ESA Climate Change Initiative "Plus" (CCI+)

Product User Guide (PUG)

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for the FOCAL XCO_2 OCO-2 Data Product CO2_OC2_FOCA (v08)

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

Table of Contents

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 product has been retrieved using University of Bremen's FOCAL algorithm.

This document describes a data set which has been retrieved with FOCAL v08. The data set covers the time period 01/2015 – 12/2018.

This document describes the FOCAL algorithm, presents an overview about the data set and its validation. In addition, information on the product file format is provided.

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

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) algorithm is described in detail by **/Reuter et al., 2017a/** and its first application to OCO-2 data by **/Reuter et al., 2017b/**. Here we only shorty describe the improvements implemented since **v06**, which has been described by **/Reuter et al., 2017b/**:

v07

- Use of OCO-2 Level 1 version 8 data
- RT now can deal with "unphysical" scattering layer heights outside the atmosphere (see **/Reuter et al., 2017a/**)
- Use of a synthetic CO_2 a priori error covariance (see **/Reuter et al., 2017a/**)
- Relaxed limits for less strict stopping iterations
- Added the capability to compute smoothing and noise error diagnostics

v08

- Levenberg-like OE-fitting
- Revised cross section database with higher resolution in the CO_2 bands (0.0026nm and 0.0044nm in the weak and strong absorption band, respectively, instead of 0.0050nm in both bands)
- HITRAN2016 for H_2O
- New dead/bad pixel mask based on OCO-2 L1B v8r 31.12.2016
- Revised pre-processor including minor bug fixes
- Use of ECMWF ERA5 hourly 0.25° x 0.25° meteorology instead of six hourly 0.75° x 0.75° ECMWF analysis.
- Revised meteorology reader

4 XCO_2 data product (FOCAL v08, 2015-2018)

In this section, we show how the new XCO_2 data product “looks like” by showing monthly maps (Sect. 4.1) including comparisons with the CAMS model (Sect. 4.2) and by giving a summary of the validation results relative to TCCON (Sect. 4.3).

4.1 Monthly maps

Figure 1 and **Figure 2** show monthly maps of the FOCALv08 OCO-2 XCO_2 data product. As can be seen, the spatial coverage depends on time due to cloud-cover (the observations correspond to cloud free scenes), sun illumination conditions, etc.

