Satellite-based atmospheric CO_2 dataset (version 4.5)

Deliverable D1.5 (update for dataset v4.5)

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About 4C

Climate-Carbon Interactions in the Coming Century (4C) is an EU-funded H2020 project that addresses the crucial knowledge gap in the climate sensitivity to carbon dioxide emissions, by reducing the uncertainty in our quantitative understanding of carbon-climate interactions and feedbacks. This will be achieved through innovative integration of models and observations, providing new constraints on modelled carbon-climate interactions and climate projections, and supporting Intergovernmental Panel on Climate Change (IPCC) assessments and policy objectives.

1 Executive Summary

This deliverable describes an atmospheric carbon dioxide (CO_2) data set derived from satellite observations of radiance spectra of solar radiation reflected by the Earth's surface in the near-infrared/shortwave-infrared spectral region. We present data product XCO2_OBS4MIPS_2x2 version 4.5. XCO_2 is the column-averaged dry-air mole fraction of atmospheric CO_2, OBS4MIPS refers to the Obs4MIPs data format, and 2x2 refers to the spatial resolution of the data product (regular 2^o latitude times 2^o longitude grid). The temporal resolution is monthly. This data product has been generated by gridding (averaging) the multi-satellite / multi-algorithm merged EMMA v4.5 XCO_2 data product, where EMMA refers to the Ensemble Median Algorithm. The ensemble of input data consists of several XCO_2 data sets as derived from the satellite sensors SCIAMACHY/ENVISAT (2003-2012), Tanso-FTS/GOSAT (since 2009), OCO-2 (since 2014) and Tanso-FTS-2/GOSAT-2 (since 2019). The XCO2_OBS4MIPS_2x2 v4.5 data product covers the time period January 2003 to December 2022. It is shown in this document that the characteristics of the product depends on time (especially the spatial coverage) due to the characteristic of the underlying input satellite data used to generate the merged XCO2_OBS4MIPS_2x2 data product. It is also shown that the spatial coverage is quite sparse due to strict quality filtering (required, e.g., to avoid biases due to cloud contamination). Product XCO2_OBS4MIPS_2x2 has been compared with ground-based Total Carbon Column Observing Network (TCCON) XCO_2 retrievals. The validation results can be summarized as follows: Overall bias: 0.46 ppm (high bias), scatter (1-sigma): 1.22 ppm, the (linear) correlation with TCCON is 0.99, i.e., very good. No significant linear bias drift has been identified (0.01 ± 0.21 ppm/year), i.e., the product is very stable. The data product presented in this deliverable report is freely accessible (see respective "data availability" section) and serves as a novel constraint for the partner work packages within the 4C project. Earlier versions of this data product have already been used within 4C for this purpose.

Keywords

Atmosphere, carbon dioxide, CO_2, satellite

2 Satellite-based atmospheric CO_2 dataset (XCO2_OBS4MIPS_2x2, version 4.5)

2.1 Overview

We present an updated version of the satellite-derived data product XCO2_OBS4MIPS_2x2. XCO_2 is the column-averaged dry-air mole fraction of atmospheric CO_2, OBS4MIPS refers to the Obs4MIPs data format, and 2x2 to the spatial resolution of the data product (regular 2^o latitude times 2^o longitude grid). The temporal resolution is monthly.

This data product has been generated by gridding (averaging) the multi-satellite / multi-algorithm merged EMMA v4.5 XCO_2 data product, where EMMA refers to the Ensemble Median Algorithm **/Reuter et al., 2013, 2020/**.

In this document only a short overview about product XCO2_OBS4MIPS_2x2 is given. Details on input data sets, the EMMA method and the validation method are given in **/Reuter et al., 2020, 2023a-c/**.

