Report on CO_2 and CH_4 Satellite Datasets: TROPOMI XCH_4 Comparison

DELIVERABLE 1.1

Author(s):	T. Hilbig, O. Schneising-Weigel, H. Bösch
Date of submission:	14-11-2023
Version:	1.0
Responsible partner:	University of Bremen
Deliverable due date:	31-06-2023
Dissemination level:	Public

Call:	HORIZON-CL5-2022-D1-02
Topic:	Climate Sciences and Responses
Project Type:	Research and Innovation Action
Lead Beneficiary:	NILU - Norsk Institutt for Luftforskning

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

Document History

Version	Date	Comment	Modifications made by
0.1	16-11-2023	First Draft	T. Hilbig, O. Schneising-Weigel, H. Bösch
0.2	21-11-2023	Internal review	R. Thompson
0.3	08-12-2023	Revision	H. Bösch, T. Hilbig
1.0	11-12-2023	Submitted to Commission	

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

Summary

This report provides an assessment of the CH_4 column data from the TROPOspheric Monitoring Instrument (TROPOMI) on board the Sentinal-5 Precursor satellite. In a later report, we will also include other CH_4 column sensors and CO_2 column instruments.

Three TROPOMI XCH_4 data products have been inter-compared and assessed against ground-based reference data from the TCCON network. The datasets include the operational, reprocessed data product RPRO version 02.04.00, the SRON RemoTeC-S5P XCH_4 scientific product version 19.446 and the University of Bremen WFM-DOAS data product version 1.8. The assessment has been carried out globally and for the European domain.

As expected, we find that the operational and the SRON data products agree very well with each other. This is expected as both are based on the same retrieval algorithm. The WFMD datasets generated by IUP Bremen also agree well with the two other datasets. There is a pronounced difference in coverage and number of data points with the WFMD product usually showing higher data volume and better coverage. Differences in the retrieved CH_4 values between WFMD and the two other datasets are more pronounced for the European domain than globally. Thus, it can be expected that surface flux inversions on a European domain will differ depending on the chosen dataset.

Differences between the WFMD and the operational dataset are also noticeable when observing emission plumes in single overpasses. Here, the often-better coverage of WFMD offers better opportunities for detection of emission plumes. Also, the magnitude of CH_4 in the columns of these single overpasses can differ which can then lead to differences in the quantification of emissions.

The comparison to European TCCON sites of the TROPOMI datasets show high correlation coefficients and low biases for all three datasets, with lowest biases obtained for the WFMD dataset (2.8 to 12.2 ppb) and the highest for the operational dataset (8.3 ppb to 17.2 ppb). Overall, the TCCON comparison demonstrates a high quality of the TROPOMI CH_4 retrievals.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

TABLE OF CONTENTS

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

1. Introduction

Methane (CH_4) total atmospheric columns are measured by several satellite missions (GOSAT/-2, TROPOMI). GOSAT provides a continuous data record since 2009, which is now complemented by GOSAT-2. GOSAT/-2 has a coarse sampling pattern where individual soundings with a diameter of 10 km are spaced out by 100-200 km. Thus, GOSAT/-2 data is useful for regional scale flux inversions but is not well suited for more localised anthropogenic emission sources.

The more recently launched (2017) TROPOspheric Monitoring Instrument (TROPOMI) on board the Sentinal-5 Precursor satellite provides much superior coverage. It provides measurements with a spatial resolution of 7km × 7km/5km and daily global coverage. Besides the more conventional surface flux inversions (e.g. Lunt et al., 2021, Tsuruta et al., 2023), this has allowed the application of TROPOMI CH_4 data to investigate localised CH_4 sources (Schneising et al., 2020, Maasakkers et al, 2022).

In this report, we evaluate the different TROPOMI CH_4 datasets that are generated by different retrievals: the operational TROPOMI product, the SRON data product and the IUP Bremen WFDM data products. The evaluation includes an inter-comparison of the data products and an assessment against ground-based reference measurements from the TCCON network for a global and European domain.

This project has received funding from the European Union's Horizon Europe
research and innovation programme under grant agreement No 101081395

2. Datasets

2.1 TROPOMI L2 XCH_4

2.1.1. Operational – reprocessed data product RPRO version 02.04.00

Retrieval:

The S5P operational CH_4 retrieval algorithm is based on RemoTeC. The methane total column-averaged dry-air mole fraction (XCH_4) is retrieved from TROPOMI measurements of sun-light backscattered by Earth's surface and atmosphere in the NIR and SWIR. The S5P RemoTeC algorithm uses the full-physics approach that simultaneously retrieves the amount of atmospheric CH_4 and the physical scattering properties of the atmosphere. (Lorente et al., 2021)

Structure and version of the data set:

The data product (http://doi.org/10.5270/S5P-3lcdqiv) is stored as NetCDF4 file containing both the data and the metadata for the product. It is stored as a single file per orbit. In this analysis data version 02.04.00 is used.

Product Identifier: L2__CH4___

Example filename:
S5P_RPRO_L2__CH4____20180501T151424_20180501T165554_02841_03_020400_20221107T155403.nc

Variables used in this analysis:

Name/Data	Symbol	Units	Description	Data type	Dimension
longitude, longitude_bounds	lon	degree	SWIR pixel longitude (center & corners)	float	1,4
latitude, latitude_bounds	lat	degree	SWIR pixel latitude (center & corners)	float	1,4
methane_mixing_ratio_bias_corrected	XCH4	ppb	bias corrected XCH_4	float	1
qa_value	QA value for CH4			int	1

Table 1: Selected contents of the output product, as used in this analysis (S5P ATBD, 2022).

Applied filter and bias correction:

Following the recommendations for data usage (S5P MPC Product Readme Methane V02.05.00):

- The TROPOMI XCH_4 bias corrected data (methane_mixing_ratio_bias_corrected) is used. The bias correction is based on the retrieved surface albedo to further improve the accuracy and the fitness for purpose of the TROPOMI CH_4 product (S5P ATBD, 2022).
- A quality assurance value qa_value > 0.5 has been chosen. It includes, since version 2.3.1, pixels both over land and over ocean. Filtering on qa_value > 0.5 does not remove all pixels considered bad. Some pixels with too low methane concentrations are still present.

Known Data Quality Issues (S5P MPC Product Readme Methane V02.05.00):

- Single TROPOMI overpasses show stripes of erroneous CH_4 values in the flight direction.
- Uncertainties estimation: Uncertainties for the XCH_4 are only based on the single sounding precision due to measurement noise. For applications requiring an overall uncertainty estimate, it is proposed

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

to multiply the provided error by a factor 2, which reflects the scatter of single sounding errors in the TCCON validation.

2.1.2. SRON RemoTeC-S5P XCH_4 scientific product version 19.446

Retrieval:

The SRON scientific product is based on the RemoTeC-S5P XCH4 retrieval algorithm. Differences between the operational and SRON product (SRON Product User Guide, 2022) are:

- Altitude DEM: SRTM 15” (SRON), GMTED2010 S5P (Operational)
- Meteorology: ECMWF reanalysis (SRON), ECMWF forecast (Operational)

Note that the impact of the difference in meteorology is very small. The impact of the change in the DEM is significant and is mainly observed around Greenland.

Structure and version of the data set:

The data is provided in netCDF format and stored in a single file per orbit. It can be freely downloaded via the ftp site ftp://ftp.sron.nl/ open-access-data-2/TROPOMI/tropomi/

Example Filename: s5p_l2_ch4_0446_<orbit number>.nc

Within this analysis the latest available data version 19_446 was used.

Applied filter and bias correction (SRON Product User Guide, 2022):

- In accordance with the operational data product, the quality assurance value qa_value > 0.5 was chosen.
- Filter setting used for the SRON scientific product are the same as applied for the operational data product.
- TROPOMI CH_4 bias corrected data has been used.

Variables used in this analysis:

Name/Data	Symbol	Units	Description	Data Type	Dimension
group: target_product					
xch4_corrected	XCH4	ppb	bias corrected XCH4	float	1
group: diagnostics					
qa_value	QA value for CH4			float	1
group: instrument					
longitude_center	lon	degree	SWIR pixel longitude (center)	float	1
latitude_center	lat	degree	SWIR pixel latitude (center)	float	1
longitude_corners		degree	SWIR pixel longitude (corners)	float	4
latitude_corners		degree	SWIR pixel longitude (corners)	float	4

Table 2: Selected contents of the output product, as used in this analysis.

This project has received funding from the European Union’s Horizon Europe research and innovation programme under grant agreement No 101081395

2.1.3. University of Bremen WFM-DOAS data product version 1.8

Retrieval:

The Weighting Function Modified Differential Optical Absorption Spectroscopy (WFMD) retrieval algorithm simultaneously retrieves the atmospheric column-averaged dry-air mole fractions XCH_4 from TROPOMI's radiance measurements in the SWIR spectral range. It is a linear least-squares method based on scaling (or shifting) pre-selected atmospheric vertical profiles. The vertical columns of the desired gases are determined from the measured sun-normalised radiance by fitting a linearised radiative transfer model to it (Schneising et al., 2019, 2023).

Structure and version of the data set:

The data is provided in netCDF format and stored in one file per day. It can be downloaded from: https://www.iup.uni-bremen.de/carbon_ghg/products/tropomi_wfmd/. We have used data version 1.8. This version includes

- Implementation of a dedicated de-striping filter, which optimally preserves the original spatial trace gas features.
- optimised quality filter reducing the number of outliers.
- improved digital elevation model, this reduces the pseudo-noise component, resulting in an improved random error.

Example Filename: ESACCI-GHG-L2-CH4-CO-TROPOMI-WFMD-20180501-fv3.nc

Applied filter and corrections:

- Quality flag = 0 ("good") was applied.
- Post-processing: machine-learning-based quality filter. In v1.8, the cloud filtering over the Arctic ocean is considerably improved.

Variables used in this analysis:

Name/Data	Symbol	Unit	Description	Data Type	Dimension
longitude	lon	degree north	centre longitude of the measurement, -90. to 90.	float	1
latitude	lat	degree east	centre latitude of the measurement -180. to 180.	float	1
longitude_corners	lon	degree north	corner longitudes of the measurement, -90. to 90.	float	4
latitude_corners	lat	degree east	corner latitudes of the measurement, -180. to 180.	float	4
xch4	XCH4	ppb	XCH_4	float	1
xch4_quality_flag	QA value for CH_4		0 - "good quality" 1 - "potentially bad quality"	int	1

Table 3: Selected contents of the output product, as used in this analysis.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

2.2. Total Carbon Column Observing Network (TCCON)

The Total Carbon Column Observing Network (TCCON) is a network of ground-based Fourier transform spectrometers. The first instrument was installed in 2004 at Park Falls, USA. The network has expanded to more than 25 operational stations worldwide. It measures direct solar spectra in the NIR to SWIR and provides atmospheric column-averaged dry-air mole fractions of CO_2, CH_4, CO, N_2O, H_2O, HDO, and HF (Wunch et al., 2015). The TCCON error assessment for the GGG2020 release estimates a total error of 0.4% (7 ppb) for CH_4 (Laughner et al., 2023).

Structure and version of the data set

The data is provided in netCDF format and can be downloaded from http://tccondata.org/. It contains the retrieved values, and ancillary data like surface pressure, temperature, averaging kernels and a priori profiles. (https://tccon-wiki.caltech.edu/Main/DataDescriptionGGG2020).

For this analysis, only European sites were selected, as summarised in Table 4: European TCCON sites used in the comparison; https://tccondata.org/ (last access: 08.11.2023 for Sodankylä site, 01.08.2023 other sites) The current data version is GGG2020.

Site	Start Date	End Date	Version	Reference
Bremen	2009-01-06	2021-06-24	GGG2020.R0	Nothold et al., 2022
Garmisch	2007-07-18	2023-05-04	GGG2020.R0	Sussmann et al., 2023
Harwell	2021-05-30	2023-09-30	GGG2020.R0	Weidmann et al., 2023
Karlsruhe	2014-01-15	2023-06-26	GGG2020.R1	Hase etal., 2023
Orléans	2009-09-06	2022-10-12	GGG2020.R0	Warneke et al., 2022
Paris	2014-09-23	2022-06-29	GGG2020.R0	Té et al., 2022
Sodankylä	2009-05-16	2023-05-30	GGG2020.R0	Kivi et al., 2022

Table 4: European TCCON sites used in the comparison; https://tccondata.org/ (last access: 08.11.2023 for Sodankylä site, 01.08.2023 other sites)

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

3. Analysis/Comparison of TROPOMI XCH_4 data products

3.1. Methodology

Three different TROPOMI XCH_4 data products, as introduced in 0, were compared. For this comparison, the data has been converted to monthly means and gridded on a 0.5° × 0.5° grid. The resulting global and European comparison maps together with the standard deviation, as a measure of the variation of the daily means, and the number of measurements available per grid box are presented in Section 3.2. Additionally, we derived the number of days with sufficient measurements per grid box and months. The limit was chosen to be 10 data points. Direct comparison of the WFMD and the SRON scientific product with the operational data set are given as scatterplots. Note that potential differences in a priori CH_4 profiles used in the different retrievals have not been corrected for this comparison.

3.2. Results and Discussion

The following sections show example maps for winter and summer months, February 2020 and August 2020 respectively, on the global scale and for Europe. The complete set of Figures for the full TROPOMI record data record from May 2018 to May 2022 is available from https://nc.uni-bremen.de/index.php/s/AZNgkQtrHrZSbgf.

3.2.1. Global Maps of monthly mean XCH_4

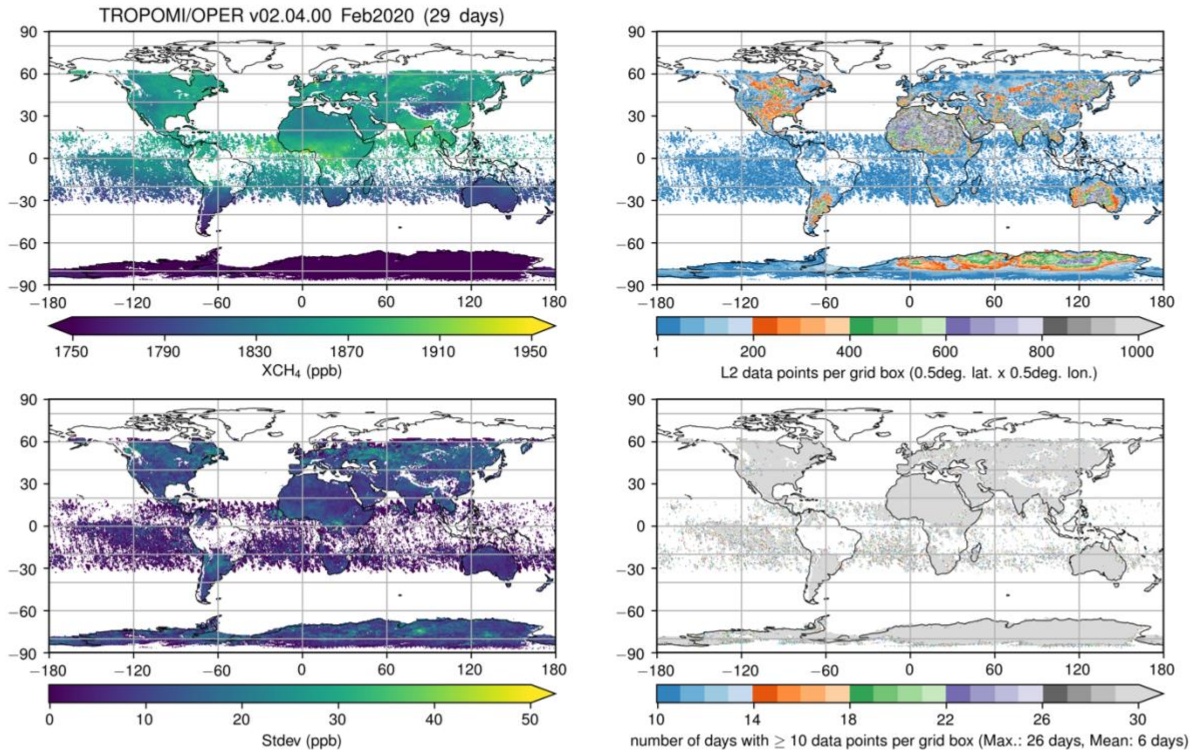


Figure 1: Left: Monthly averages of the operational (reprocessed) data product RPRO version 02.04.00 (top panel) and corresponding standard deviation for February 2020 (bottom panel). Right: Number of measurements contained in monthly mean as shown in the left panel (top panel) and number of days with more than 10 measurements per grid cell (bottom panel).