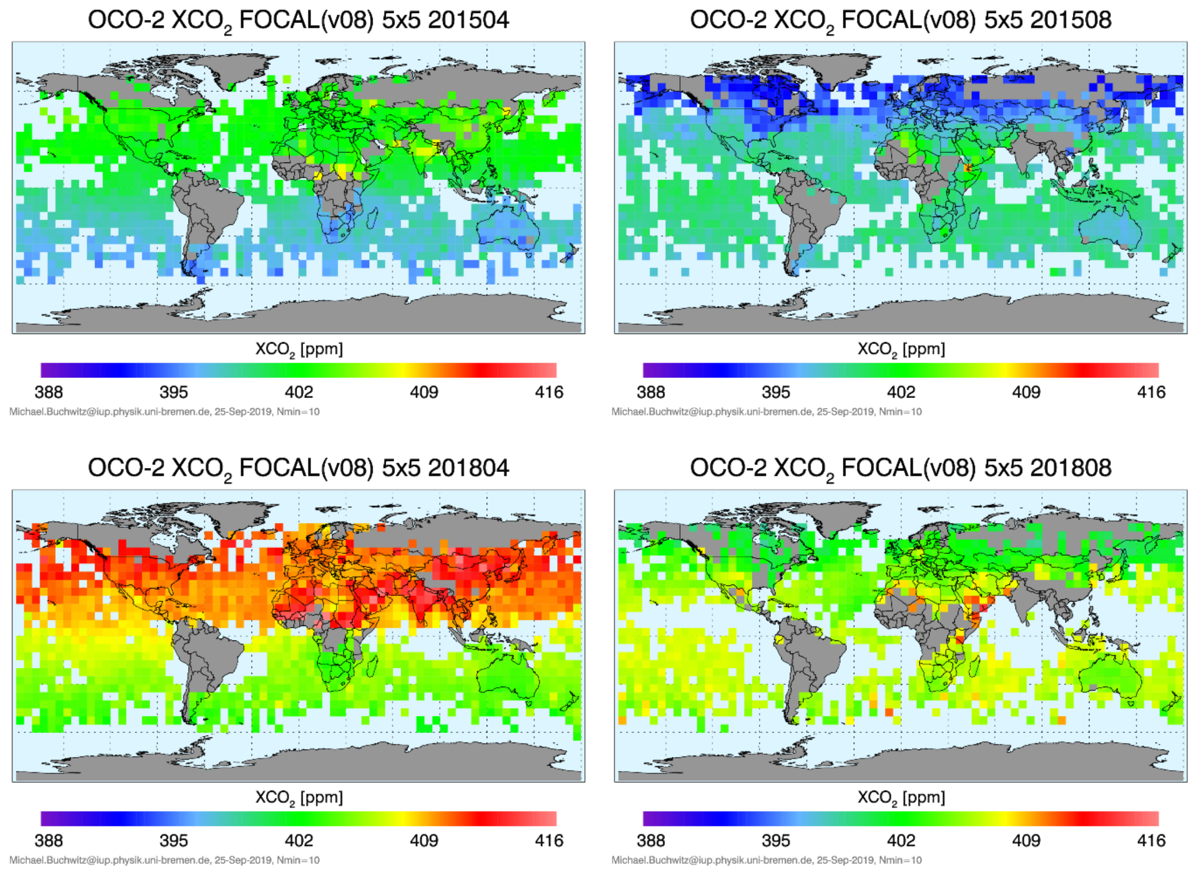

Figure 1: Monthly maps of the FOCALv08 OCO-2 XCO_2 data product. Top: April (left) and August (right) 2015. Bottom: April (left) and August (right) 2018. To generate these maps the Level 2 (individual soundings) data product has been gridded (averaged) to monthly time and 5°x5° spatial resolution.

