ESA Climate Change Initiative "Plus" (CCI+)

Product User Guide Version 5 (PUGv5)

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for the FOCAL XCO$_2$ OCO-2 Data Product CO2_OC2_FOCA (v11)

for the Essential Climate Variable (ECV)

Greenhouse Gases (GHG)

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Change log

Version Nr.	Date	Status	Reason for change
Version 1	8. Oct. 2018	Final	New document for FOCAL v08 initial data set 2015-2016
Version 2	29. Nov. 2019	Final	Update for FOCAL v08 extended data set 2015-2018
Version 3 Draft	16. Nov. 2020	Draft	New data set FOCAL v09 2015-2019
Version 3	25. Jan. 2021	Final	Updated equation numbering
Version 4	06. Feb. 2023	As submitted	New data set FOCAL v10 2014-2021
Version 4.1	21. Apr. 2023	Final	Updated data set FOCAL v10.1 with improved bias correction
Version 5	05.07.2024	Final	Updated document for FOCAL v11

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1 Purpose of document

The purpose of this document is to describe a global atmospheric carbon dioxide (CO$_2$) data set as retrieved from NASA's OCO-2 satellite mission. The data product is the column-averaged dry-air mole fraction of CO$_2$, denoted XCO$_2$ (in parts per million, ppm). The XCO$_2$ data set has been retrieved using University of Bremen's FOCAL algorithm for OCO-2 v11.

This document describes the data set, including the product file format, and provides the user with important information on how to use the FOCAL data.

2 Orbiting Carbon Observatory 2 (OCO-2)

The Orbiting Carbon Observatory-2 (OCO-2) (e.g., **/Eldering et al., 2017/** and references given therein) was launched in 2014 aiming at continuing and improving XCO_2 observations from space. XCO_2 is the column-averaged dry-air mole fraction of carbon dioxide (CO_2) (typically reported in parts per million (ppm)).

As part of the A-train satellite constellation, OCO-2 flies in a sun-synchronous orbit crossing the equator at 13:36 local time. OCO-2 measures one polarization direction of the solar backscattered radiance in three independent wavelength bands: the O_2-A band at around 760 nm (band1) with a spectral resolution of about 0.042 nm and a spectral sampling of about 0.015 nm, the weak CO_2 band at around 1610 nm (band2) with a spectral resolution of about 0.080 nm and a spectral sampling of about 0.031 nm, and the strong CO_2 band at around 2060 nm (band3) with a spectral resolution of about 0.103 nm and a spectral sampling of about 0.040 nm.

OCO-2 is operated in a near-push-broom fashion and has eight footprints across track measured with an integration time of 0.333 s (i.e., 3 across track scan lines per second). The instrument's spatial resolution at ground is 1.29 km across track and 2.25 km along track.

For more information on the OCO-2 instrument please see **/Eldering et al., 2017/** and references given therein and NASA's OCO-2 website (https://www.nasa.gov/mission_pages/oco2/index.html).

3 Retrieval algorithm FOCAL

The fast atmospheric trace gas retrieval (FOCAL) for OCO-2 has been setup to retrieve XCO_2 by analyzing hyper spectral solar backscattered radiance measurements of NASA's OCO-2 satellite. FOCAL includes a radiative transfer model which has been developed to approximate light scattering effects by multiple scattering at an optically thin scattering layer. This reduces the computational costs by several orders of magnitude. FOCAL's radiative transfer model is utilized to simulate the radiance and its derivative according to several geophysical parameters in all three OCO-2 spectral bands.

FOCAL's radiative transfer and retrieval technique has initially been described by **/Reuter et al., 2017a/** and its first application to OCO-2 data by **/Reuter et al., 2017b/**. Since then, many minor and major algorithm improvements have been implemented and documented in the most recent version of the CO2_OC2_FOCA algorithm theoretical basis document **/ATBDv5, 2024/**. Furthermore, the most recent version of the end-to-end ECV uncertainty budget document for the CO2_OC2_FOCA data product **/E3UBv5, 2024/** comprises important information on the data reliability. This includes an assessment of stochastic and potential systematic uncertainties based on results of a thorough validation, analyses of simulated observations, and a model comparison.