In **/Reuter et al., 2023a-c/**, the generation of the EMMA input data set is described (but for an earlier version) and how it has been used to generate an XCO_2 product in Obs4MIPs format at 5^ox5^o resolution. The product described in this document, i.e., product XCO2_OBS4MIPS_2x2, is essentially identical with the 5^ox5^o resolution product, except for the higher spatial resolution (2^ox2^o) of product XCO2_OBS4MIPS_2x2.

The XCO2_OBS4MIPS_2x2 v4.5 data product covers the time period January 2003 to December 2022. This new data product is an update of the XCO2_OBS4MIPS product used in **/Gier et al., 2020/** for comparisons with climate models.

It is shown in this document that the characteristics of the product depends on time (especially the spatial coverage) due to the characteristic of the underlying input satellite data used to generate the merged XCO2_OBS4MIPS_2x2 data product. It is also shown that the spatial coverage is quite sparse due to strict quality filtering (required, e.g., to avoid biases due to cloud contamination)

Product XCO2_OBS4MIPS_2x2 has been compared with ground-based Total Carbon Column Observing Network (TCCON) XCO_2 version GGG2020 retrievals (https://tccondata.org/, last access: 28-June-2023). The validation results can be summarized as follows: Overall bias: 0.46 ppm (high bias), scatter (1-sigma): 1.22 ppm, the (linear) correlation with TCCON is 0.99, i.e., very good. No significant linear bias drift has been identified (0.01 ± 0.21 ppm/year), i.e., the product is very stable. The data product presented in this deliverable report is freely accessible (see respective “data availability” section) and serves as a novel constraint for the partner work packages within the 4C project.

2.2 Input data

The XCO2_OBS4MIPS_2x2 v4.5 data product has been obtained by gridding (averaging) the XCO2_EMMA v4.4 XCO_2 data product.

The EMMA product and its validation is described in detail in **/Reuter et al., 2023a-c/** (but for an earlier version).

In short, the EMMA product is a Level 2 data product containing for each satellite footprint (i.e., single observation) detailed information on geolocation (latitude, longitude), time, XCO_2, XCO_2 uncertainty, XCO_2 averaging kernel, etc. The EMMA product has been generated using an ensemble of individual satellite sensor data products, i.e., the EMMA product is a multi-sensor / multi-algorithm merged data product. The satellite sensors are (see also **/Reuter et al., 2020/** for details):

- SCIAMACHY / ENVISAT (ESA; 2003-2012)
- TANSO-FTS / GOSAT (JAXA/NIES, since 2009)
- OCO-2 (NASA, since 2014)
- TANSO-FTS-2 / GOSAT-2 (JAXA/NIES, since 2019)

2.3 Algorithm

The algorithm which has been used to generate the XCO2_OBS4MIPS_2x2 v4.5 data product is essentially the same algorithm as used to generate the XCO2_OBS4MIPSv4.4 data product **/Reuter et al., 2023a/**, which has a spatial resolution of 5^ox5^o.

2.4 Product description

Product XCO2_OBS4MIPS_2x2 v4.5 consists of a single NetCDF file:

xco2_c3s_l3_v45_200301_202212_2x2.nc (size: 365 MB)

The product is self-explaining as it contains all relevant information (description of all variables incl. corresponding units, etc.). A detailed product description including product format is given in **/Reuter et al., 2023c/.** For data access see Sect. 2.7.

2.5 Maps and time series

In this section, we show how product XCO2_OBS4MIPS_2x2 “looks like”.

Figure 1 presents an overview about this product in terms of time series and spatial maps. As can be seen, XCO_2 increases with time (primarily due to burning of fossil fuels) and shows a seasonal cycle, especially over the northern hemisphere (primarily due to uptake and release of atmospheric CO_2 by terrestrial vegetation).

As can be seen from the spatial maps, the spatial coverage depends on time. This is due to the different characteristics of the underlying satellite data (see, e.g., **/Reuter et al., 2020/** for details).