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

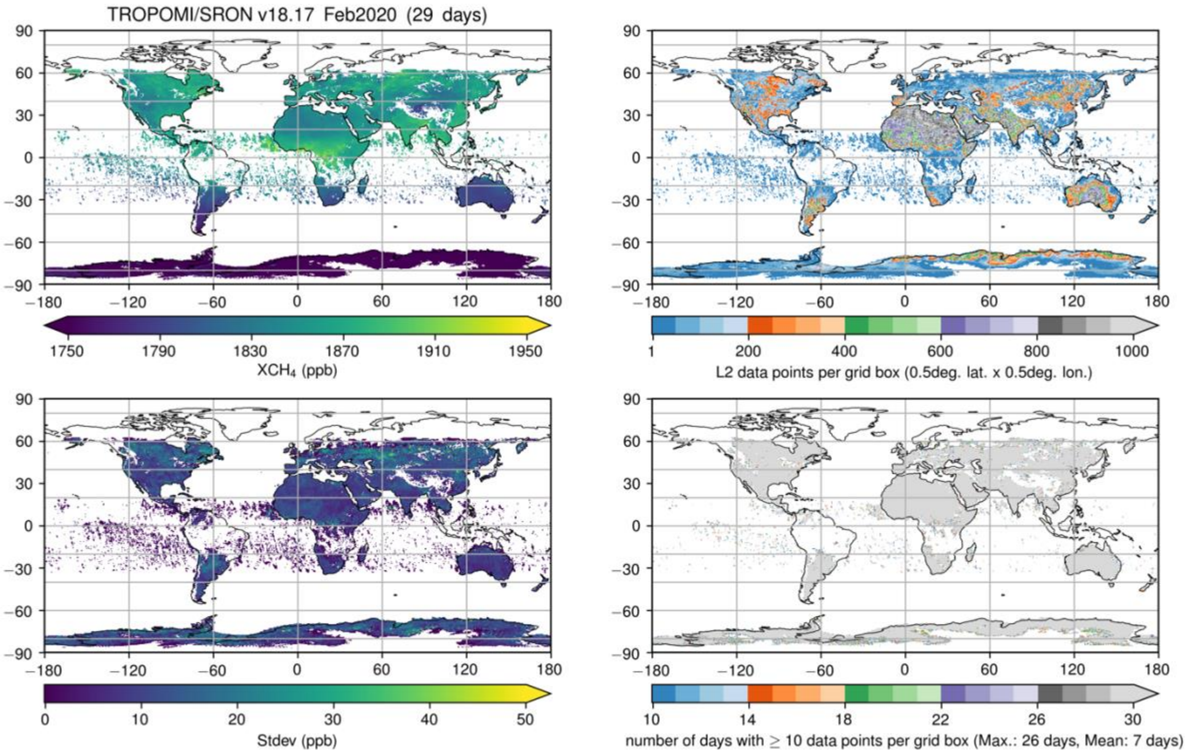


Figure 2: As Figure 1 but for SRON RemoTeC-S5P XCH4 scientific product version 19.446

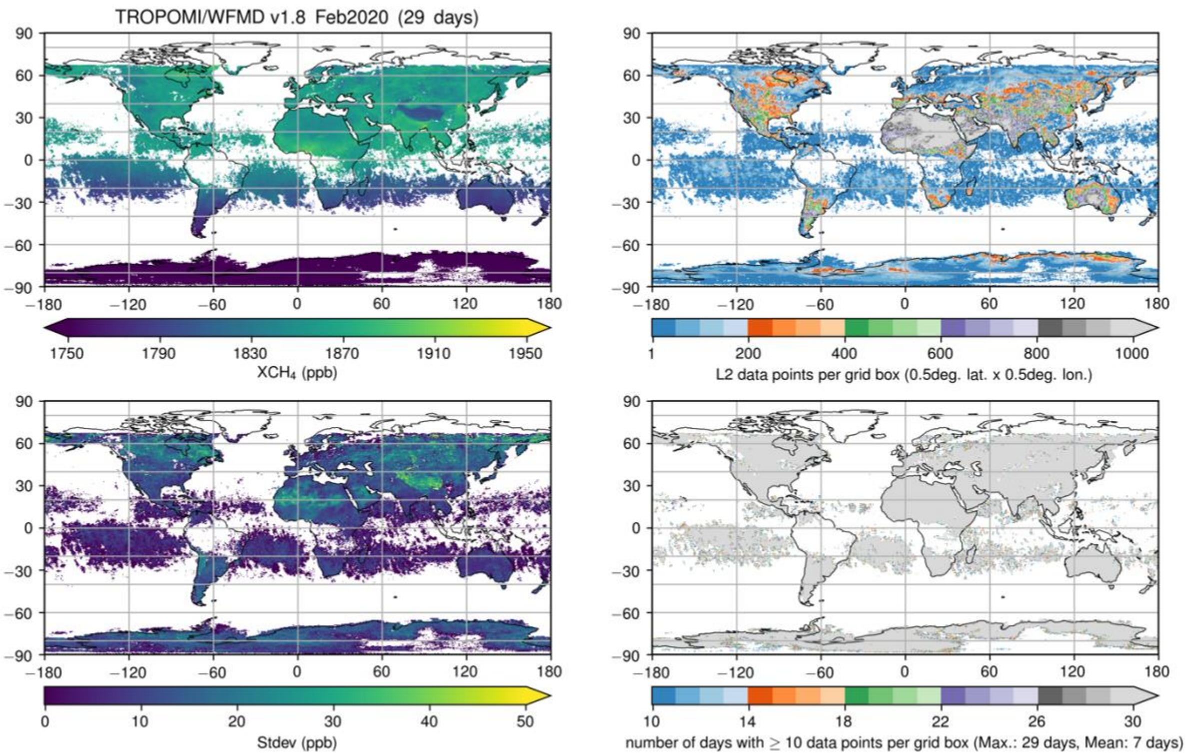


Figure 3: As Figure 1 but for the University of Bremen WFM-DOAS data product version 1.8

This project has received funding from the European Union's Horizon Europe
research and innovation programme under grant agreement No 101081395

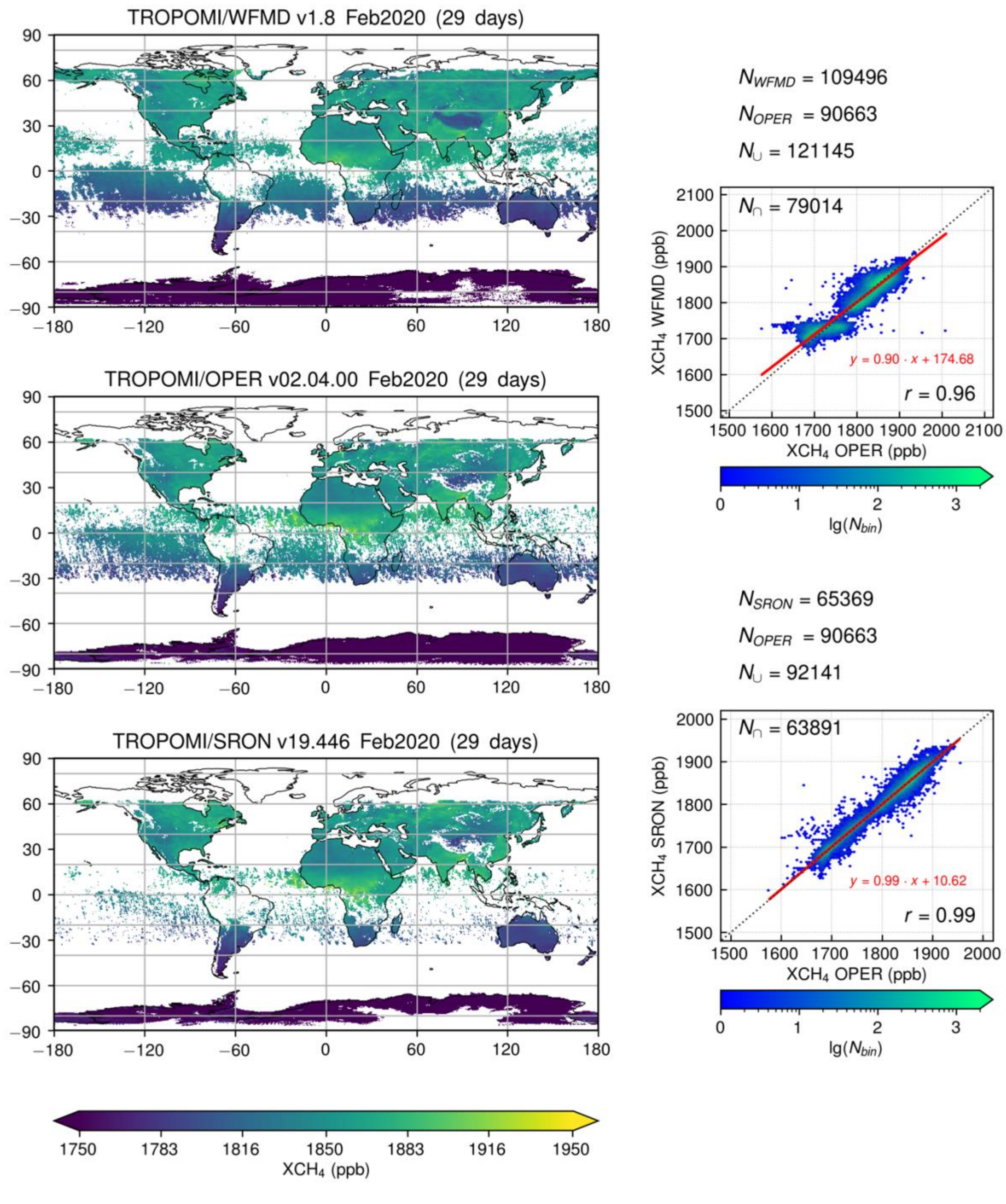


Figure 4: Comparison of TROPOMI monthly mean XCH_4 for three data products as shown in Figure 1 to Figure 3 complemented with scatterplots. N_0 gives the number of data points and r the correlation coefficient. Also given is a linear fit.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

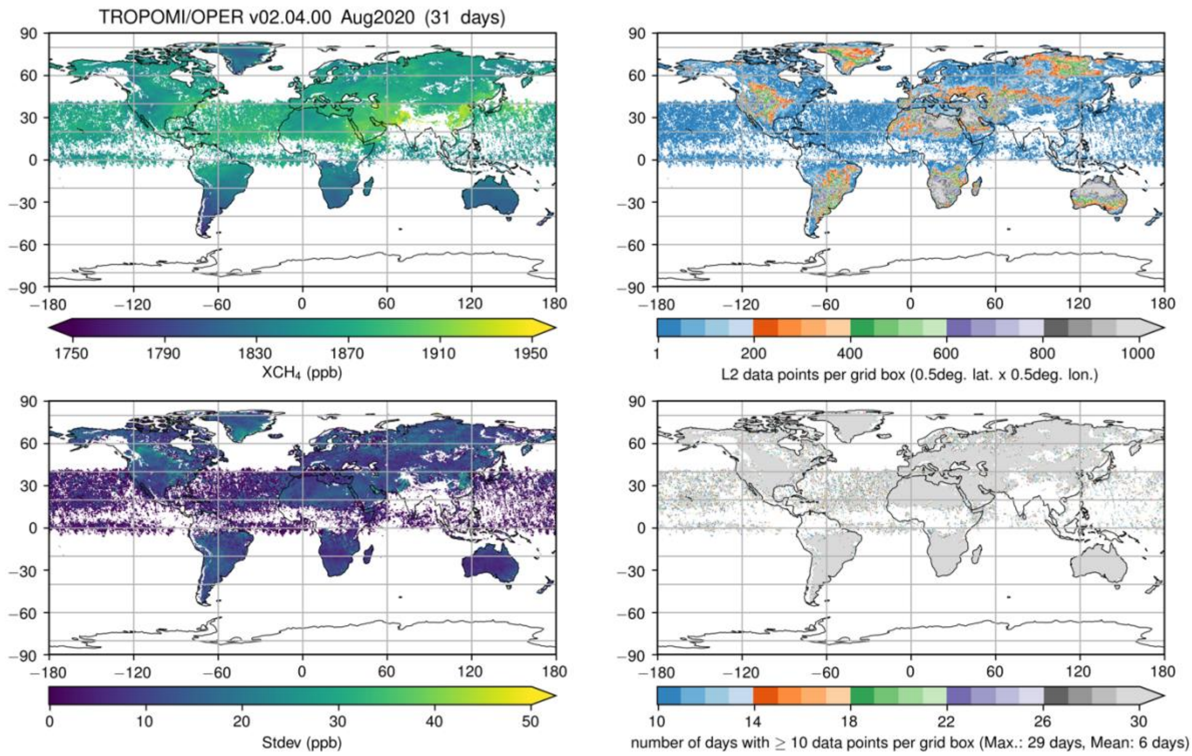


Figure 5: Left: Monthly averages of the operational (reprocessed) data product RPRO version 02.04.00 and corresponding standard deviation for August 2020. Right: Number of measurements contained in monthly mean as shown in the left panel (top) and number of days with more than 10 measurements per grid cell (bottom).

