ESA Climate Change Initiative "Plus" (CCI+)

Product User Guide Version 3 (PUGv3)
-
for the FOCAL XCO₂ OCO-2 Data Product
CO2_OC2_FOCA (v09)

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	26. Jan. 2021	Final	Updated equation numbering

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

This document describes a data set which has been retrieved with FOCAL v09. The data set covers the time period 01/2015 – 12/2019.

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).

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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/**:

v09

- Generation of a global 5-years data set (2015-2019) based on OCO-2 v8 L1b data with an extension till 05/2020 based on OCO-2 v10 L1b data.
- Migration of L2 processor from IDL to Python.
- Usage of previous results as first guess state vector (except for albedo) in order to improve convergence behavior. This acceleration is only applied for soundings of the same orbit having distances below 25km. Additionally, the maximum number of successive accelerated soundings is limited to 25.
- Bug fixes.

v08

- Generation of a global 4-years data set.
- Improved cross section data bases with finer temperature, pressure, and wavelength grid in the wCO2 (0.0026nm) and sCO2 (0.0044nm) band.
- Quadratic wavelength and linear pressure interpolation of the cross section data base.
- Usage of HITRAN2016 as H2O spectroscopy.
- Allowing unphysical values of the height of the scattering layer for improved convergence behavior.
- Widened limits for improved convergence behavior.
- Improved smoothing and noise error diagnostics.
- Usage of ECMWF ERA5 meteorological data.
- Bug fixes.

4 XCO₂ data product (FOCAL v09, 2015-2019)

In this section, we show how the FOCAL XCO₂ data product "looks like" by showing monthly maps including a comparisons with the CAMS model (Section 4.1) and by giving a summary of the validation results relative to TCCON (Section 4.2).

4.1 Monthly maps

In this section, we show six months (Feb., Apr., Jun., Aug., Oct., and Dec. 2015) of post-filtered and bias corrected FOCAL v09 data on a 5°×5° grid (**Figure 4.1**) and corresponding CAMS v15r4 model data considering FOCAL's column averaging kernels **/PUGS, 2017/** and sampled as FOCAL (**Figure 4.2**). 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.