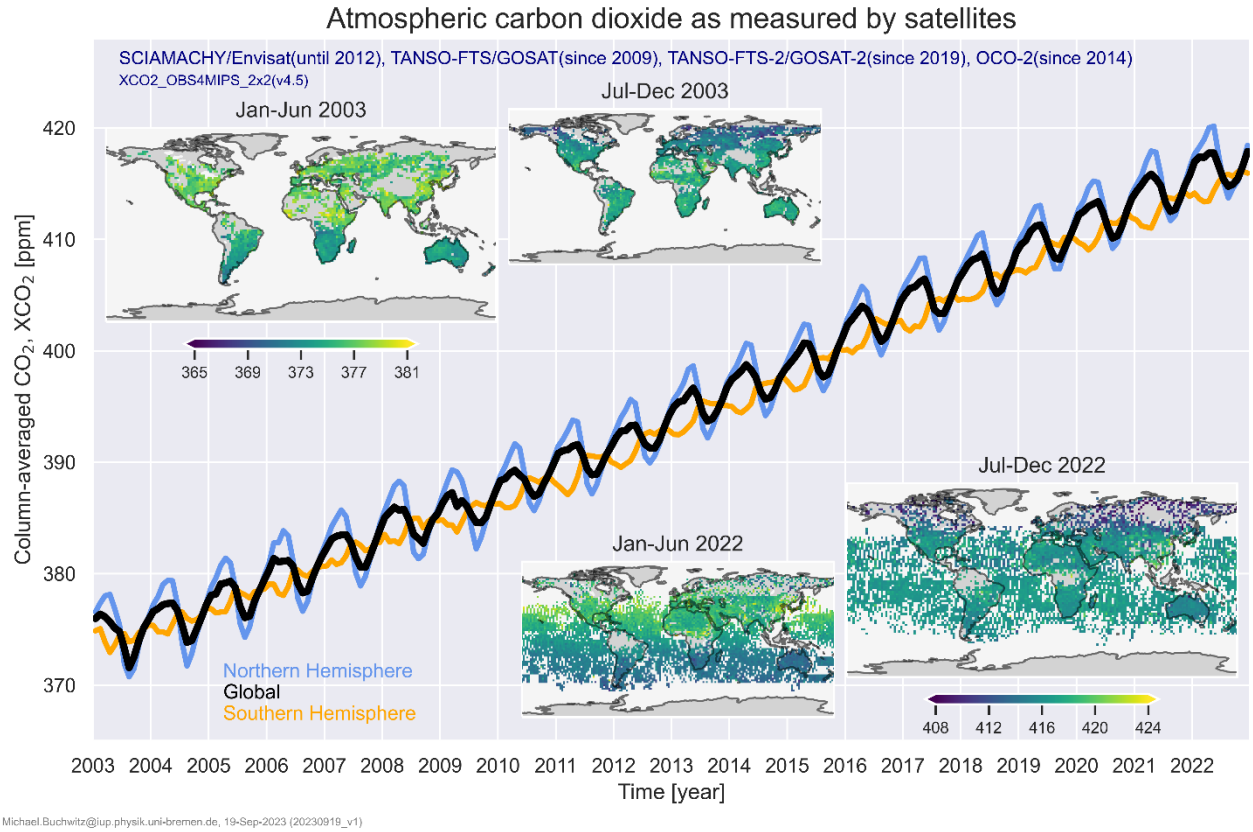


Figure 1: Overview of product XCO2_OBS4MIPS_2x2 in terms of time series for three latitude bands and half-yearly global maps.

Figure 2 (a) to (d) shows XCO_2 and related quantities for August in different years: (a) 2003, (b) 2010, (c) 2015, (d) 2022. The top left maps show XCO_2, the top right maps show the (reported) XCO_2 uncertainty (1-sigma; standard error), the bottom left maps show the number of observations per 2^ox2^o grid cell and the bottom right maps show the standard deviation of the (input) Level 2 observations within each grid cell. (b) to (d): as (a) but for 2010, 2015, 2022.