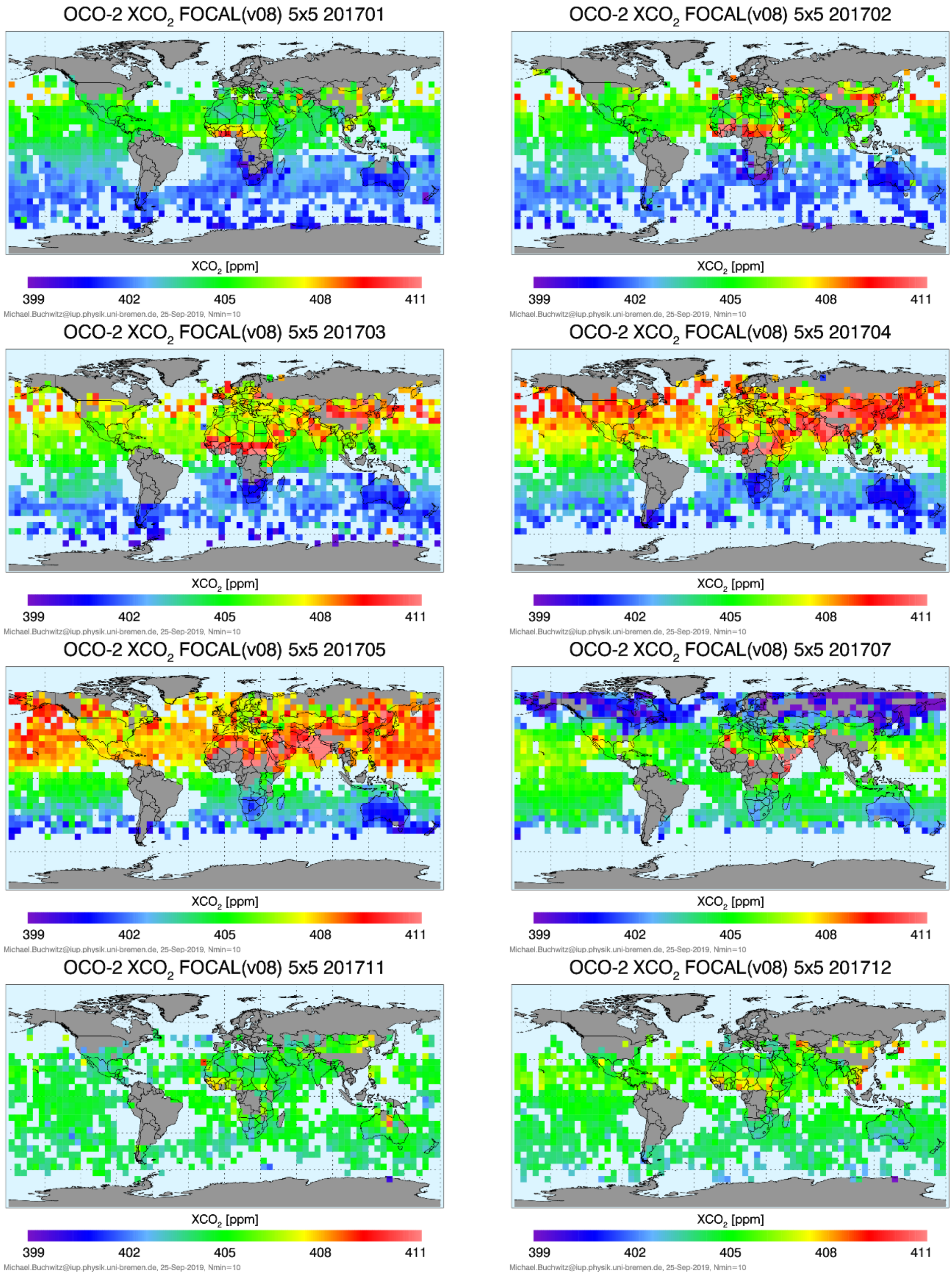

Figure 2: As **Figure 1** but for selected months of the year 2017.

4.2 Comparison with CAMS

In this section, we compare two months (April and August 2015) of post-filtered and bias corrected FOCAL v08 XCO_2 results with corresponding values of the CAMS v15r4 model accounting for FOCAL's column averaging kernels.

Figure 3 shows 5° x 5° monthly gridded values for both months, FOCAL, and CAMS. The main spatial and temporal patterns are similar for FOCAL and CAMS with largest and smallest values in the northern hemisphere in April and August, respectively.

Differences become larger at smaller scales, e.g., FOCAL sees larger values in natural and anthropogenic source regions of Sub-Saharan Africa and Asia in April but also above the Sahara in August. However, it shall be noted that often only few data points are in the corresponding grid boxes. In grid boxes with more than about 100 soundings, the standard error of the mean becomes negligible (<0.1 ppm). Therefore, the difference between FOCAL and CAMS in such grid boxes can be interpreted as systematic temporal and regional mismatch or bias. The standard deviation of this systematic mismatch (including also representation errors) amounts to 0.9 ppm. The standard deviation of the single sounding mismatch after subtracting the systematic mismatch amounts to 1.1 ppm which agrees reasonably well with the average reported uncertainty of 1.2 ppm.