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 East Asia, e.g., in April but also above the Sahara, e.g., 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 100 soundings, the standard error of the mean becomes negligible (~0.1ppm). 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 1.0ppm. The standard deviation of the single sounding mismatch after subtracting the systematic mismatch amounts to 1.2 ppm which is consistent with the average reported uncertainty of 1.2 ppm.
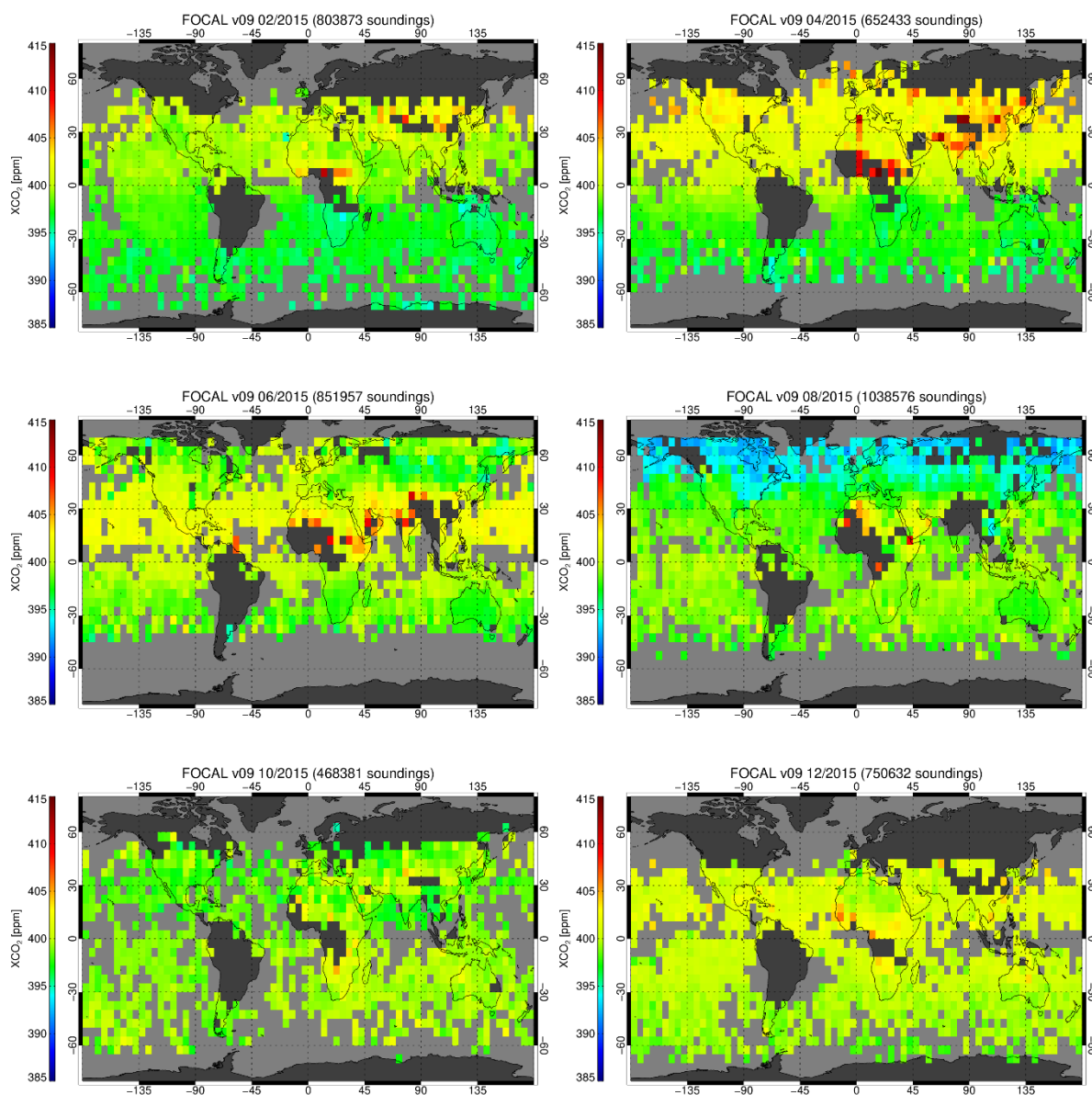
Figure 4.1: FOCAL v09 monthly mean XCO₂ gridded to 5°×5°. From top/left to bottom/right: Feb., Apr., Jun., Aug., Oct., and Dec. 2015.
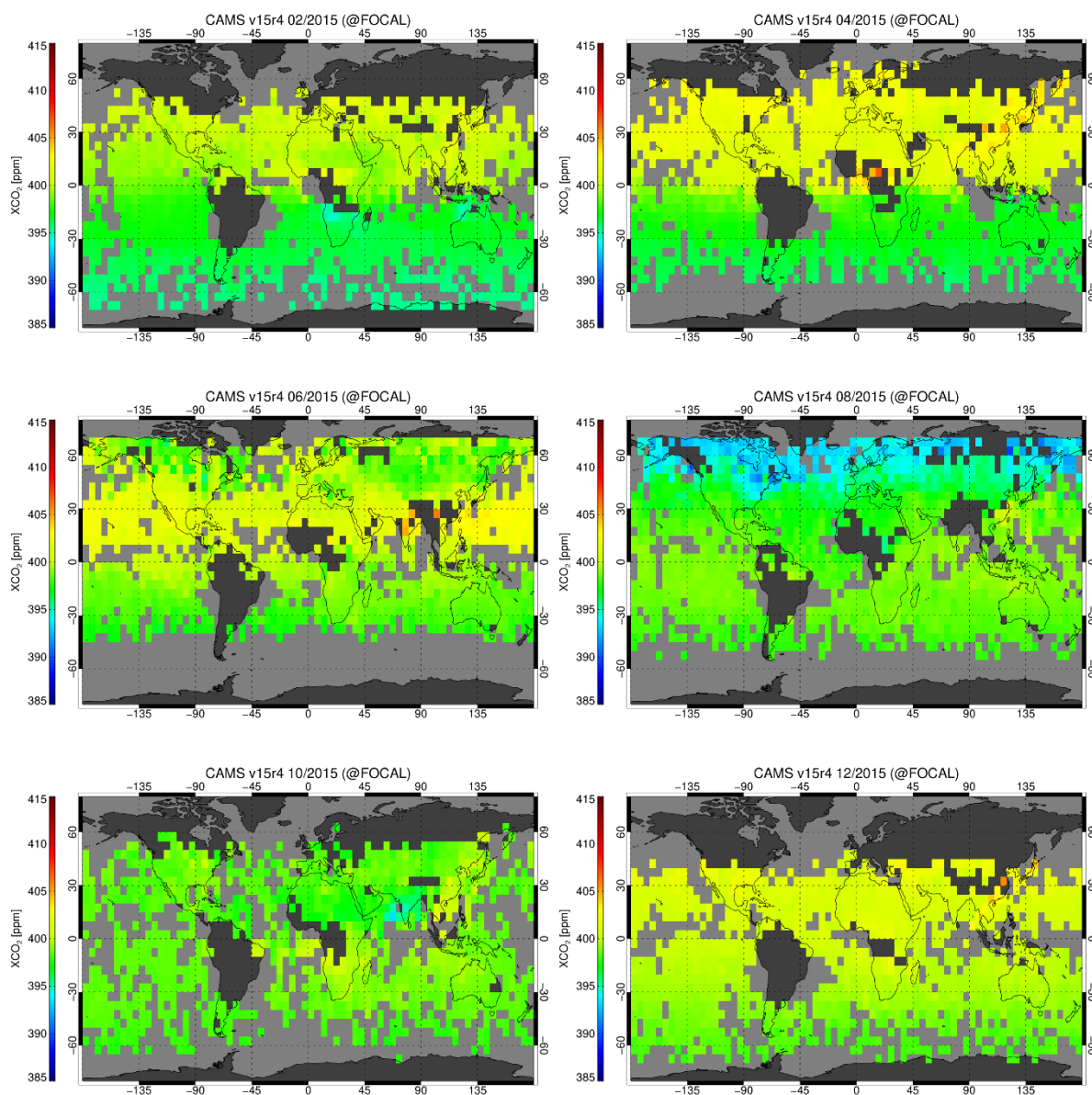
Figure 4.2: CAMS v15r4 monthly mean XCO₂ sampled as FOCAL and gridded to 5°×5°. From top/left to bottom/right: Feb., Apr., Jun., Aug., Oct., and Dec. 2015.