Figure 2 (a) shows the data product for August 2003. This part of the product is only based on a single XCO_2 data product from one satellite instrument, namely SCIAMACHY on ENVISAT, retrieved using the BESD algorithm (see **/Reuter et al., 2020, 2023a-c/** for details). Data coverage is limited to observations over land.

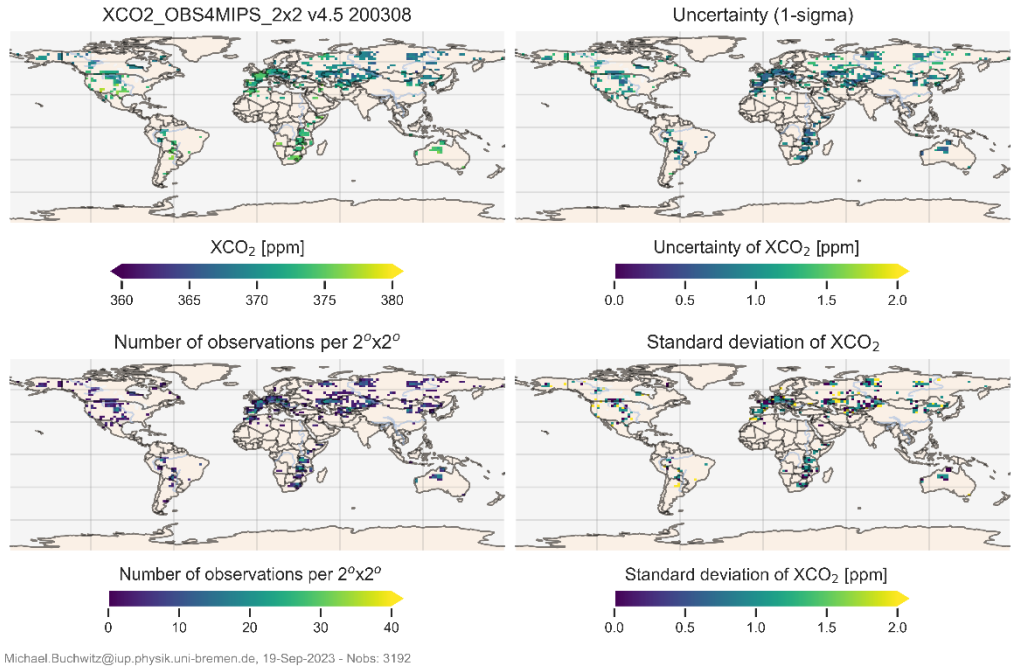
Figure 2 (b) shows the data product for August 2010. Here in addition to the SCIAMACHY/BESD product an ensemble of GOSAT product has been used in addition (see **/Reuter et al., 2020, 2023a-c /** for details). As can be seen, there is now also some ocean coverage.

Figure 2 (c) shows the data product for August 2015, based on an ensemble of GOSAT and OCO-2 products (see **/Reuter et al., 2020, 2023a-c /** for details).

Figure 2 (d) shows the data product for August 2022, based on an ensemble of GOSAT, GOSAT-2 and OCO-2 products (see **/Reuter et al., 2020, 2023a-c /** for details but related to an earlier version).

The lat/lon 10^ox10^o block like structure of the data visible most clearly in Figures 2 (c) and (d) is a feature of the underlying Ensemble Median Algorithm (EMMA) algorithm (explained in detail in **/Reuter et al., 2013/** and /**Reuter et al., 2020, 2023a-c**/), which selects from the ensemble of Level 2 products input data a single product (the median; after harmonization of all products in terms of bringing them to the same CO_2 a priori) for each month and each 10^ox10^o lat/lon region and then essentially transferring all information contained in the original Level 2 products (not only XCO_2 but also its uncertainty, it averaging kernels, etc.) into the EMMA Level 2 product files, which contain the merged products. The EMMA Level 2 product files are then gridded and stored in Obs4MIPS format **/Reuter et al., 2020/** to generate the product described in this document.