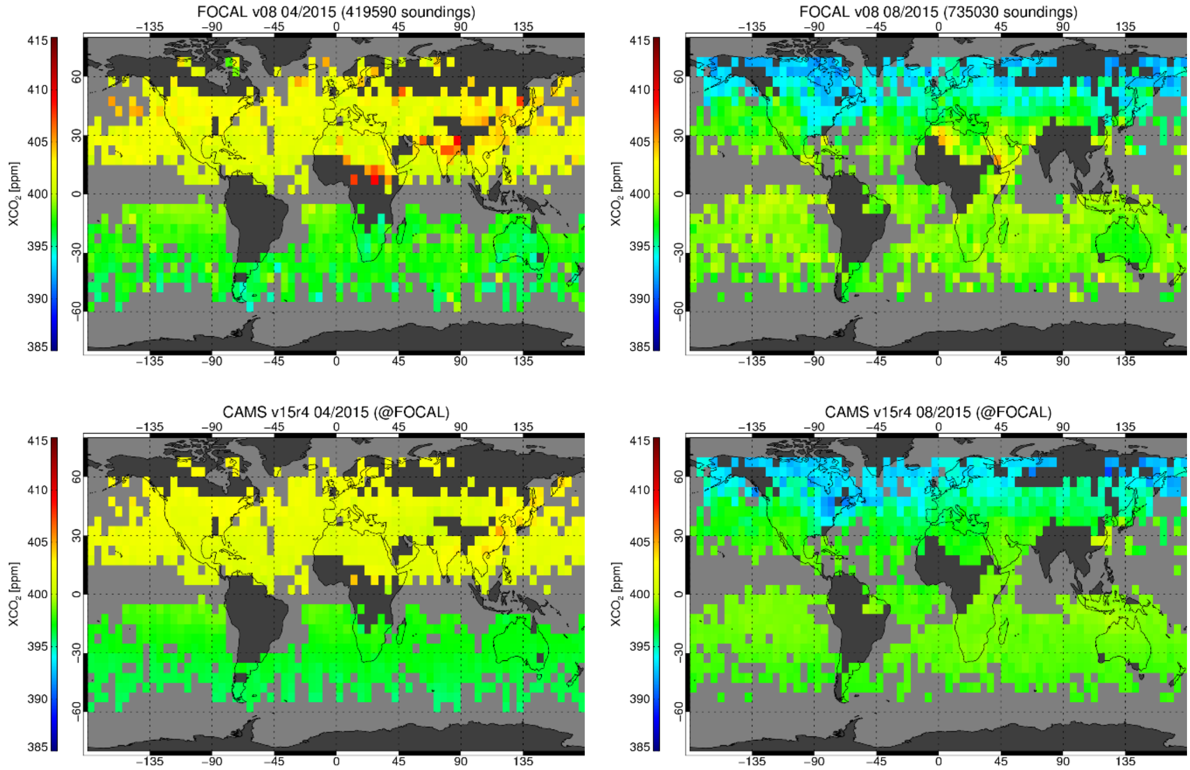

Figure 3: Monthly mean XCO_2 at 5° x 5°. Top: FOCAL v08. Bottom: CAMSv15r4 sampled as FOCAL. Left: April 2015. Right: August 2015.

4.3 Validation with TCCON

This section summarizes the main validation results presented in the FOCAL OCO-2 ESA GHG CCI+ End-to-End ECV Uncertainty Budget Version 1 **/E3UBv1, 2019/** document.

We used ground based TCCON GGG2014 **/Wunch et al., 2011/** data obtained from *http://tccon.ornl.gov* as reference data set and considered the column averaging kernels according to **/PUGS, 2017/**. We co-located OCO-2 and TCCON measurements with a maximum time difference of 2h, a maximum distance of 500 km, and a maximum surface elevation difference of 250m.

In cases with multiple TCCON measurements of the same site co-locating with an OCO-2 sounding, we averaged the TCCON measurements. In total, we found about 600000 co-locations with TCCON during the four-year validation period 2015-2018.

Figure 4 shows the co-locations of all 24 sites with more than 250 co-locations. Per site statistics (bias and scatter, i.e., single sounding precision measured by the standard deviation of the difference to TCCON after removing systematic effect, see **/E3UBv1, 2019/** for more details) are shown from north to south by **Figure 5**.

Note that a global offset of -0.31 ppm has been removed from the FOCAL data set. The standard deviation of the site biases is 0.64 ppm. TCCON's site-to-site consistency is about 0.4 ppm (1s) **/Wunch et al., 2011/**. The site-to-site pattern for the scatter shows somewhat lower values for the southern hemispheric sites (except for Lauder) probably due to smaller natural variability and, consequently, smaller representation errors. The average scatter relative to TCCON amounts to 1.52 ppm.

The validation results can be summarized as follows:

- Single observation random error ("precision", 1-sigma): 1.52 ppm
- Overall bias (global offset): -0.31 ppm
- Spatial bias: 0.64 ppm
- Temporal (seasonal) bias: 0.38 ppm
- Spatio-temporal bias ("relative accuracy"): 0.74 ppm