Additional information on FOCAL can also be obtained from the FOCAL website (http://www.iup.uni-bremen.de/~mreuter/focal.php).

4 Description of data format

The data product is a level 2 (L2, i.e., individual soundings) product, i.e., it contains detailed information such as XCO_2 and its uncertainty, time, latitude, longitude, averaging kernel, a priori profile, etc. for each individual satellite sounding. Additionally, the data product includes information on XH_2O which is a by-product of the XCO_2 retrieval.

The data content is conform with ESA's Product Specification Document (PSD) for the Essential Climate Variable (ECV) Greenhouse Gases (GHG) **/Buchwitz et al., 2014/**. It is the baseline for the satellite-derived Level 2 XCO_2 data products generated in the framework of ESA's Climate Change Initiative (https://climate.esa.int/en/projects/ghgs/) (e.g., **/Buchwitz et al., 2017/**) and, more recently, for the Copernicus Climate Change Service (C3S, https://climate.copernicus.eu) (e.g., **/Buchwitz et al., 2018/**).

The data format is NetCDF-4 classic (Network Common Data Format 4 classic) and the product is in-line with CF (Climate and Forecasting) convention 1.6. NetCDF is a binary machine-independent file format widely used for storing and exchanging scientific data. It is supported and maintained by the Unidata Program Center (https://www.unidata.ucar.edu/software/netcdf/). Programming interfaces exist for basically all wide-spread higher programming languages such as C++, Fortran, Java, Python, IDL, MATLAB, R, etc. There are also cross-platform tools like NASA's Panoply (https://www.giss.nasa.gov/tools/panoply) or HDFView from the HDF Group (https://www.hdfgroup.org/downloads/hdfview) allowing to browse through the content of NetCDF files and visually inspect the included data.

All stored FOCAL parameters are explained in each file making the product essentially self-explaining. For each day one separate file has been generated. The data set has a yearly volume of typically 7.3GB and covers the time period 09/2014 – 02/2022. The file names consist of the processing institute (IUP = Institute of Environmental Physics, University of Bremen), the essential climate variable (GHG = greenhouse gases), processing level (L2), primary target gas (CO2), sensor (OCO-2), retrieval algorithm (FOCAL), date (YYYYMMDD), and the retrieval algorithm version (v11) all separated by hyphens (-). The file name extension is ".nc".

Example: IUP-GHG-L2-CO2-OCO-2-FOCAL-20210112-v11.0.nc

Beside several descriptive meta data entries, the FOCAL L2 NetCDF files include the data arrays listed and explained in Table 4.1.

Table 4.1: Data arrays within the FOCAL L2 NetCDF data files. Name: Name of the data array. Type: Primitive data type. Dimension: Dimension of data array with n being the number of soundings within the file and m the number of profile layers which is always five for FOCAL v11. Unit: Physical unit. Description: Short description of the variable. All profiles are ordered from surface to TOA (top of atmosphere) and profile values represent layer averages within the corresponding pressure levels (layer boundaries).

Name	Type	Dimension	Unit	Description
sounding_id	64bit int.	n	-	Unique identifier for each sounding as in NASA's OCO-2 L1b data.
footprint_index	64bit int.	n	-	Footprint index of the sounding (0-7).
operation_mode	string	n	-	Two-letter abbreviation of the science acquisition mode: GL=glint, ND=nadir, TG=target, XS=transition.
time	64bit float	n	second	Measurement time in seconds since 01.01.1970 00:00:00
longitude	32bit float	n	degree east	Center of the measurement. Range: [-180°, 180°].
vertex_longitude	32bit float	n x 4	degree east	Corner longitudes (average of OCO-2's three spectral bands).
latitude	32bit float	n	degree north	Center of the measurement. Range: [-90°, 90°].
vertex_latitude	32bit float	n x 4	degree north	Corner latitudes (average of OCO-2's three spectral bands).