(a)



(b)

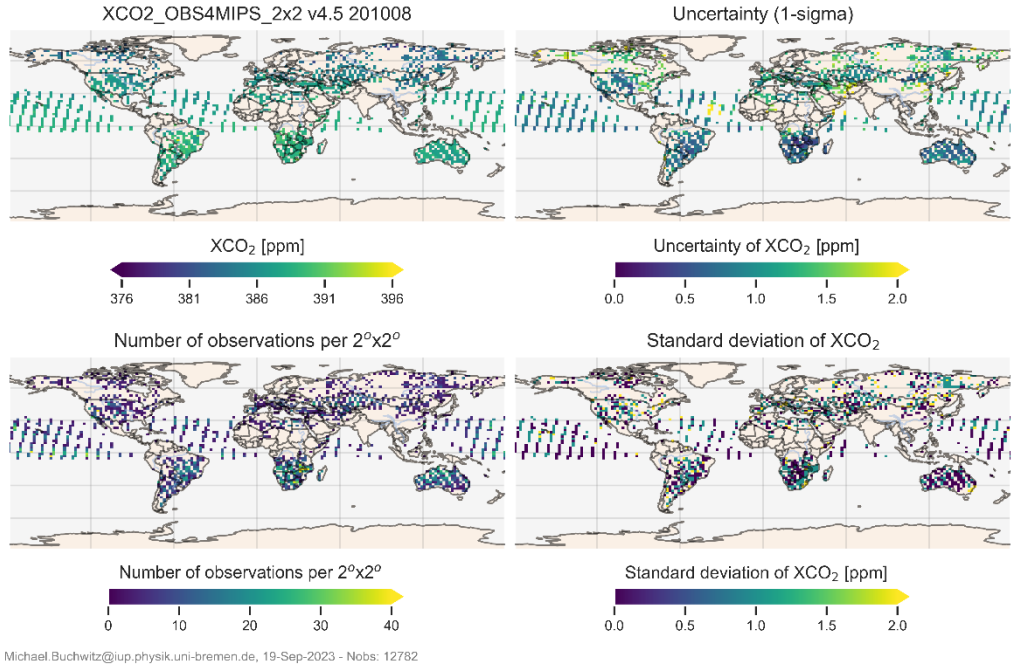
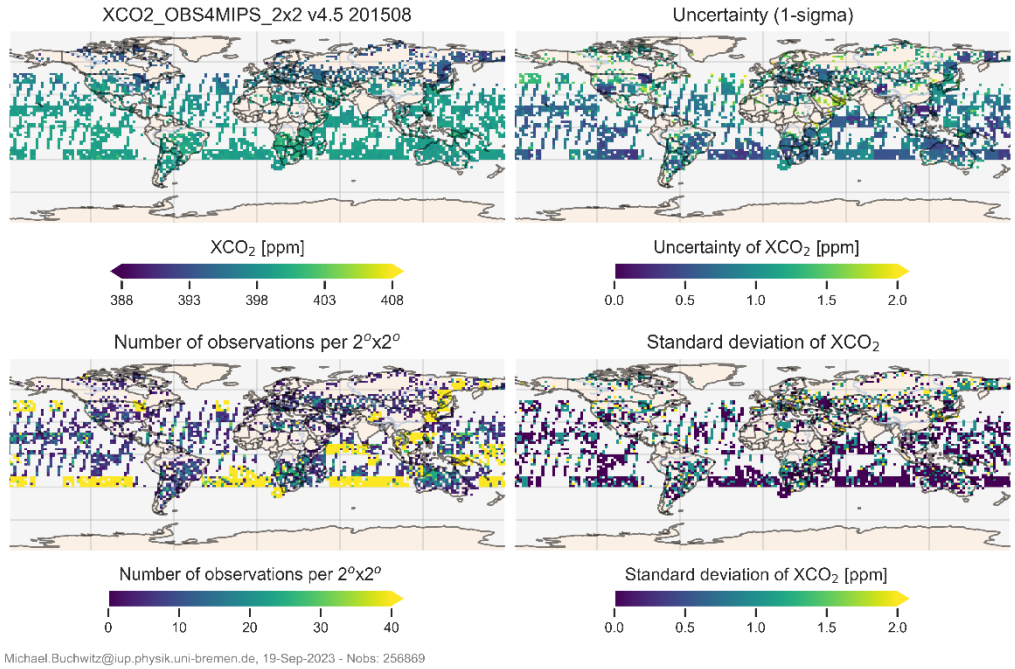


Figure continued on next page.