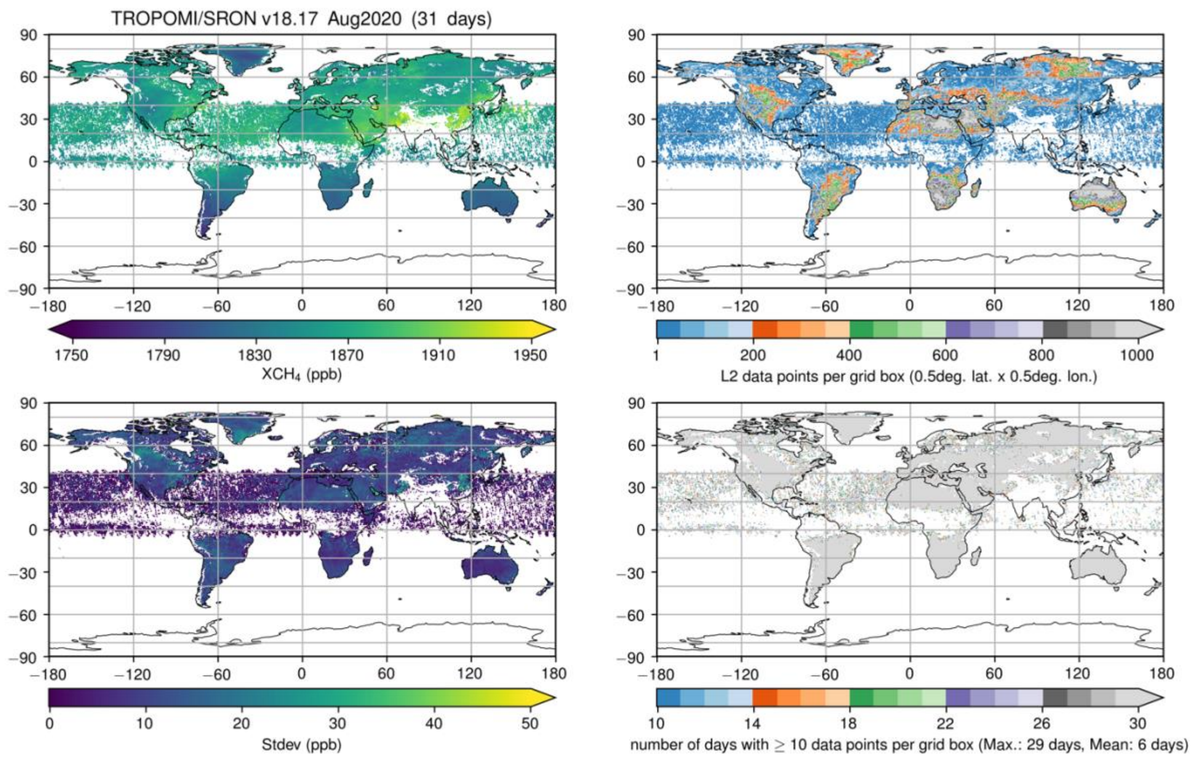


Figure 6: As Figure 5 but for SRON RemoTeC-S5P XCH_4 scientific product version 19.446

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

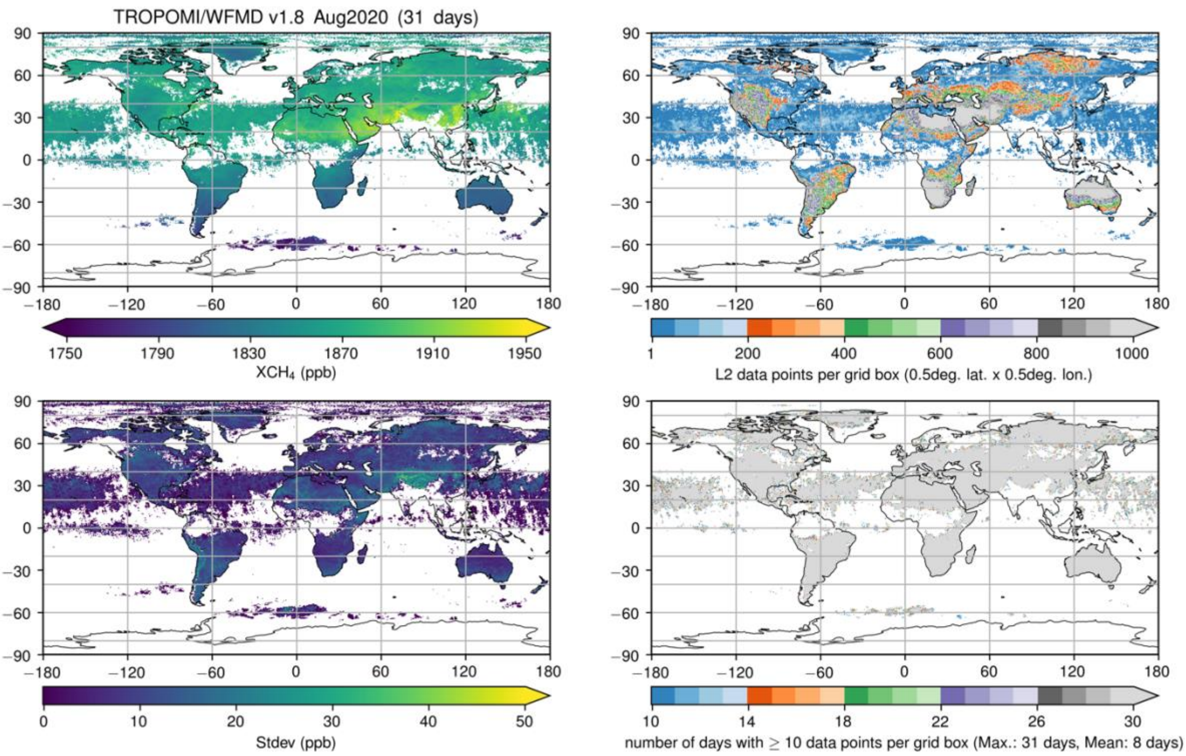


Figure 7: As Figure 5 but the University of Bremen WFM-DOAS data product version 1.8.

Overall, the global maps of TROPOMI XCH_4 are good agreement between the three data products, the operational (reprocessed) data product RPRO version 02.04.00, the SRON RemoTeC-S5P XCH_4 scientific product version 19.446 and the University of Bremen WFM-DOAS data product version 1.8. The WFMD data provides typically provides more data points and better coverage. This is well visible at high latitudes or over water. As expected, the operational product and the SRON product show high agreement as they are based on the same algorithm. As shown by the scatter plots, slightly larger differences are observed between the WFMD dataset and the operational dataset and the correlation coefficient is typically a bit reduced. The WFMD dataset shows a larger standard deviation over some regions which is likely the result of the more relaxed quality filter the subsequent higher data throughput.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

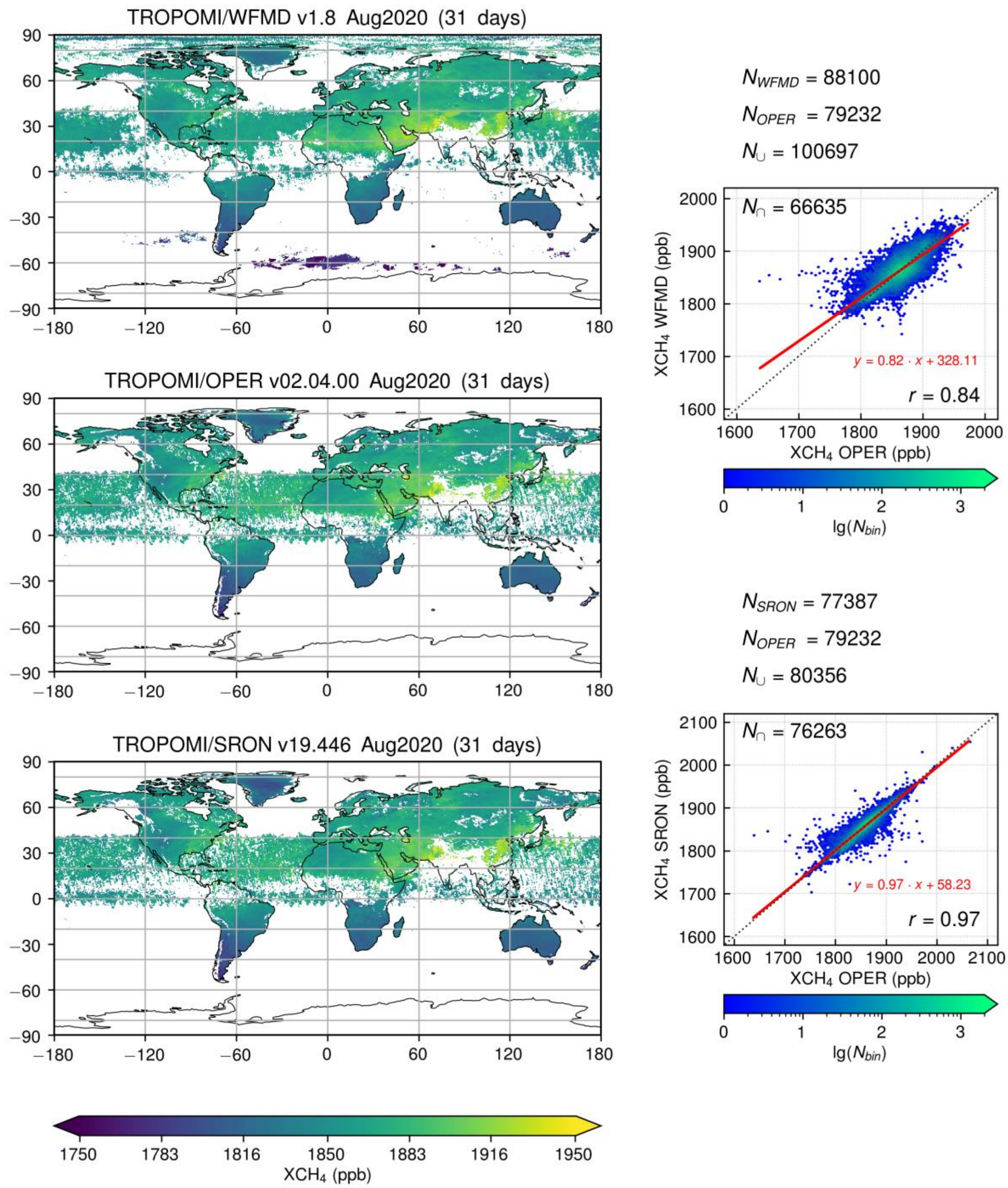


Figure 8: Comparison of TROPOMI monthly mean XCH_4 for three data products as shown in Figure 5 complemented with scatterplots. N_0 gives the number of data points and r the correlation coefficient. Also given is a linear fit.

3.2.2. Maps of monthly mean XCH_4 – Europe

We have repeated the global analysis from Section 3.2.1 but for the European domain. This was chosen to cover the longitudes 20°W to 50°E and the latitudes 30°N to 75°N. Note the changed colour scale in comparison to Section 3.2.1.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

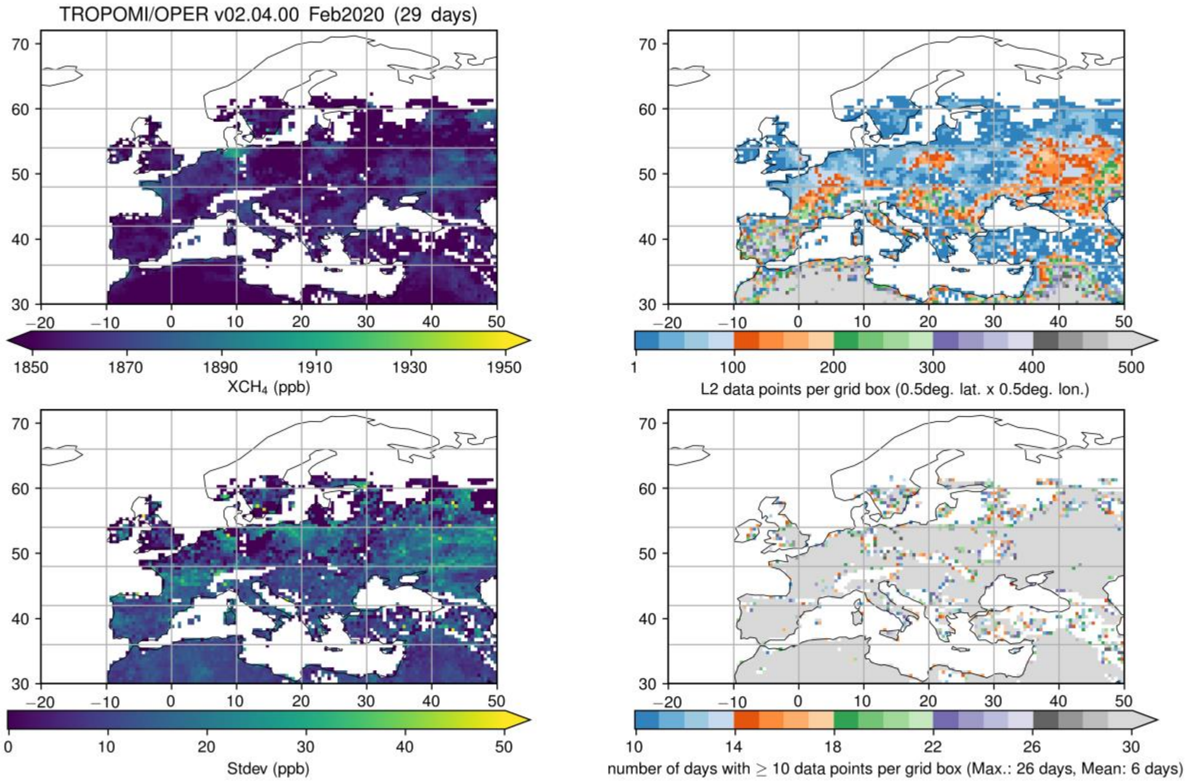


Figure 9: Left: Monthly averages of the operational (reprocessed) data product RPRO version 02.04.00 and corresponding standard deviation for February 2020. Right: Number of measurements contained in monthly mean as shown in the left panel (top) and number of days with more than 10 measurements per grid cell (bottom).

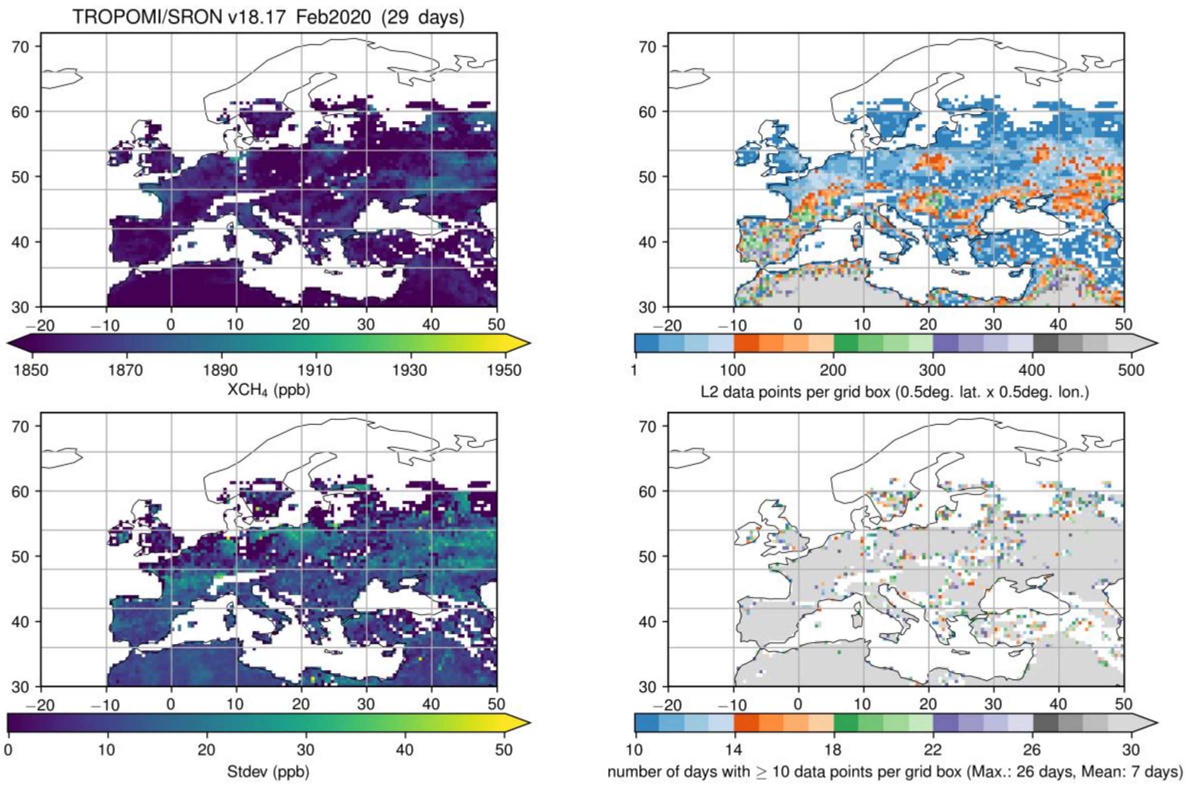


Figure 10: As Figure 9 but for the SRON RemoTeC-S5P XCH_4 scientific product version 19.446