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4.2 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 **/E3UBv2, 2020/** 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 FOCAL 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 total, we found more than 700000 co-locations with TCCON during the five-year validation period 2015-2019.

Figure 4.3 shows the co-locations of all 22 sites with more than 250 co-locations spanning over at least 2 years. 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 **/E3UBv2, 2020/** for more details) are shown from north to south by **Figure 4.4**.

Note that a global offset of -0.15ppm has been removed from the FOCAL data set. The standard deviation of the site biases is 0.57ppm. TCCON's site-to-site consistency is about 0.4ppm (1σ) **/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 1.48ppm.

The validation results can be summarized as follows:

- Single observation random error ("precision", 1σ): 1.48ppm
- Overall bias (global offset): -0.15ppm
- Spatial bias: 0.57ppm
- Temporal (seasonal) bias: 0.37ppm
- Spatio-temporal bias ("relative accuracy"): 0.68ppm

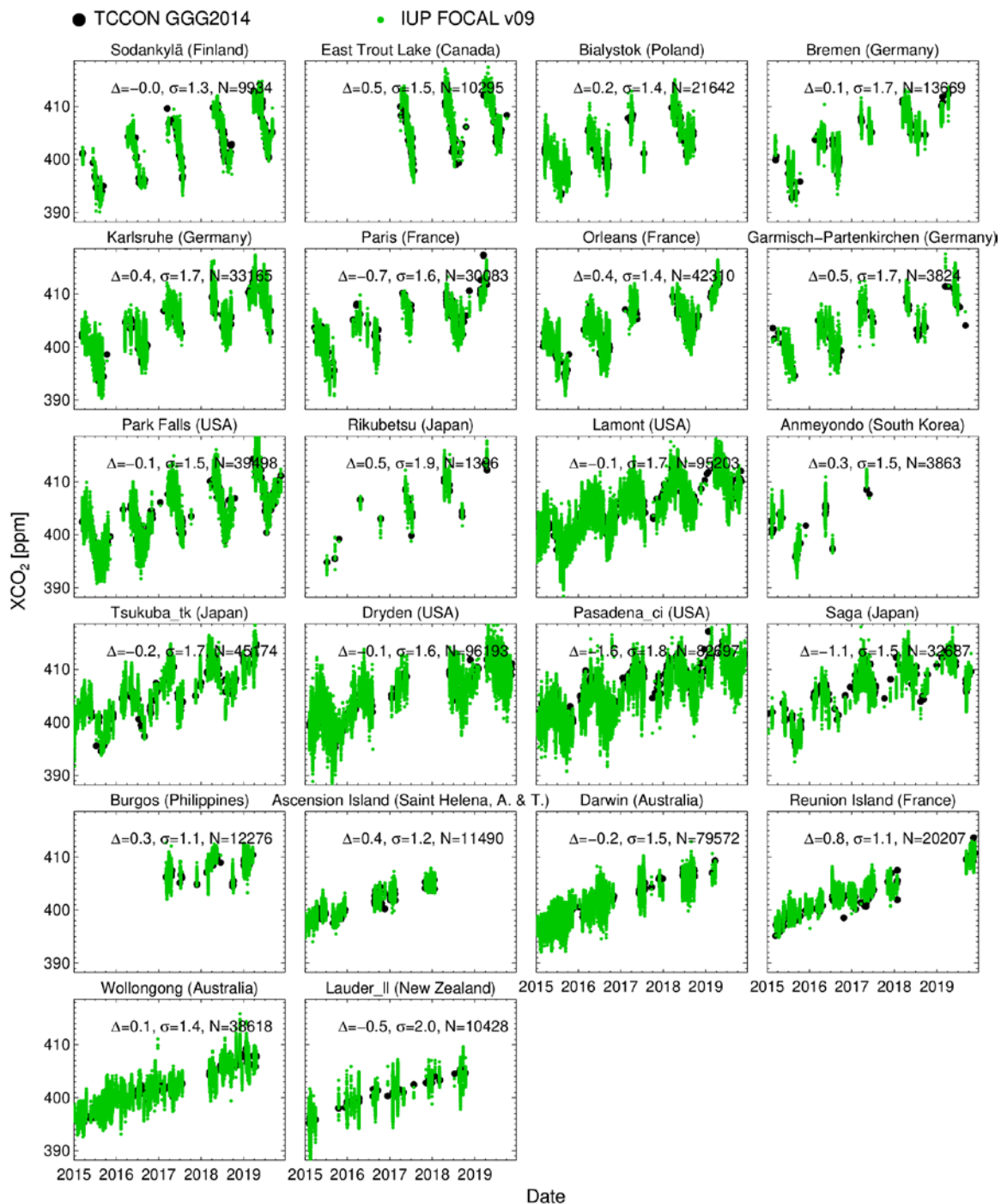|	ESA Climate Change Initiative "Plus" (CCI+)	Page 11