(c)



(d)

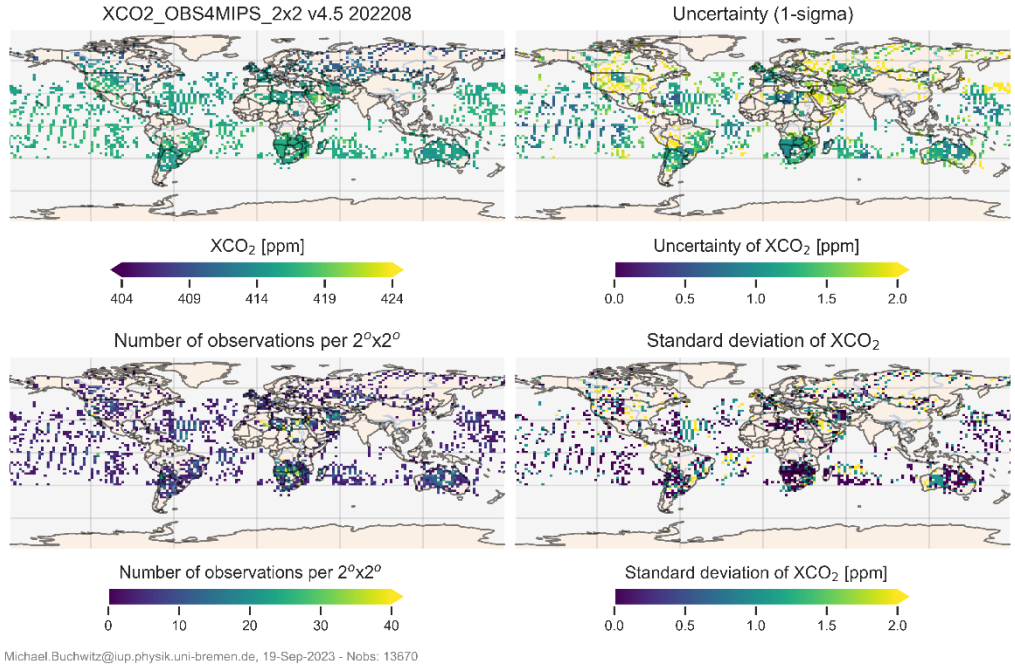


Figure 2: (a) XCO_2 and related quantities for August 2003. Top left: XCO_2. Top right: XCO_2 uncertainty (1-sigma; standard error). Bottom left: Number of observations per 2°x2° grid cell. Bottom right: standard deviation of the (input) Level 2 observations within each grid cell. (b) to (d): as (a) but for 2010, 2015, 2022.

2.6 Validation

Product XCO2_OBS4MIPS_2x2 has been compared with ground-based Total Carbon Column Observing Network (TCCON) XCO_2 retrievals **/Wunch et al., 2011/** using version GGG2020 (https://tccondata.org/, last access: 28-June-2023) **/Laughner et al., 2021/**. The overall validation results are shown in Fig. 3. The validation method is explained in **/Reuter et al., 2020/**.

The validation results can be summarized as follows: Overall bias: 0.46 ppm (high bias), scatter (1-sigma): 1.22 ppm, the (linear) correlation with TCCON is 0.99, i.e., very good. No significant linear bias drift has been identified (0.01 ± 0.21 ppm/year), i.e., the product is very stable.