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

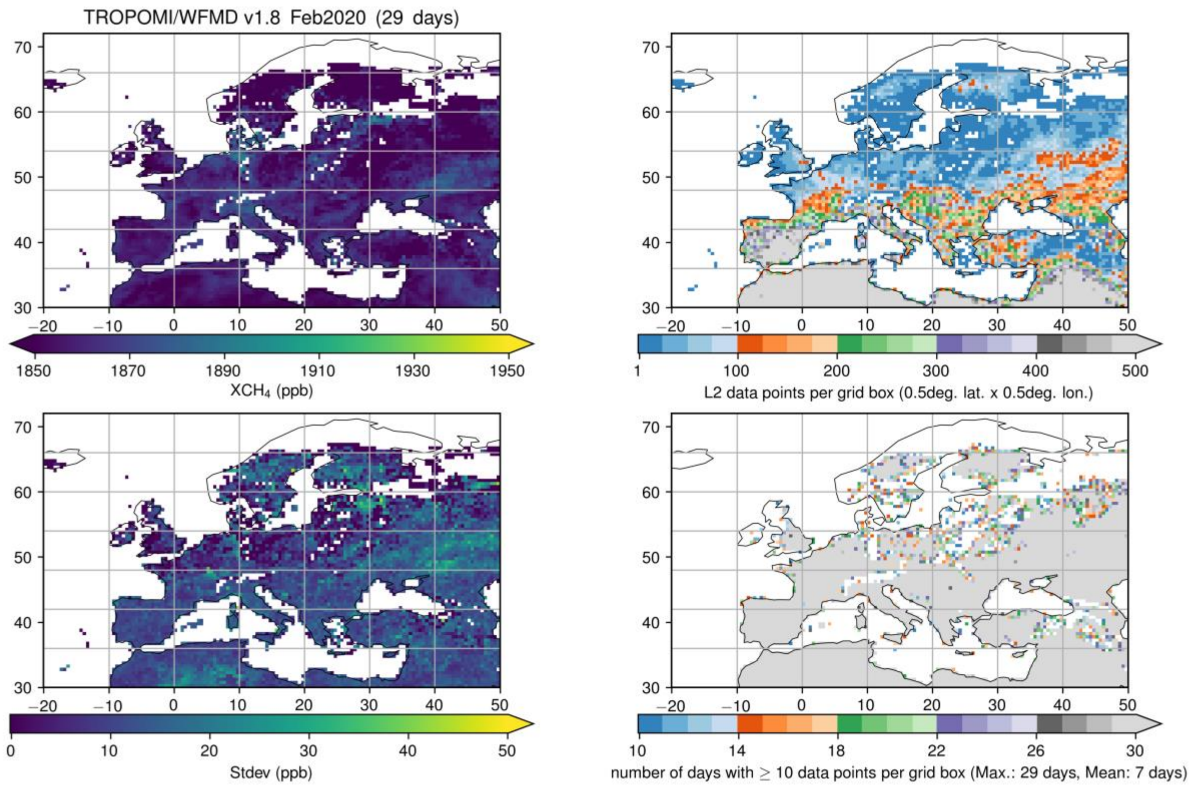


Figure 11: As Figure 9 but for the Bremen WFM-DOAS data product version 1.8

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

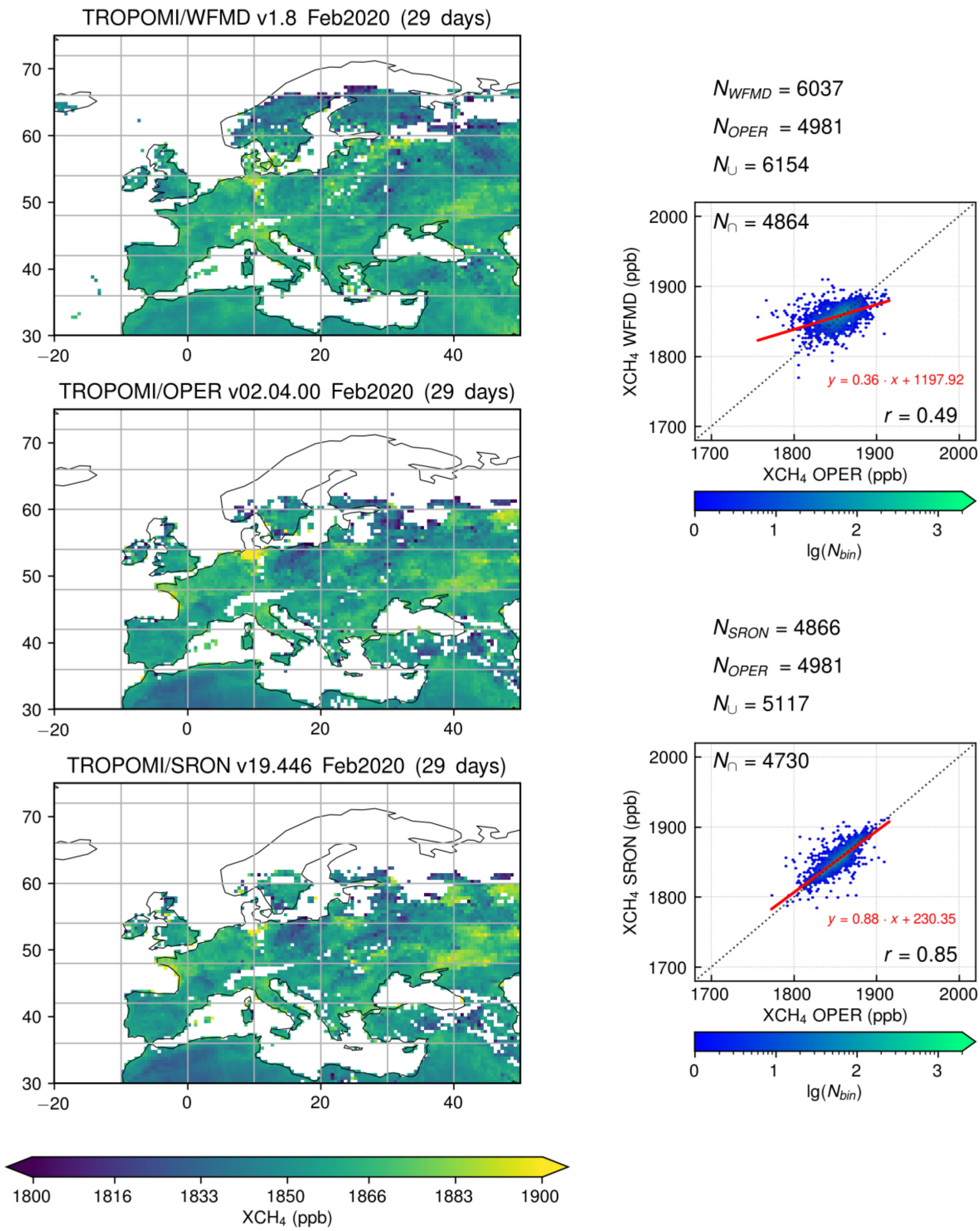


Figure 12: Comparison of TROPOMI monthly mean XCH_4 for three data products as shown in Figure 9 complemented with scatterplots. N_0 gives the number of data points and r the correlation coefficient. Also given is a linear fit.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

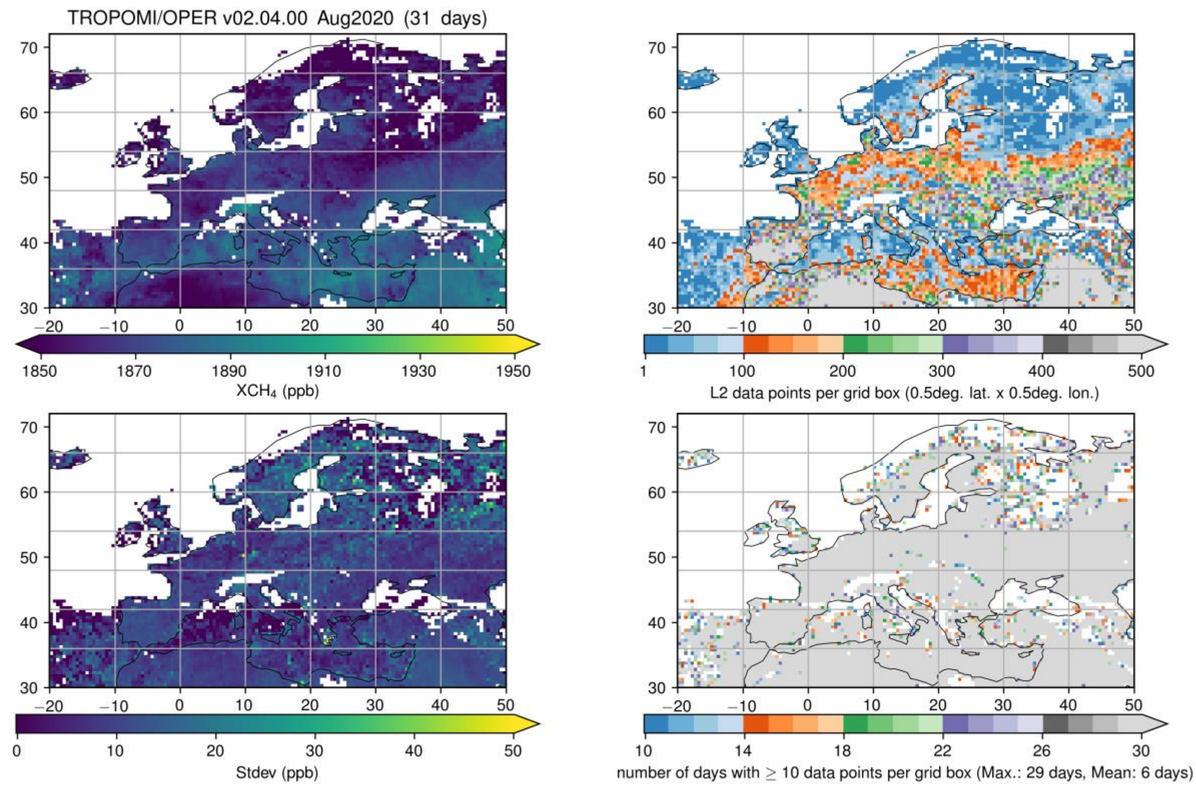


Figure 13: Left: Monthly averages of the operational (reprocessed) data product RPRO version 02.04.00 and corresponding standard deviation for August 2020. Right: Number of measurements contained in monthly mean as shown in the left panel (top) and number of days with more than 10 measurements per grid cell (bottom).

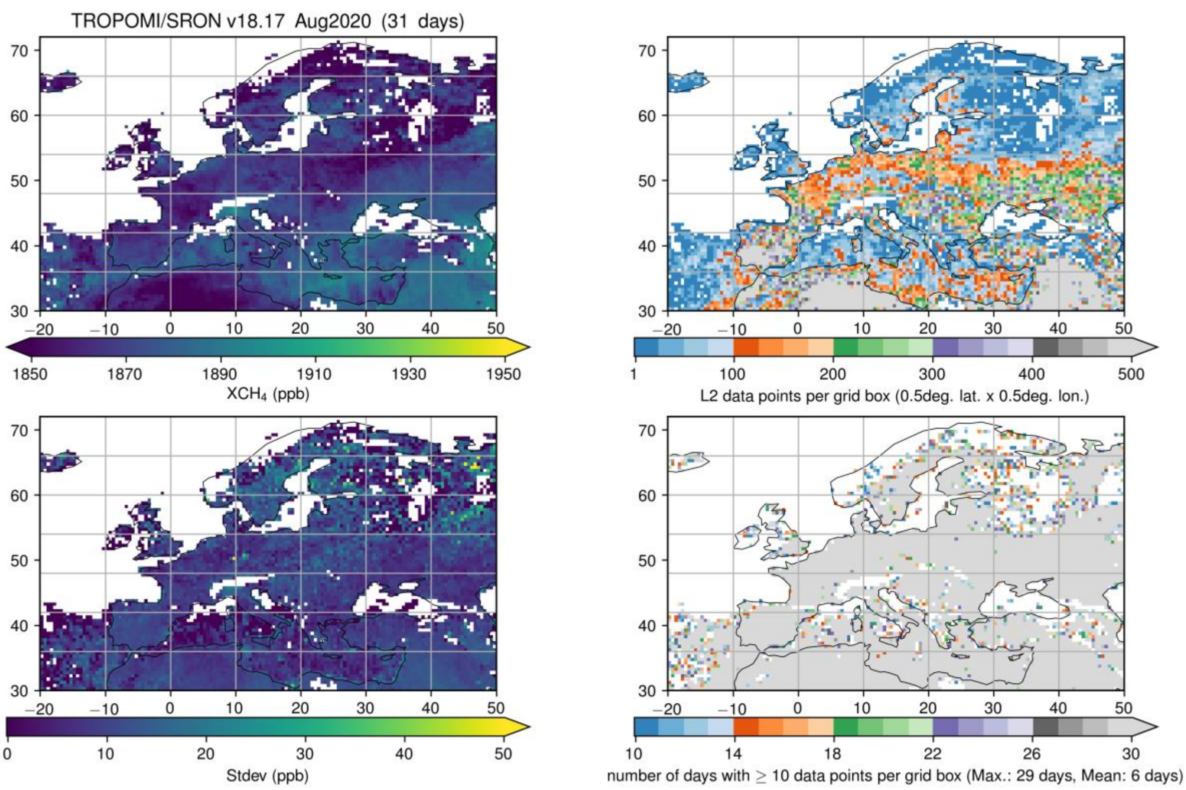


Figure 14: As for Figure 13 but for the SRON RemoTeC-S5P XCH_4 scientific product version 19.446 .

This project has received funding from the European Union's Horizon Europe
research and innovation programme under grant agreement No 101081395

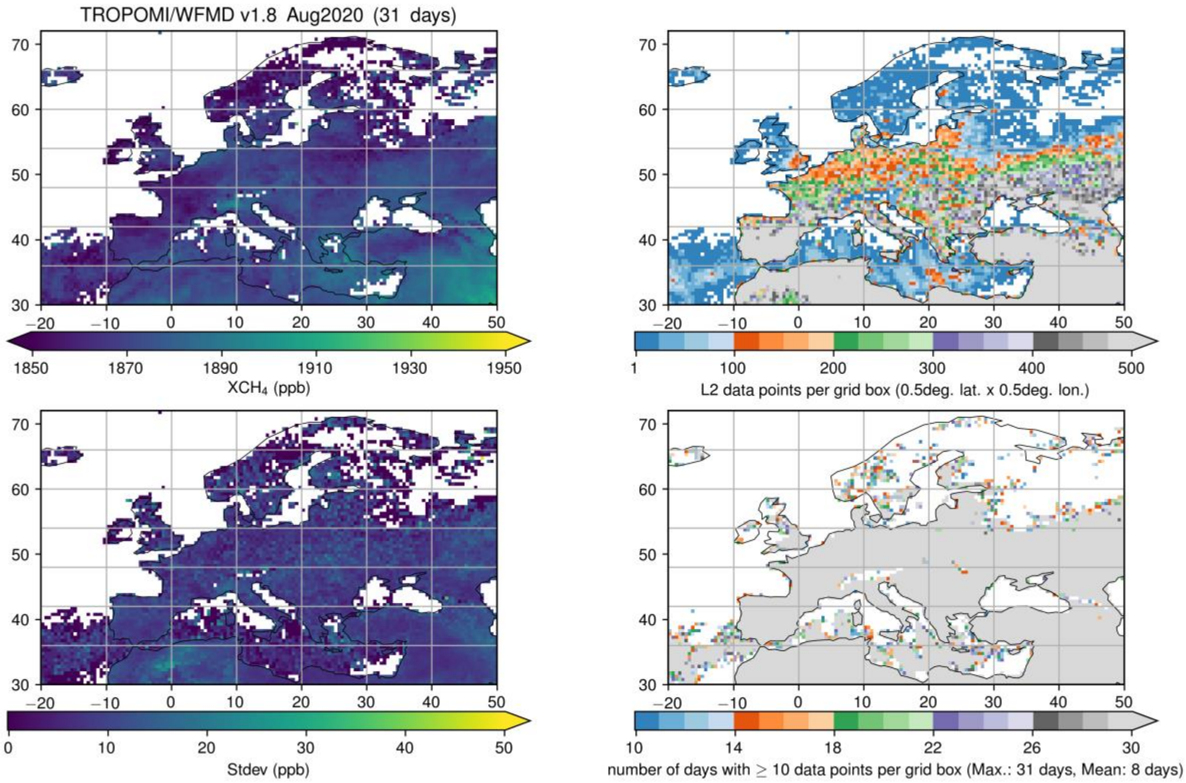


Figure 15: As for Figure 13 but for the University of Bremen WFM-DOAS data product version 1.8