Name	Type	Dimension	Unit	Description
land_fraction	32bit float	n	-	Range: [0, 1]
sensor_zenith_angle	32bit float	n	degree	The angle between the line of sight to the sensor and the local vertical.
solar_zenith_angle	32bit float	n	degree	The angle between the line of sight to the sun and the local vertical.
pressure_levels	32bit float	n x (m+1)	hPa	Boundaries of the averaging kernel and mole fraction profile layers (1st element = surface pressure).
pressure_weight	32bit float	n x m	-	Layer dependent weights needed to apply the averaging kernels.
xco2	32bit float	n	ppm	Retrieved column-average dry-air mole fraction of atmospheric carbon dioxide (XCO$_2$).
xco2_uncertainty	32Bit float	n	ppm	1-sigma uncertainty of the retrieved XCO$_2$.
xco2_quality_flag	8bit int.	n	-	0=good, 1=bad
xco2_averaging_kernel	32Bit float	n x m	-	Normalized column-averaging kernel representing the sensitivity of the retrieved XCO$_2$ to the atmospheric CO$_2$ mole fraction profile. Values near one are ideal and indicate that the influence of the a priori is minimal.
co2_profile_apriori	32Bit float	n x m	ppm	CO$_2$ a priori dry-air mole fraction profile needed to apply the XCO$_2$ averaging kernel.

Name	Type	Dimension	Unit	Description
xh2o	32Bit float	n	ppm	Retrieved column-average dry-air mole fraction of atmospheric water vapor (XH_2O).
xh2o_uncertainty	32Bit float	n	ppm	1-sigma uncertainty of the retrieved XH_2O.
xh2o_quality_flag	8bit int.	n	-	0=good, 1=bad
xh2o_averaging_kernel	32Bit float	n x m	-	Normalized column-averaging kernel representing the sensitivity of the retrieved XH_2O to the atmospheric H_2O mole fraction profile. Values near one are ideal and indicate that the influence of the a priori is minimal.
h2o_profile_apriori	8bit int.	n x m	ppm	H_2O a priori dry-air mole fraction profile needed to apply the XH_2O averaging kernel.

5 Usage of averaging kernels

Each FOCAL XCO_2 retrieval comes with an estimate for its corresponding normalized column-averaging kernel representing the sensitivity of the retrieved XCO_2 to the atmospheric CO_2 mole fraction profile. Values near one are ideal and indicate that the influence of the a priori is minimal. A data user should consider making use of the averaging kernel (AK) information whenever highly accurate comparisons with models or other measurements with differing height sensitivities are in the study focus. Typical applications are the validation with other measurements, e.g., from the Total Carbon Column Observing Network (TCCON) or surface flux inverse modelling. For these applications, the correct usage of the AK information reduces the influence of the a priori, especially in situations with reduced sensitivity. For FOCAL this is typically the case in higher altitudes (e.g., within the stratosphere).

The same mathematical formalism as explained in the following sections can also be applied to FOCAL's XH_2O data which is a byproduct of the XCO_2 retrieval. However, due to the usually lower accuracy and precision requirements of XH_2O, it is less common to use the AK information.

5.1 Comparison with models

When comparing the satellite-retrieved XCO_2 data product with model simulations the altitude sensitivity, i.e., the AKs of the satellite retrievals should be taken into account in order to achieve the most reliable results. The same is true for the observation operator of an inverse model computing surface fluxes (e.g., **/Bergamaschi el al., 2007/**).

Usually and as also described in **/PUGS, 2019/**, the AKs are used to compute the model's XCO_2 ($\hat{x}^{mod}$) as the satellite would "see" it.

