors_cci+_D2.2_E3UB_02_03
- Product Validation and Intercomparison Report: Precursors_cci+_D4.2_PVIR_02_00
- Climate Assessment Report: Precursors_cci+_D5.1_CAR_02_00