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

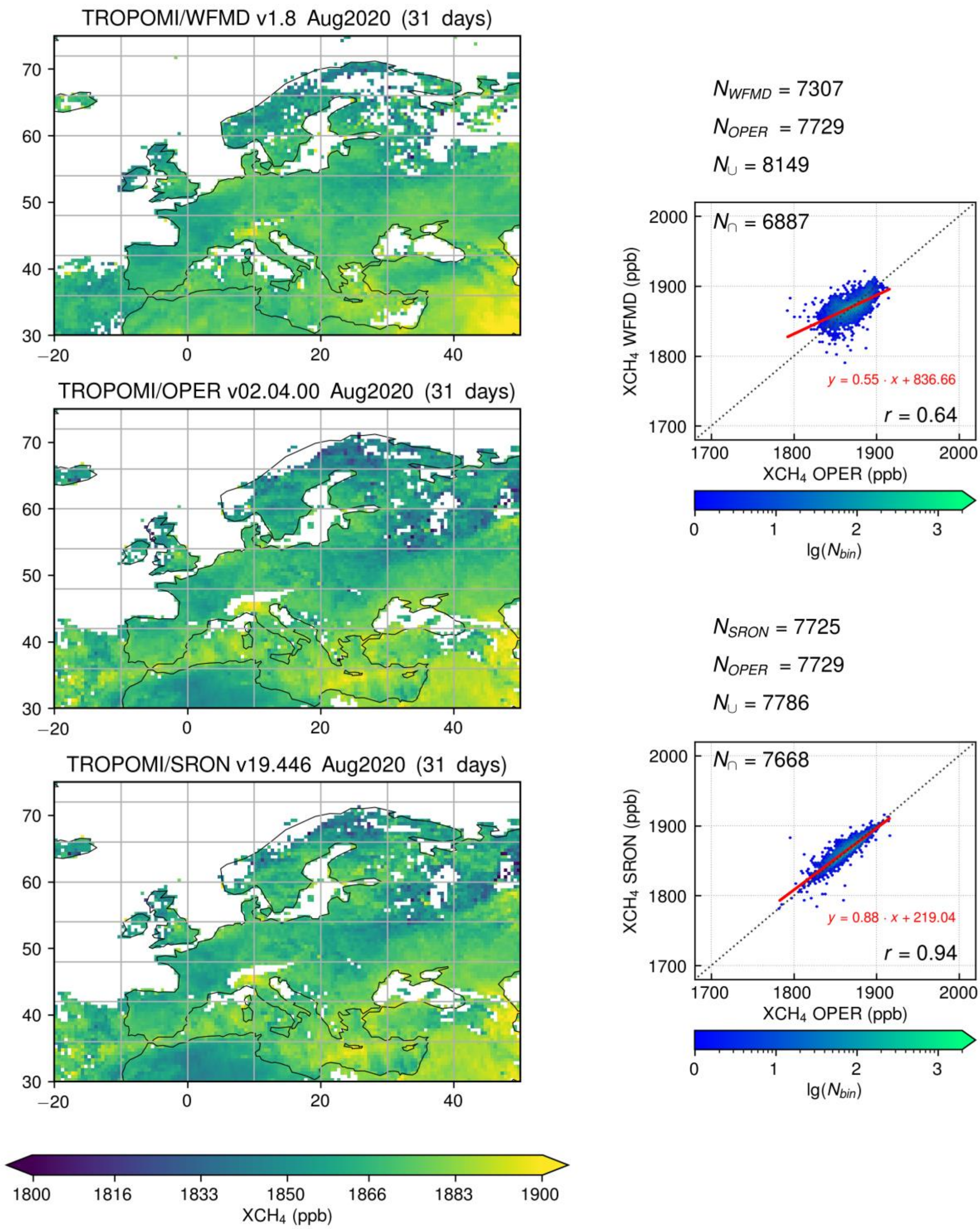


Figure 16: Comparison of TROPOMI monthly mean XCH_4 for three data products as shown in Figure 13 complemented with scatterplots. N_0 gives the number of data points and r the correlation coefficient. Also given is a linear fit.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

The European comparison shows very similar features as for the global comparison. The WFMD dataset shows typically higher data volume and better coverage. This is very pronounced in winter while in summer the WFMD dataset surprisingly shows somewhat lower number of days with data over high latitudes. This is likely caused by the chosen threshold of 10 soundings and it appears that in the case of WFMD, this threshold is missed while it is just passed in the SRON and operational products. Again, we find the expected excellent agreement between the operational and the SRON product. Differences to the WFMD product are now more enhanced on this smaller scale and we obtain a modest correlation with coefficients of 0.49 and 0.64. It is possible that differences in a priori CH_4 profiles between the retrievals contribute to the lower correlation in winter. This indicates that that the choice of data product will be important and we can expect different results when they are used in surface flux inversions.

3.2.3 Time series

Figure 17 shows time series of the globally and monthly averaged XCH_4, for the time period from May 2018 till May 2022. All datasets show the seasonal cycle and the annual increase in global methane. As already observed earlier, the operational and the SRON product agree very well. However, the WFMD product shows higher values in northern hemispheric winter and thus a lower seasonal amplitude. This is likely a consequence of the different coverage of the different datasets.

The number of contributing measurements is in general higher for the Bremen WFMD data product. The operational and the SRON scientific product show much larger variations throughout a year in the number of data points. Both datasets consist nearly of the same number of data points with a few exceptions in winter 2019 and 2020.

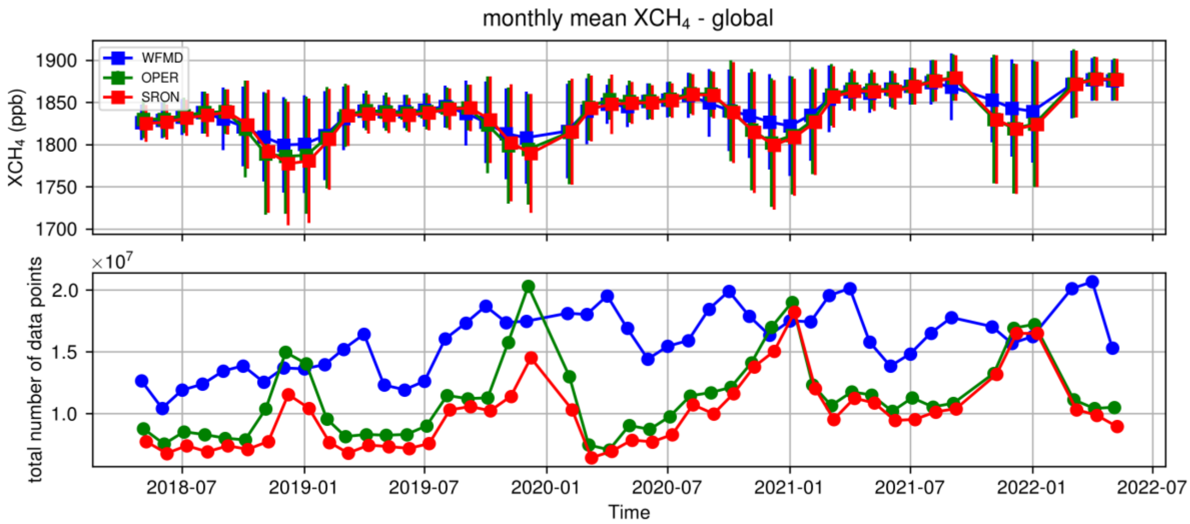


Figure 17: Upper panel: Time series of TROPOMI monthly mean XCH_4 for the 3 data products on a global scale. Lower panel: corresponding number of measurements. The error bars give the standard-deviation of the monthly data.

The time series for the European domain is given in Figure 18. All 3 datasets show similar trend with a tendency by the WFMD dataset to show higher values throughout most the time period. The datasets agree better in winter. The observed differences are likely again the result of differences in spatial coverage. For the European domain, we find that WFMD consistently has roughly 50% more data compared to the operational and SRON product.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

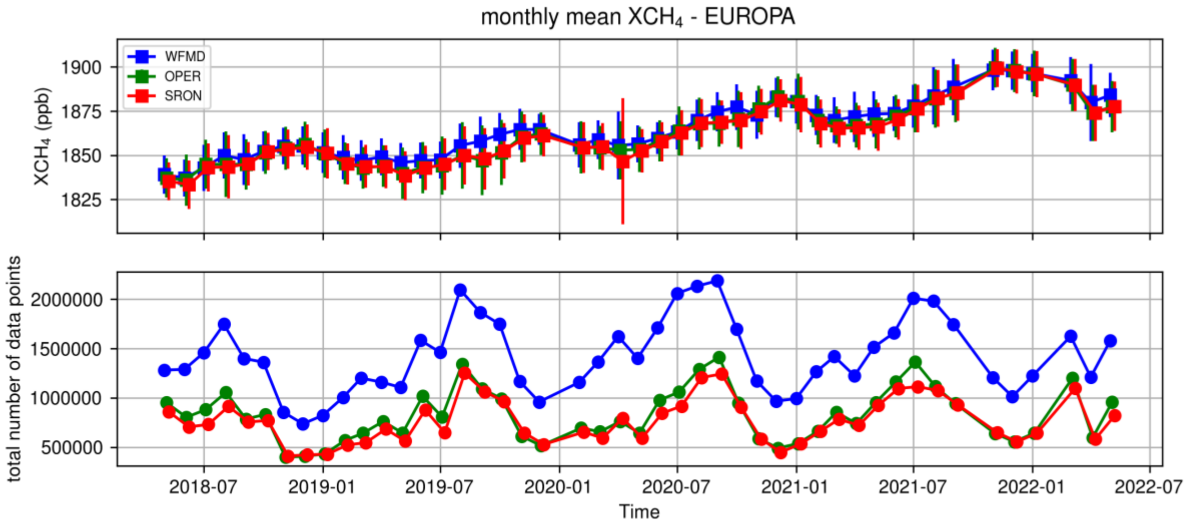


Figure 18: Upper panel: Time series of TROPOMI monthly mean XCH_4 representative for the European domain. Lower panel: corresponding number of measurements. The error bars give the standard-deviation of the monthly data.

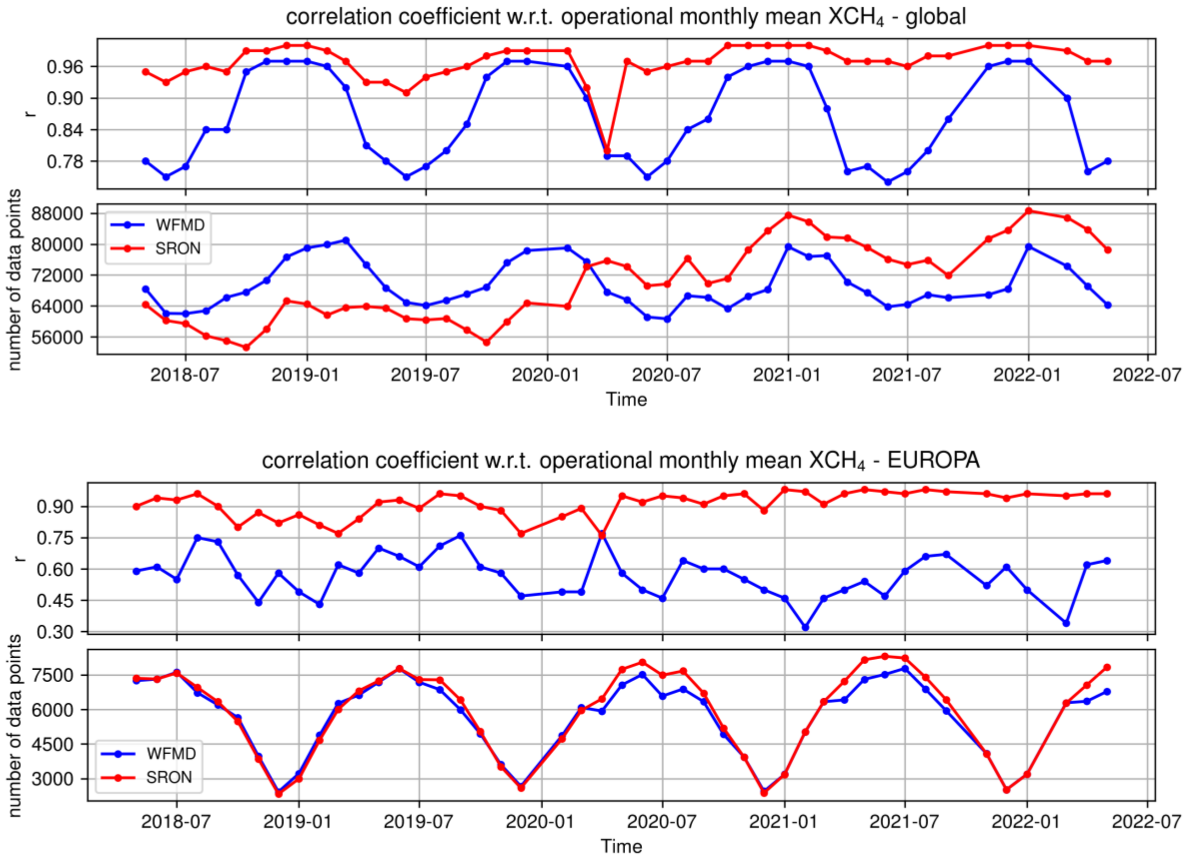


Figure 19: Time Series of the correlation coefficient r for the comparison WFMD - operational (blue lines) and SRON – operational (red lines) as shown in Figure 4: Comparison of TROPOMI monthly mean XCH4 for three data products as shown in Figure 1 to Figure 3 complemented with , Figure 8Top: global; Bottom: Europe.

Figure 19shows the correlation coefficient between the SRON and the WFMD product with the operational product globally and for Europe. As already mentioned, we expect a high correlation between

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

the SRON product and the operational product and this is also observed on both domains but with an outlier in spring 2020. The correlation between WFMD and the operational product is lower. For the global domain, we observe a summer – winter difference with much higher correlations for winter than for summer. This pattern is not visible for the European domain where the correlation coefficient scatters around a value of 0.5. The number of common datapoints with the operational product is initially higher for WFMD but this changes in the second half of the time series. Over the European domain, the common datapoints is similar between the SRON and WFMD product.

3.2.3. Single Orbits – Plume Studies

Figure 20display examples for single overpass measurements over regions with strong local hotspot emissions. This includes the Upper Silesian Coal Basin in Poland and the Permian, USA and Turkmenistan. The figures compare results for the Bremen WFMD XCH_4 data product and the operational (RPRO v02.04.00) dataset.