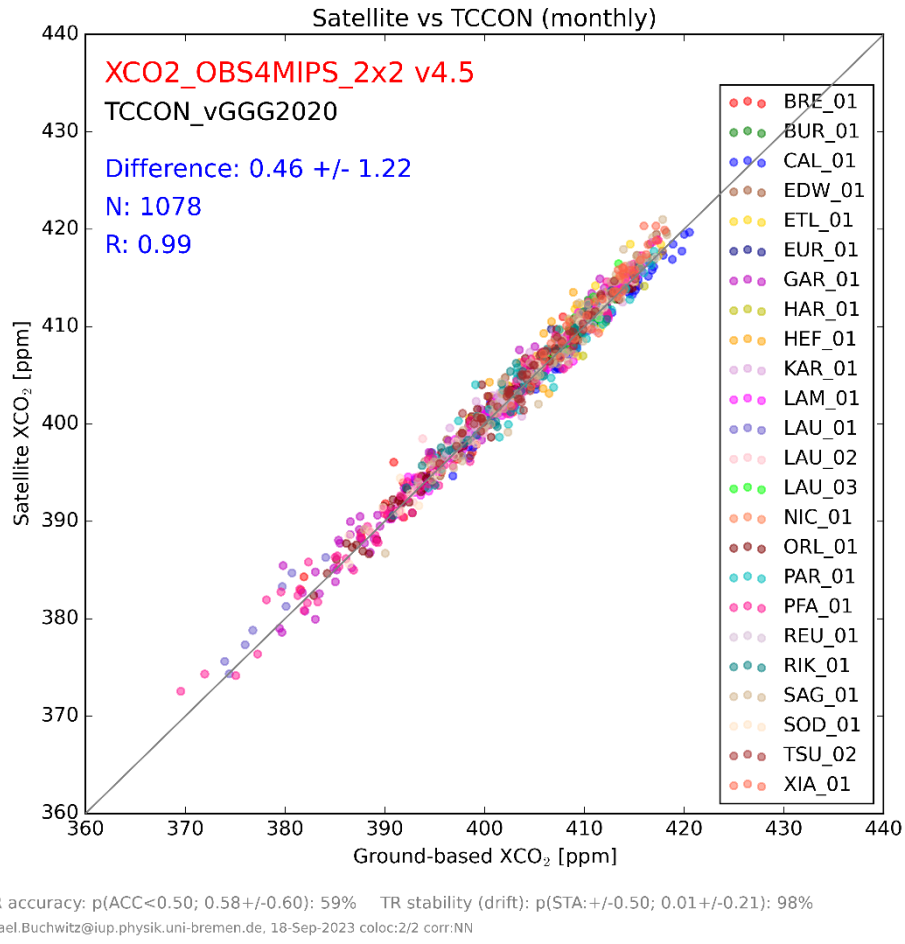


Figure 3: Validation of product XCO2_OBS4MIPS_2x2 version 4.5 by comparison with TCCON ground-based XCO_2 observations. Each symbol denotes a comparison of a monthly value at a given TCCON sites (N = 1078 combinations; each color corresponds to a certain TCCON site; the used TCCON sites are listed on the right hand side).

2.7 Data availability

Access and use of data product XCO2_OBS4MIPS_2x2 version 4.5 does not require registration and is free of charge. However, if the data product is used for any type of presentation or publication it is required to add the following acknowledgement:

“The XCO2_OBS4MIPS_2x2 version 4.5 data product has been generated by University of Bremen using funding from the European Commission H2020 project 4C (Climate-Carbon Interactions in the Current Century, Grant Agreement No. 821003).”