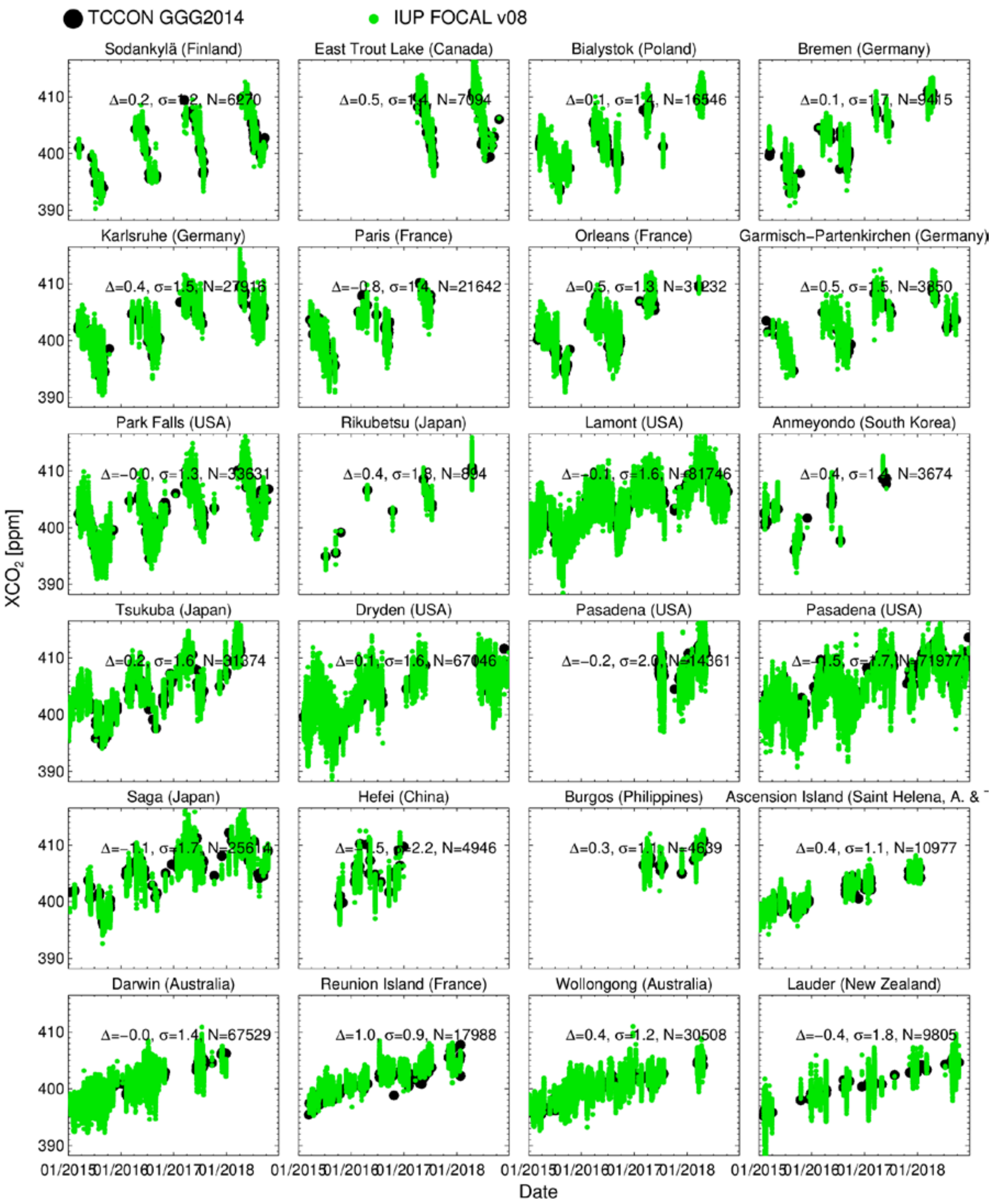

Figure 4: Validation of single soundings of FOCAL (**green**) with co-located TCCON measurements (**black**) at all TCCON sites with more than 250 co-locations and covering a time period of at least one year. Numbers in the figures: Δ = station bias, i.e., average of the difference; σ = single measurement precision, i.e., standard deviation of the difference; N = number of co-locations.