In general, an emission plume is visible in all cases with both datasets. The WFMD product tends to have higher coverage (except in overpass over the Silesian Coal Basin on 6 June 2018) which is important for the plume detection. In the operational product, an across-track striping feature is visible. Possible stripes of erroneous CH_4 value in flight direction is mentioned in the S5P MPC Product Readme document. This has been removed in the WFMD dataset. The scatter plot shows good agreement between both datasets with typical correlation coefficients of around 0.8. However, in some cases, clear offsets are observed (e.g. in the upper example shown in Figure 20). To what extent this will impact the emission estimation still needs to be studied.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

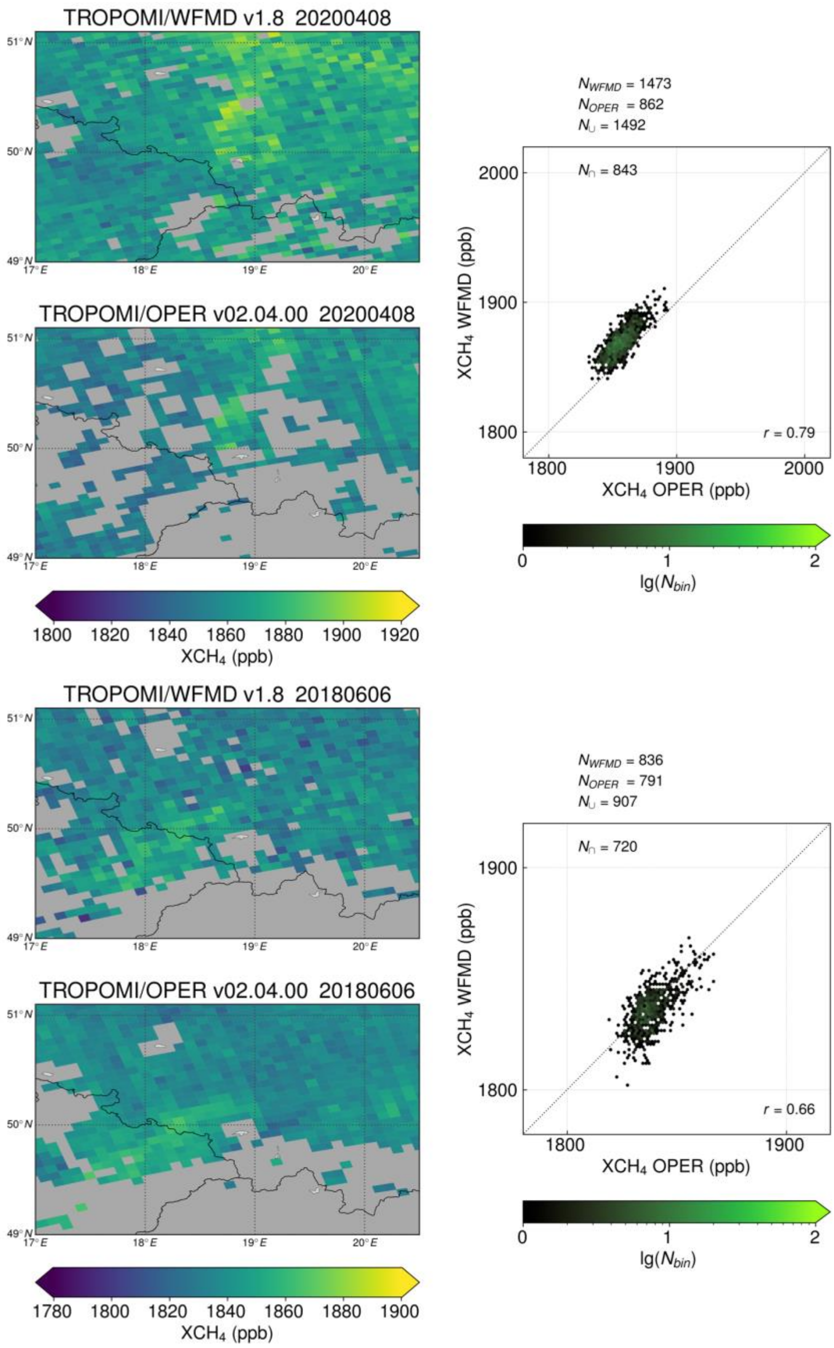


Figure 20: Single overpass, Upper Silesian Coal Basin in Poland

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

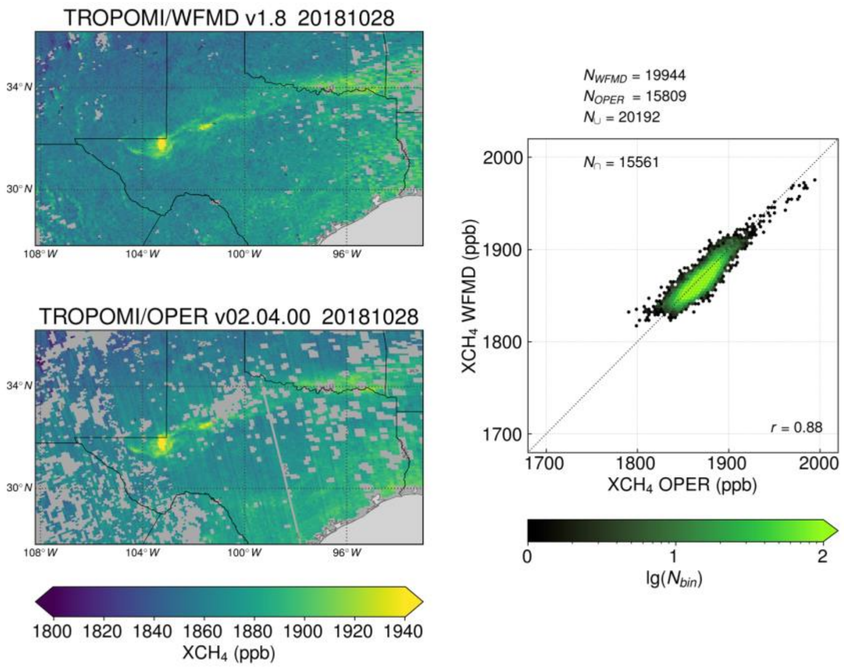


Figure 21: Single orbit data. Permian, USA with enhancements due to emissions from the oil and gas industry.

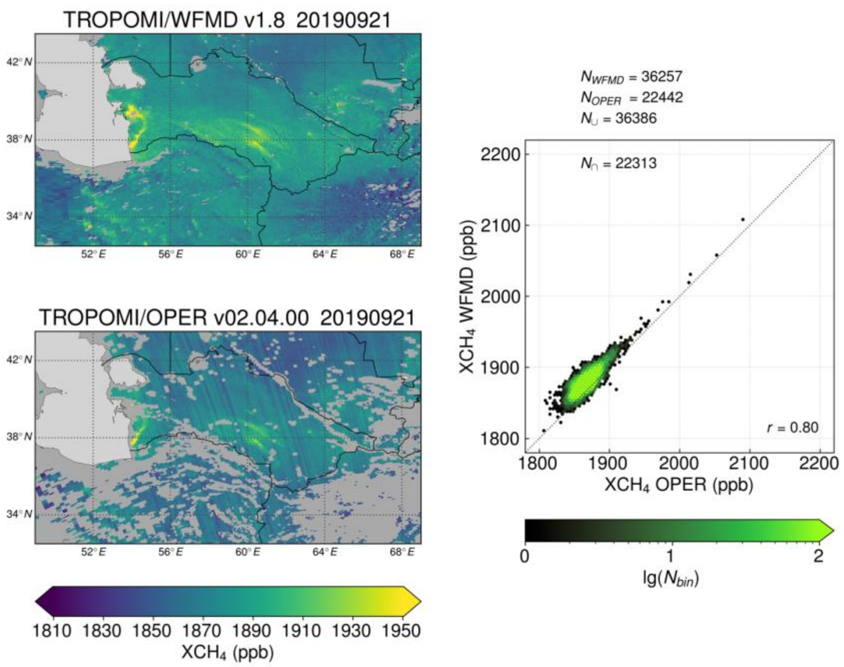


Figure 22: Single orbit data. Turkmenistan with enhancements due to emissions from the oil and gas industry.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

4. Comparison with TCCON XCH_4

4.1. Methodology

The focus of the comparison to TCCON data is for Europe and only European sites were considered and listed in Table 4: European TCCON sites used in the comparison; https://tccondata.org/ (last access: 08.11.2023 for Sodankylä site, 01.08.2023 other sites). A set of co-location criteria were defined for the comparison: The spatial co-location requires the TROPOMI measurement to be within a radius of 100km around the TCCON station. The altitude collocation is defined by a maximum hight difference of 250m. The temporal collocation is set to ± 2h and TCCON data over this window is averaged.

For a comparison between TCCON and the satellite data, it has to be taken into account that the sensitivities of both instruments differ from each other and that different a priori profiles are used to determine the best estimate of the true atmospheric state, respectively. Therefore, the measurements are adjusted to a common a priori profile to correct for the a priori contribution to the smoothing equation (Schneising et al., 2012; Dils et al., 2014). The TCCON prior is used as the common a priori profile for all measurements (Schneising et al. 2019).

The results are plotted as time series and scatterplots of the individual measurements for the different TROPOMI XCH_4 products in comparison to the TCCON data. N indicates the number of co-locations. The correlation coefficient r, the mean of the difference $\mu(\Delta)$ and the standard deviation $\sigma(\Delta)$ are given in the scatterplots.

4.2. Results and Discussion

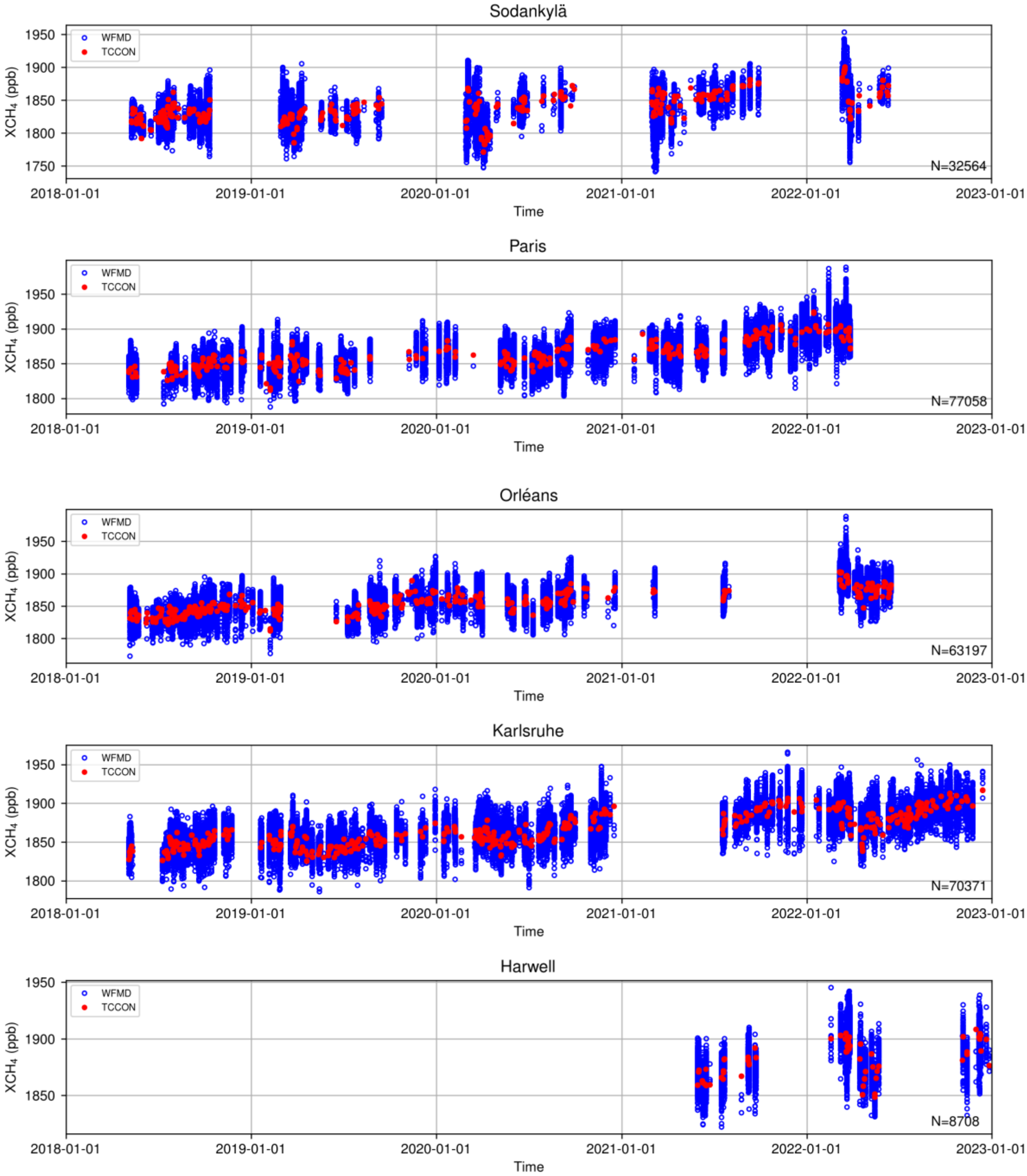
Time series and scatter plots for all selected TCCON sites are given in Figure 23 for the comparison with TROPOMI/WFMD data, in Figure 25 and Figure 26 for the SRON RemoTeC product and in Figure 27 and Figure 28 for the TROPOMI/operational (RPRO) product. The complete set of Figures is available from https://nc.uni-bremen.de/index.php/s/AZNgkQtrHrZSbgf.

The comparison of the WFMD datasets to TCCON shows overall good agreement. We find a good correlation ($r \geq 0.7$) and low biases of 6.2 ppb or less for the different sites. The exception is Garmisch where the bias is larger (12.2 ppb) and the correlation is lower ($r = 0.58$). This is likely caused by the difficult location of the site

The comparison for the SRON product shows good agreement with TCCON as well. The obtained correlation coefficients are very similar to those from the WFDM comparison but biases are higher for all sites. This is most pronounced for the Sodankylä site where the bias increases from 2.8 ppb for WFMD to 11.4 ppb for SRON. The number of datapoints available for the TCCON comparison is higher for the WFMD product than for the SRON product, except for Sodankylä where the SRON product has almost 30% more data. This higher data yield at Sodankylä in the SRON product might be related to the increased bias observed for this site as differences in data yield are primarily the result of the applied quality filter and a stricter filter can lead to a lower bias.

The comparison for the operational dataset is, as expected, similar to the SRON comparison with very similar correlation coefficients. The number of data points and the obtained biases are slightly larger for the operational product compared to the SRON product for all sites except for Sodankylä where the bias is comparable.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395



This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

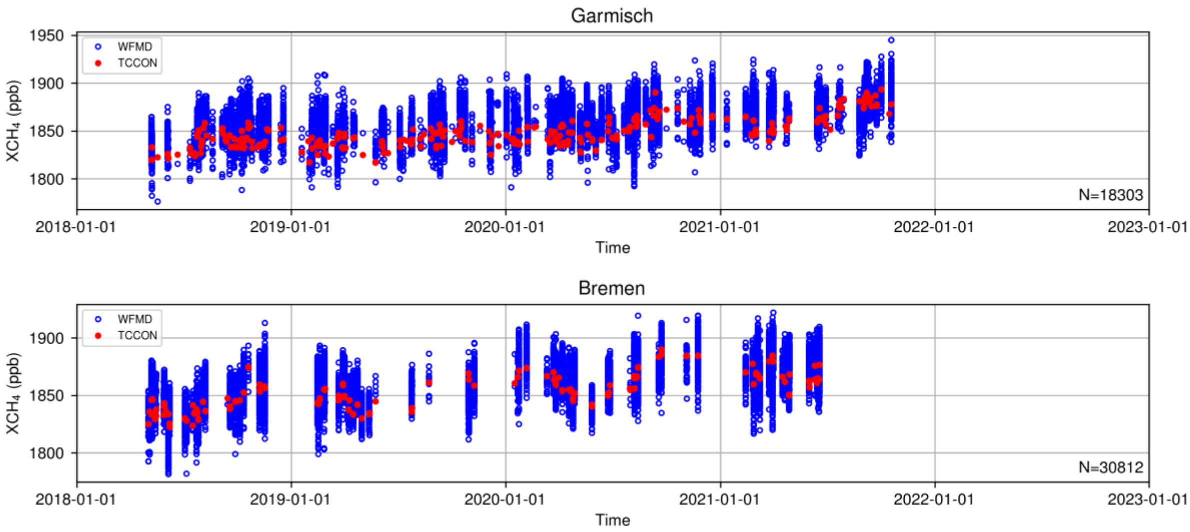


Figure 23: Comparison of the TROPOMI/WFM-DOAS v.1.8 XCH4 time series (blue) with ground-based TCCON measurements (red). N indicates the number of co-locations.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