5-1
$$\hat{x}^{mod} = \sum_{i=1}^{m} \left[C_i^{apr} + A_i \left(C_i^{mod} - C_i^{apr} \right) \right] w_i$$

Here C^{apr} and C^{mod} represent the atmospheric CO_2 dry-air mole fraction profiles of the a priori of the satellite retrieval and of the model simulation, respectively. A is the

averaging kernel of the satellite retrieval, and w the pressure weight. The summation goes over all $m = 5$ layers of the FOCAL retrieval.

C^{apr}, A, and w come from the FOCAL satellite product without the need for modifications. Usually only the model's CO₂ dry-air mole fraction profile layering has to be adapted in advance to match FOCAL's layering. This can be achieved by using FOCAL's pressure levels in order to compute the model's average CO₂ dry-air mole fraction in-between each of two consecutive FOCAL pressure levels.

In this step, one should pay attention to maintain the number of particles in the atmospheric column. As a cross-check, it should be ensured that the XCO₂ of the unmodified model profile agrees with the XCO₂ of the new profile with FOCAL layering. The XCO₂ of the new profile simply corresponds to the profile's average, because FOCAL's layering is defined to have the same number of dry-air particles within each layer.

5.2 Comparison with other measurements

Also when comparing the satellite-retrieved XCO₂ data product with other measurements with a different altitude sensitivity, the AKs should be taken into account in order to achieve the most reliable results. This is usually done, e.g., for validation studies like that of **/Reuter et al. (2020)/** comparing multiple satellite retrieved data sets with TCCON ground based remote sensing data.

A common approach is to adjust the different data sets as if they all share a common a priori. If the common a priori is that of FOCAL, no modifications of the FOCAL data are needed. As this is generally not the case, the following equation can be used to approximate the XCO₂ ($\hat{x}^{foc}$) that FOCAL would have retrieved when using the atmospheric CO₂ dry-air mole fraction profile C^{com} as (common) a priori instead of FOCAL's original a priori profile C^{apr}.

5-2
$$\hat{x}^{foc} = X^{foc} + \sum_{i=1}^{m}(1 - A_i)\,(C_i^{com} - C_i^{apr})\,w_i$$

X^{foc} is FOCAL's unmodified XCO₂ retrieval result, A is the averaging kernel of the FOCAL retrieval, and w its pressure weight. The summation goes over all $m = 5$ layers of the FOCAL retrieval.

C^{apr}, A, and w come from the FOCAL satellite product without the need for modifications. Usually only the common a priori CO₂ dry-air mole fraction profile

layering has to be adapted in advance to match FOCAL's layering. This can be achieved by using FOCAL's pressure levels in order to compute the average CO_2 dry-air mole fraction of the common a priori in-between each of two consecutive FOCAL pressure levels.

In this step, one should pay attention to maintain the number of particles in the atmospheric column. As a cross-check, it should be ensured that the XCO_2 of the unmodified common a priori profile agrees with the XCO_2 of the adapted common a priori profile with FOCAL layering. The XCO_2 of the adapted profile corresponds simply to the profile's average, because FOCAL's layering is defined to have the same number of dry-air particles within each layer.

If the adjusted FOCAL XCO_2 ($\hat{x}^{foc}$) is going to be compared with other remote sensing retrieval results sharing the same common a priori C^{com}, the influence of the smoothing error can be reduced according to **/Wunch et al., 2011/**. Analog to Eq. 5-1), one can compute what FOCAL would "see" given the retrieved profile of the other measurement as truth.

5-3
$$\hat{x}^{mea} = \sum_{i=1}^{m}[C_i^{com} + A_i\ (C_i^{mea}\ -\ C_i^{com})]\ w_i$$

In this equation, $\hat{x}^{mea}$ is the adjusted other measurement as FOCAL would "see" it, C^{com} the common a priori profile, A FOCAL's averaging kernel, w FOCAL's pressure weight, and C^{mea} the retrieved CO_2 profile of the measurement to be compared with.