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Figure 4.3: Validation of single soundings of FOCAL (**green**) with co-located TCCON measurements (**black**) at all TCCON sites with more than 250 co-locations and covering a time period of at least two years. 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.
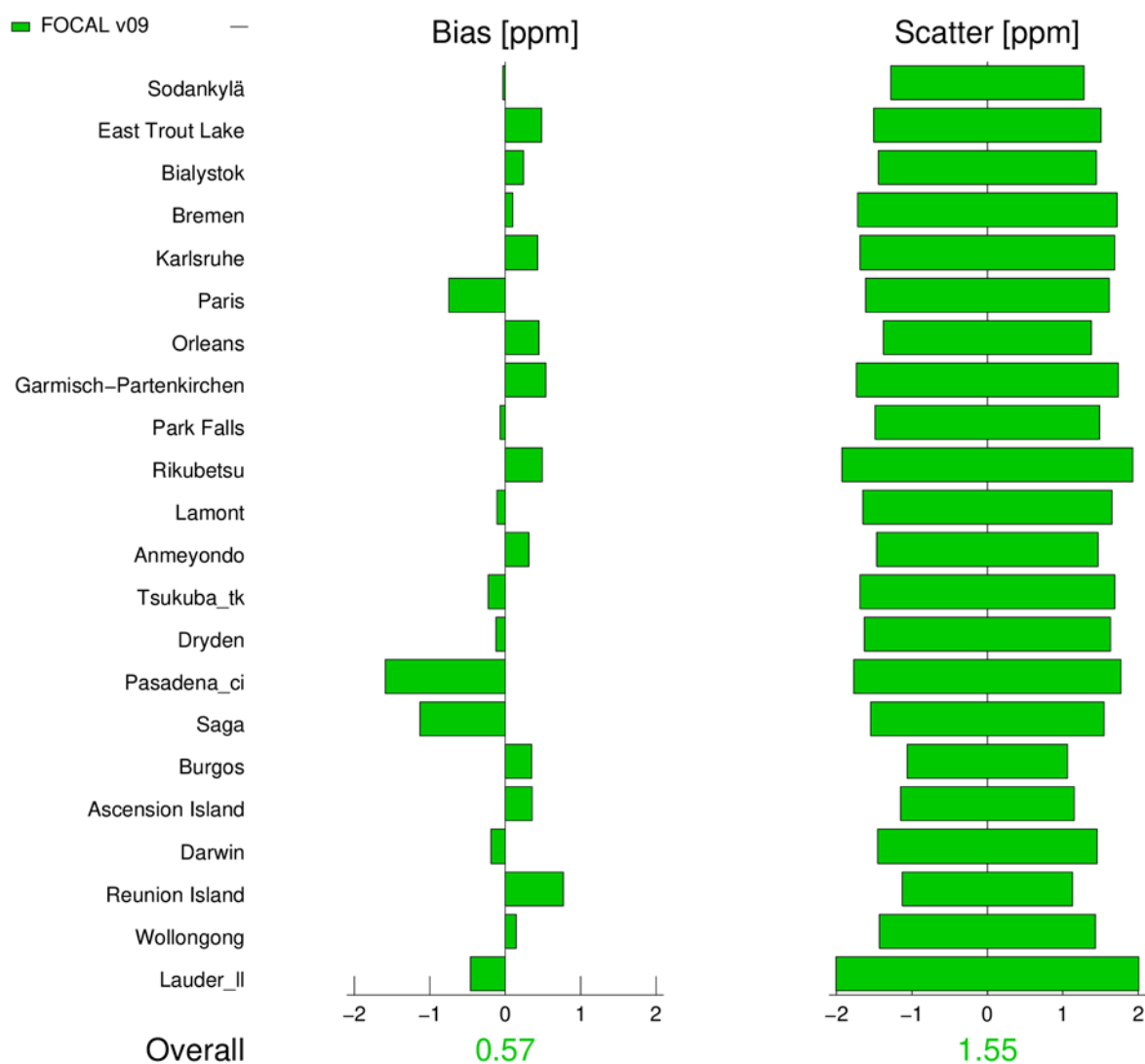
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Figure 4.4: Validation statistics for FOCALv09: bias (**left**) and scatter (**right**) per TCCON site with more than 250 co-locations and covering at least two years. The summarizing values ("overall") represent the standard deviation of the site 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 analyzed in how far variations in the reported uncertainty correspond to variations in the scatter relative to TCCON.

Summarizing the results presented in **/E3UBv2, 2020/**, we suggest that users who are interested in more realistic uncertainty estimates, shall apply the following error parameterization:

$$\sigma_{\text{corrected}}^{\text{XCO}_2} = \sigma_{\text{v09}}^{\text{XCO}_2} \cdot 1.361 - 0.133 \text{ppm} \tag{4-1}$$

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 (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) 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 in FOCAL's Product Specification Document (PSD) **/Buchwitz et al., 2014/**.

6 Acknowledgements

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