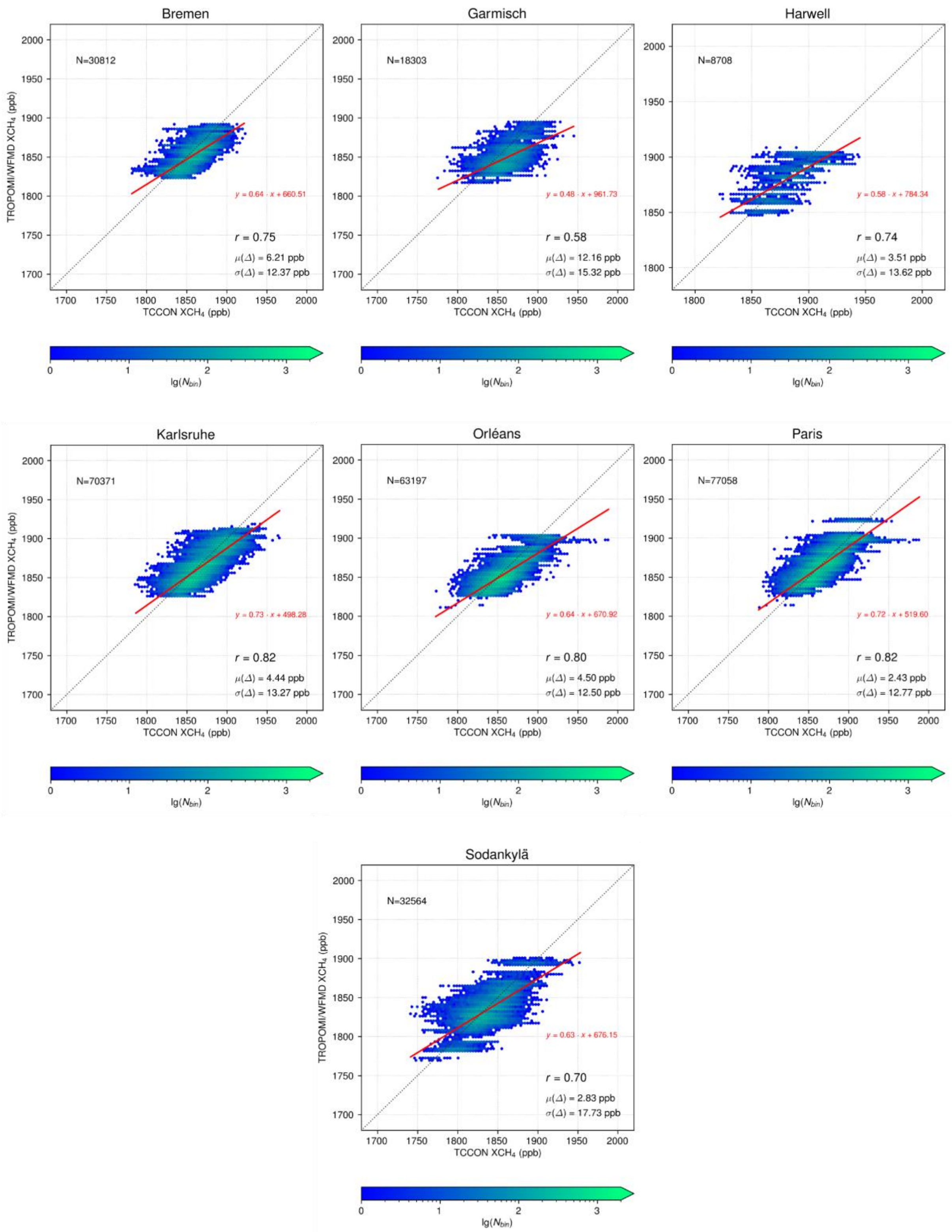
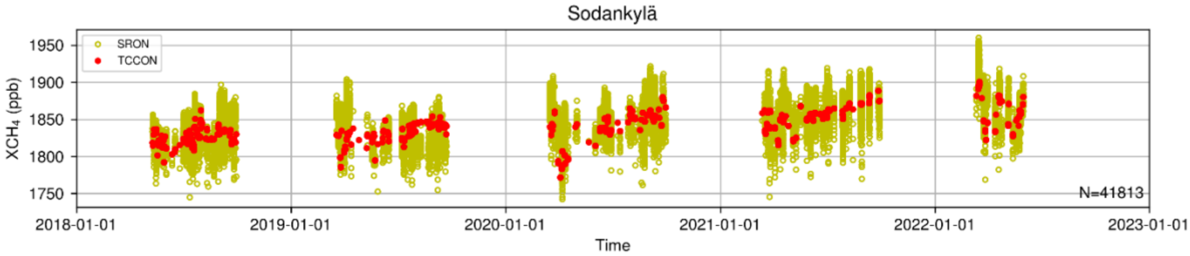
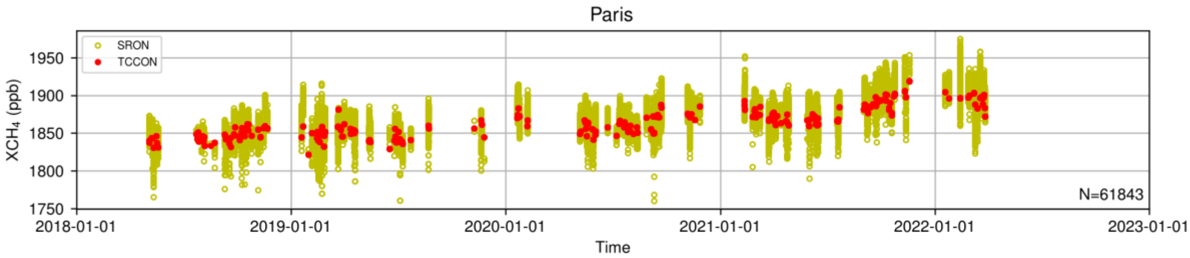
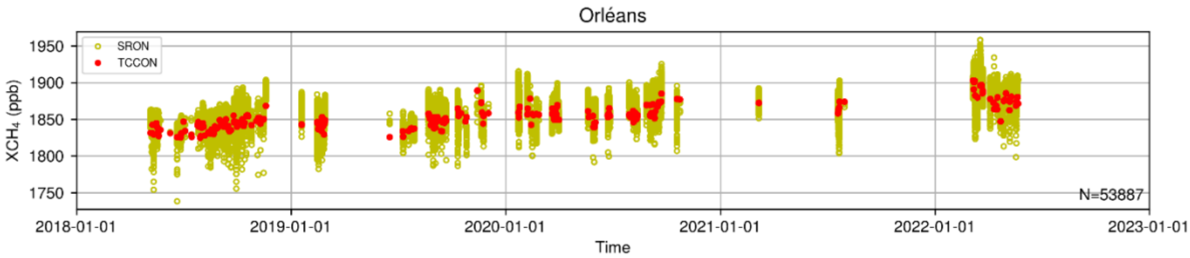


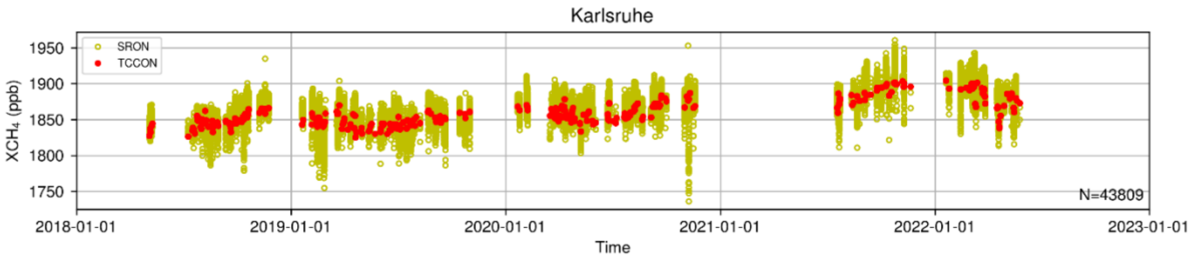
Figure 24: Comparison of TROPOMI/WFMD and TCCON XCH4 for European sites. The number of co-locations N, the correlation coefficient r, the mean of the difference μ(Δ) and the standard deviation σ(Δ) are indicated.

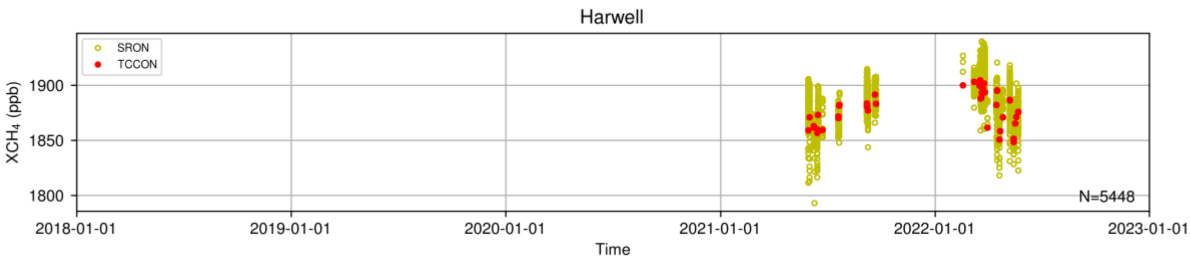
This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

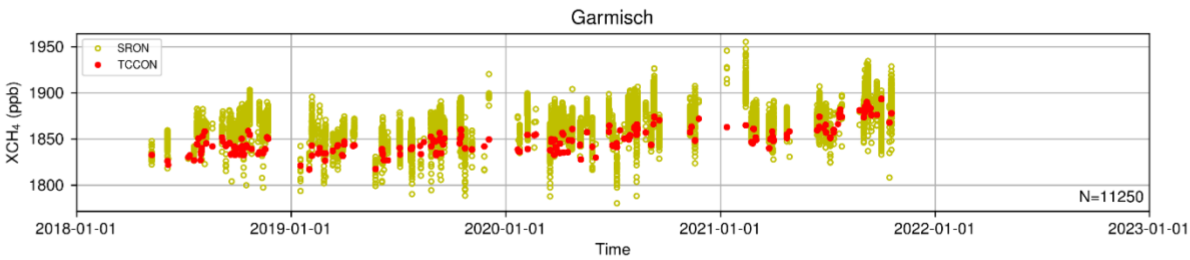












This project has received funding from the European Union's Horizon Europe
research and innovation programme under grant agreement No 101081395

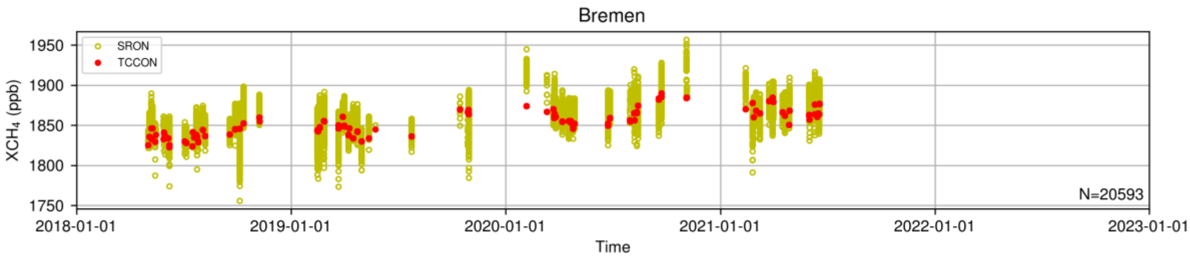


Figure 25: Comparison of the SRON RemoTeC-S5P XCH_4 scientific product version 19.446 time series (yellow) with ground-based TCCON measurements (red). N indicates the number of co-locations.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

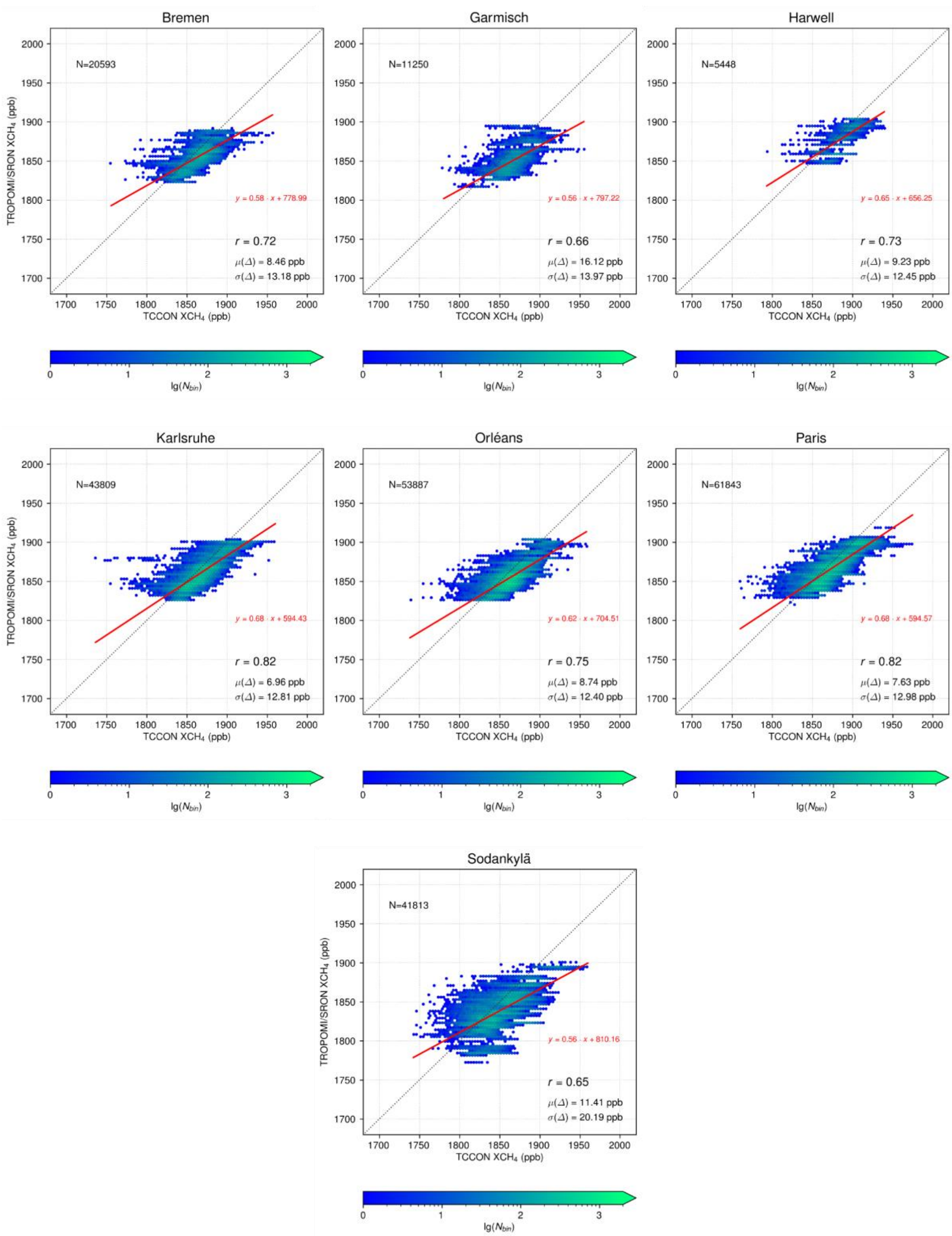
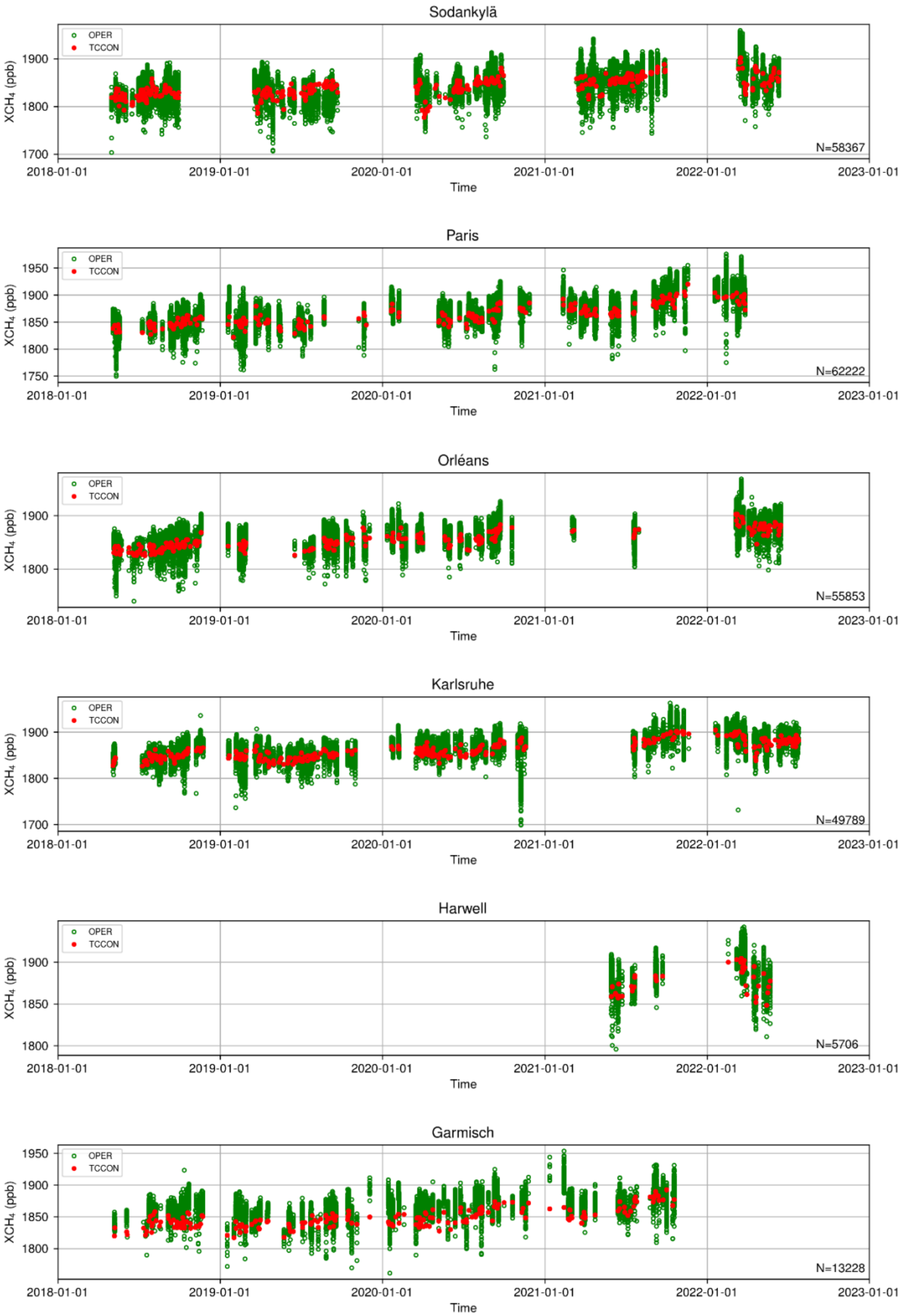