Of course, this is only possible if C^{mea} is known, which is not always the case. If the other measurement is based on a profile scaling retrieval (as for example TCCON GGG2014), one can compute C^{mea} from the retrieved scaling factor $\gamma = X^{mea}/X^{com}$ by:

5-4
$$C^{mea} = \gamma\ C^{com} = \frac{X^{mea}}{X^{com}}\ C^{com}$$

with X^{mea} being the unmodified XCO_2 of the profile scaling retrieval before applying Eq. 5-3. Generally, it cannot be expected that C^{mea} has the same layering as the FOCAL profiles, therefore it has to be adapted in advance to match FOCAL's layering as described above. It shall be noted that the influence of applying Eq. 5-3 is usually very minor.

6 Quick looks

In this section, we show how the quality filtered and bias corrected FOCAL XCO_2 data product "looks like" by showing a selection of overpasses of local CO_2 enhancements, global monthly maps, and time series in three latitude bands. New users may find it helpful to reproduce some of these figures to ensure that no obvious errors are being made when reading and handling the FOCAL data.

The scenes of the local XCO_2 enhancements (Figure 6.1) are the same as two of the scenes analyzed by **/Reuter et al., 2019/** who found similarly large enhancements in NASA's operational bias-corrected OCO-2 L2 Lite XCO_2 product v9 **/Kiel et al., 2019/**.
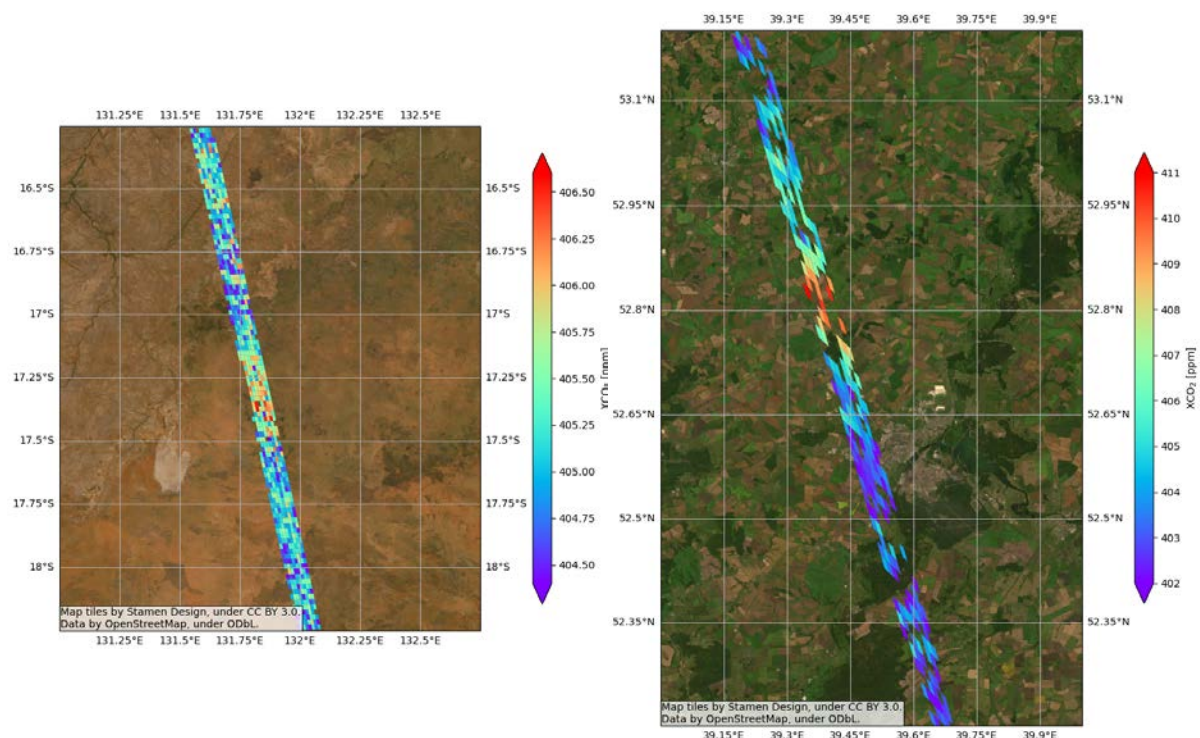
Figure 6.1: **Left)** Local XCO_2 enhancement due to emissions of Australian wildfires (May 5, 2018, 05:00 UTC). **Right)** Local XCO_2 enhancement due to the emissions of the TEC-2 Lipetsk power plant in Russia (August 25, 2018, 10:15 UTC).