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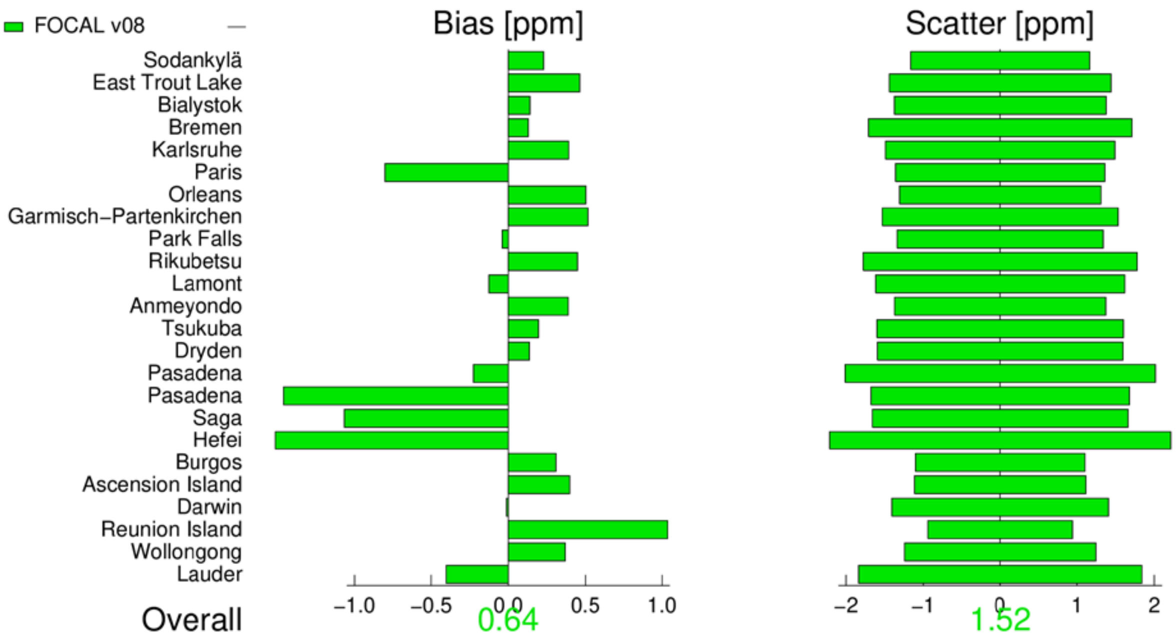

Figure 5: Validation statistics bias (**left**) and scatter (**right**) per TCCON site with more than 250 co-locations for FOCALv08 (bias corrected). The summarizing values (“overall”) represent the standard deviation of the site biases and the average scatter relative to TCCON. The sites are ordered from north (top) to south (bottom).

Additionally, to the validation of XCO2 values, also the reported uncertainty has been validated using TCCON. For this purpose, we analysed in how far variations in the reported uncertainty correspond to variations in the scatter relative to TCCON.

Summarizing the results presented in **/E3UBv1, 2019/**, we suggest that users who are interested in more realistic uncertainty estimates, shall apply the following error parameterization:

$$\sigma_{\text{corrected}}^{\text{XCO}_2} = \sigma_{\text{v08}}^{\text{XCO}_2} \cdot 1.128 + 0.128\text{ppm}$$

5 Description of data format

The data product is a Level 2 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 footprint. Additionally, the data product includes information on XH_2O and SIF, which are by-products of the XCO_2 retrieval.

The data format is conform with the satellite-derived Level 2 XCO_2 data products generated in the framework of ESA's Climate Change Initiative (http://www.esa-ghg-cci.org) (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) and the product is in-line with CF (Climate and Forecasting) convention 1.6. Each parameter is explained in each file and the product is, therefore, essentially self-explaining. For each day one separate file has been generated.

The data format is described in detail by **/Buchwitz et al., 2014/**. This Product Specification Document (PSD) is available via this link:

http://www.esa-ghg-cci.org/index.php?q=webfm_send/160

6 Acknowledgements

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The OCO-2 data were produced by the OCO-2 project at the Jet Propulsion Laboratory, California Institute of Technology, and obtained from the OCO-2 data archive maintained at the NASA Goddard Earth Science Data and Information Services Center. Additionally, NASA provided the MODIS L2 collection 6 MYD35 cloud mask data, the OMI L3 OMAERUVd v003 UV aerosol index data, and the absorption cross section database ABSCO.

ECMWF provided the used meteorological profiles.

The used solar spectra were made available by R. L.Kurucz and G.C. Toon.

The used chlorophyll fluorescence spectrum has been published by U.Rascher.

TCCON data were obtained from the TCCON Data Archive, hosted by the Carbon Dioxide Information Analysis Center (CDIAC).

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