Information about the underlying (earlier version) satellite Level 2 input data and the generation of a corresponding XCO2_OBS4MIP product at 5ºx5º resolution can be obtained from this peer-reviewed publication:

Reuter, M., Buchwitz, M., Schneising, O., Noel, S., Bovensmann, H., Burrows, J. P., Boesch, H., Di Noia, A., Anand, J., Parker, R. J., Somkuti, P., Wu, L., Hasekamp, O. P., Aben, I., Kuze, A., Suto, H., Shiomi, K., Yoshida, Y., Morino, I., Crisp, D., O'Dell, C., Notholt, J., Petri, C., Warneke, T., Velazco, V., Deutscher, N. M., Griffith, D. W. T., Kivi, R., Pollard, D., Hase, F., Sussmann, R., Te, Y. V., Strong, K., Roche, S., Sha, M. K., De Maziere, M., Feist, D. G., Iraci, L. T., Roehl, C., Retscher, C., and Schepers, D., Ensemble-based satellite-derived carbon dioxide and methane column-averaged dry-air mole fraction data sets (2003-2018) for carbon and climate applications, Atmos. Meas. Tech., 13, 789-819, https://doi.org/10.5194/amt-13-789-2020, 2020.

Data product XCO2_OBS4MIPS_2x2 version 4.5 can be downloaded from here (single NetCDF file, 365 MB):

https://www.iup.uni-bremen.de/carbon_ghg/data/xco2_c3s_l3_v45_200301_202212_2x2.nc

2.8 Acknowledgements

This research has received funding from the European Union (EU) Horizon 2020 (H2020) research and innovation programme project 4C (formerly CCiCC) grant agreement number 821003.

The generation of the presented satellite data product and its validation would not have been possible without the availability of several input data sets and funding from other projects and agencies: The generation of the EMMA Level 2 input data set and the corresponding data analysis has been funded primarily by the EU via the Copernicus Climate Change Service (C3S, https://climate.copernicus.eu/) managed by the European Centre for Medium-range Weather Forecasts (ECMWF). That work strongly benefited from additional funding by the European Space Agency (ESA) via ESA's Climate Change Initiative (CCI, http://www.esa-ghg-cci.org/) projects GHG-CCI/GHG-CCI+. The further development of the FOCAL retrieval algorithm used to generate the OCO-2/FOCAL XCO2 input data product would not have been possible without co-funding from the EU H2020 projects CHE (Grant Agreement No. 776186) and VERIFY (Grant Agreement No. 776810). We thank several space agencies for making available satellite Level 1 (L1) input data: ESA/DLR for SCIAMACHY L1 data, JAXA for GOSAT Level 1B data and NASA for the OCO-2 L1 data product. We also thank ESA for making the GOSAT L1 product available via the ESA Third Party Mission (TPM) archive. We thank NIES for the operational GOSAT XCO2 and XCH4 Level 2 products and the NASA team for the GOSAT and OCO-2 ACOS Level 2 XCO_2 products. TCCON data were obtained from the TCCON Data Archive, hosted by CaltechDATA, California Institute of Technology (https://tccondata.org/).

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/Reuter et al., 2023b/ Reuter, M., Buchwitz, M., and Schneising-Weigel, O.: Product Quality Assessment Report (PQAR) – ANNEX D for products XCO2_EMMA, XCH4_EMMA, XCO2_OBS4MIPS, XCH4_OBS4MIPS (v4.4, 01/2003-12/2021), Technical Report Copernicus Climate Change Service (C3S), version 6.3, 02-Mar-2023, pp. 52, in review, final approved version will be made available via Copernicus Climate Data Store (https://cds.climate.copernicus.eu/), 2023.

/Reuter et al., 2023c/ Reuter, M., Buchwitz, M., and Schneising-Weigel, O.: Product User Guide and Specification (PUGS) – ANNEX D for products XCO2_EMMA, XCH4_EMMA, XCO2_OBS4MIPS, XCH4_OBS4MIPS (v4.4, 01/2003-12/2021), Technical Report Copernicus Climate Change Service (C3S), version 6.2, 14-Feb-2023, pp. 33, in review, final approved version will be made available via Copernicus Climate Data Store (https://cds.climate.copernicus.eu/), 2023.

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