Each sub-figure of Figure 6.2 shows one month of FOCAL XCO_2 data arithmetically averaged on a 2.5° x 2.5° grid. The figures illustrate for two years (2018 and 2020) and two months (April and August) the sampling and large scale XCO_2 patterns of the FOCAL data. As to be expected, FOCAL shows larger XCO_2 values in the northern hemisphere than in the southern hemisphere at the beginning of the growing season in April and vice versa at the end of the growing season in August. As an additional information, the sub-figures also show the number of soundings. The sampling of the FOCAL data is sparser in Brasilia partly because of the south Atlantic anomaly and in high latitudes because of the unfavorable illumination conditions in these regions. Sampling and large scale XCO_2 patterns are similar in 2018 and 2020.
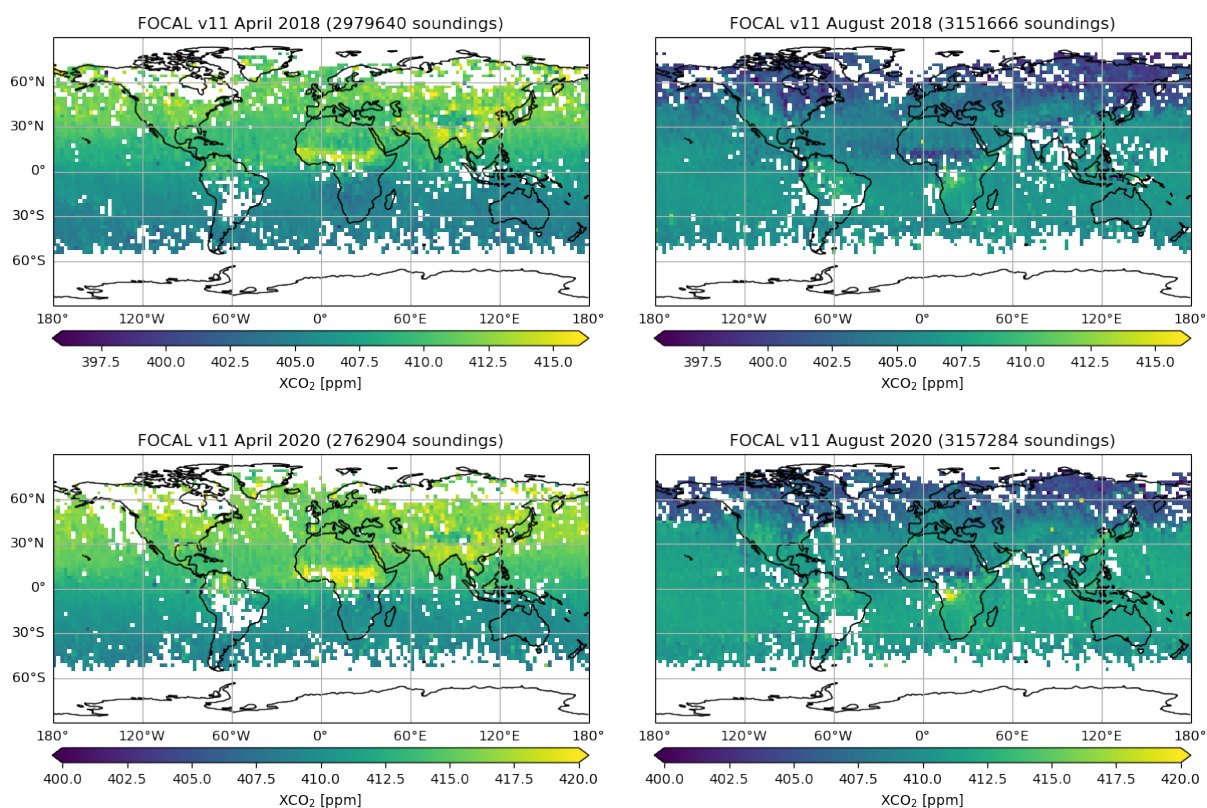

Figure 6.2: FOCAL XCO_2 data of April 2018 (top, left), August 2018 (top right), April 2020 (bottom, left), and August 2020 (bottom, right) gridded 2.5° x 2.5° by arithmetic averaging.

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Figure 6.3 shows a time series of daily FOCAL XCO_2 averages of all soundings of the northern hemisphere, tropics, and the southern hemisphere. One can clearly see the distinct seasonal cycle of the northern hemisphere which is mainly caused by photosynthesis and respiration of the terrestrial vegetation. One can also see the continuous year-to-year increase due to the anthropogenic CO_2 emissions and also that the northern hemispheric CO_2 values are larger on average than the southern hemispheric values, because of the majority of anthropogenic sources being located on the northern hemisphere.
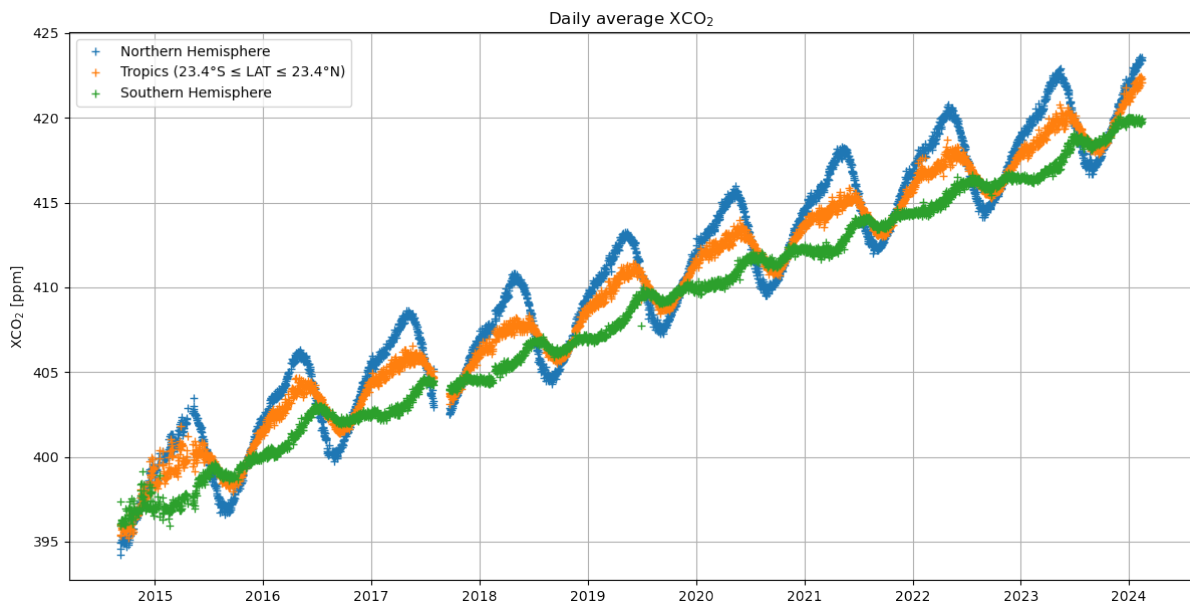

Figure 6.3: FOCAL XCO_2 daily averages of the northern hemisphere (latitude ≥ 0°N), southern hemisphere (latitude < 0°N), and the tropics (-23.4°N ≤ latitude ≤ 23.4°N).

7 Acknowledgements

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