Figure 26: Comparison of RemoTeC-S5P XCH_4 scientific product version 19.446 and TCCON XCH_4 for European sites. The number of collocations N, the correlation coefficient r, the mean of the difference μ(Δ) and the standard deviation σ(Δ) are indicated.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395



This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

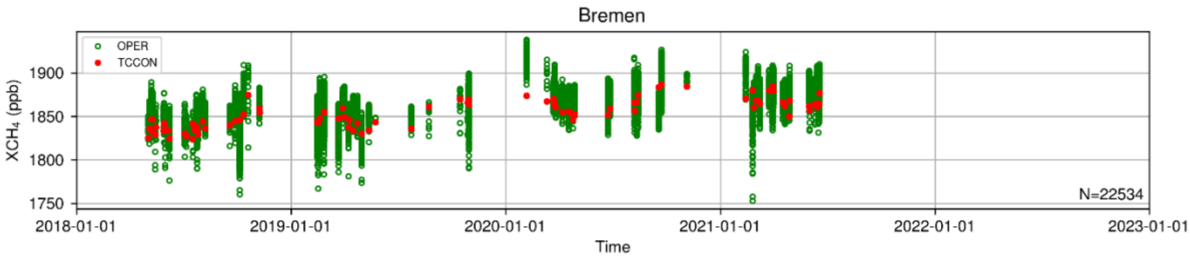


Figure 27: Comparison of the operational (reprocessed) data product RPRO version 02.04.00 time series (green) with ground-based TCCON measurements (red). N indicates the number of collocations.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

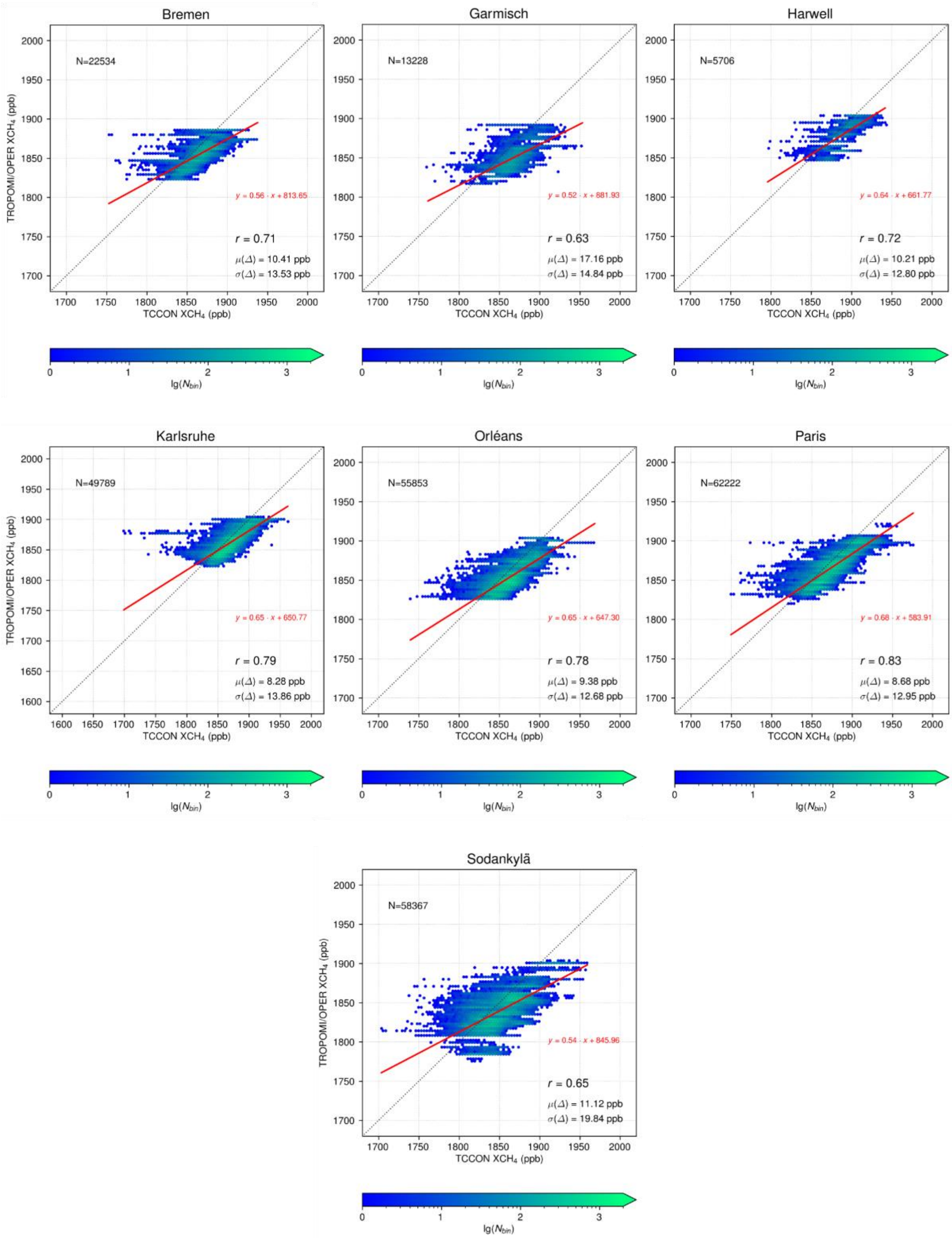


Figure 28: Comparison of TROPOMI/operational (RPRO) and TCCON XCH_4 for European sites. The number of collocations N, the correlation coefficient r, the mean of the difference μ(Δ) and the standard deviation σ(Δ) are indicated.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

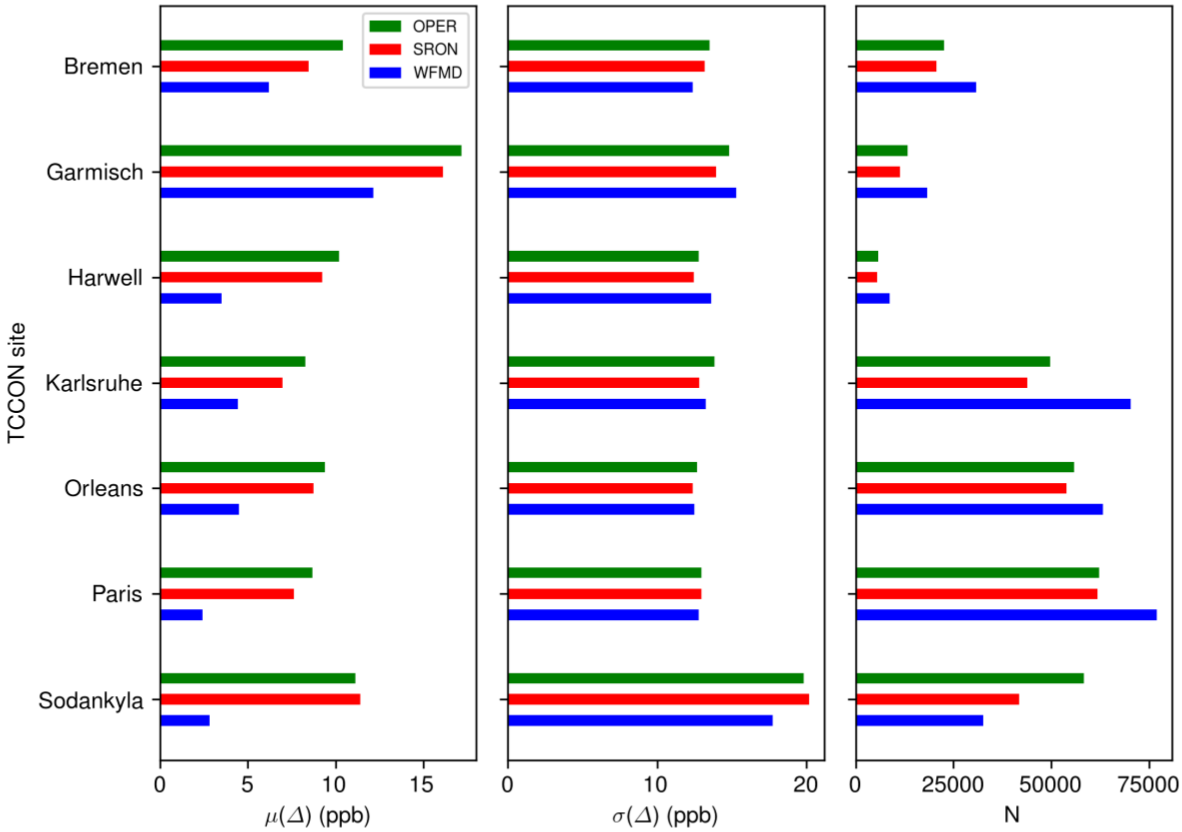


Figure 29: Mean of the difference μ(Δ), the standard deviation σ(Δ) and number of soundings (N) of the TCCON and TROPOMI XCH_4 comparison for three different products for European sites.

Figure 29 gives an overview over the obtained biases and scatter obtained from the comparison to TCCON for the three different datasets for all European sites. This shows again the behaviour already described above. For all sites, we find lower biases for the WFMD dataset compared to the SRON and operational datasets with the largest difference being found for Sodankylä. The operational datasets show the largest biases of all three datasets compared to TCCON. The observed scatter is typically between 12 and 15 ppb and is similar for all three products. Larger scatter is observed for the Sodankylä site. The number of data point is largest for the WFMD dataset, except for Sodankylä where the SRON and operational datasets have significantly more data.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

5. Conclusions

Three TROPOMI XCH_4 data products have been inter-compared and assessed against ground-based reference data from the TCCON network. The datasets include the operational, reprocessed data product RPRO version 02.04.00, the SRON RemoTeC-S5P XCH_4 scientific product version 19.446 and the University of Bremen WFM-DOAS data product version 1.8. The assessment has been carried out globally and for the European domain.

As expected, we find that the operational and the SRON data products agree very well with each other. This is expected as both are based on the same retrieval algorithm. The WFMD datasets generated by IUP Bremen shows also good agreement with the two other datasets. There is a pronounced difference in coverage and number of data points with the WFMD product usually showing higher data volume and better coverage. Differences in the retrieved CH_4 values between WFMD and the two other datasets are more pronounced for the European domain than globally. Thus, it can be expected that surface flux inversions on a European domain will differ depending on the chosen dataset.

Differences between the WFMD and the operational dataset are also noticeable when observing emission plumes in single overpasses. Here, the often-better coverage of WFMD offers better opportunities for detection of emission plumes. Also, the magnitude of the CH_4 columns in these single overpasses can differ which can then lead to differences in the quantification of emissions.

The comparison to European TCCON sites of the TROPOMI datasets show high correlation coefficients and low biases for all three datasets, with lowest biases obtained for the WFMD dataset (2.8 to 12.2 ppb) and the highest for the operational dataset (8.3 ppb to 17.2 ppb). Overall, the TCCON comparison demonstrates a high quality of the TROPOMI CH_4 retrievals.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

Acknowledgements

Acknowledgement of the TCCON science team. The TCCON data were obtained from the TCCON Data Archive, hosted by CaltechDATA, California Institute of Technology (https://tccondata.org/).

References

Dils, B., et al., (2014)., The Greenhouse Gas Climate Change Initiative (GHG-CCI): comparative validation of GHG-CCI SCIAMACHY/ENVISAT and TANSO-FTS/GOSAT CO_2 and CH_4 retrieval algorithm products with measurements from the TCCON, Atmos. Meas. Tech., 7, 1723–1744, https://doi.org/10.5194/amt-7-1723-2014

Hase, F., Herkommer, B., Groß, J., Blumenstock, T., Kiel, M. ä ., & Dohe, S. (2023). TCCON data from Karlsruhe (DE), Release GGG2020.R1 (Version R1) [Data set]. CaltechDATA. https://doi.org/10.14291/tccon.ggg2020.karlsruhe01.R1

Kivi, R., Heikkinen, P., & Kyrö, E. (2022). TCCON data from Sodankylä (FI), Release GGG2020.R0 (Version R0) [Data set]. CaltechDATA. https://doi.org/10.14291/tccon.ggg2020.sodankyla01.R0

Lunt et al., Rain-fed pulses of methane from East Africa during 2018–2019 contributed to atmospheric growth rate, 2021 Environ. Res. Lett.,16, 024021

Maasakkers, J.D. et al., (2022). Using satellites to uncover large methane emissions from landfills, Sci. Adv.8, DOI:10.1126/sciadv.abn9683

Notholt, J., Petri, C., Warneke, T., & Buschmann, M. (2022). TCCON data from Bremen (DE), Release GGG2020.R0 (Version R0) [Data set]. CaltechDATA. https://doi.org/10.14291/tccon.ggg2020.bremen01.R0

Sussmann, R., & Rettinger, M. (2023). TCCON data from Garmisch (DE), Release GGG2020.R0 (Version R0) [Data set]. CaltechDATA. https://doi.org/10.14291/tccon.ggg2020.garmisch01.R0

Té, Y., Jeseck, P., & Janssen, C. (2022). TCCON data from Paris (FR), Release GGG2020.R0 (Version R0) [Data set]. CaltechDATA. https://doi.org/10.14291/tccon.ggg2020.paris01.R0

Warneke, T., Petri, C., Notholt, J., & Buschmann, M. (2022). TCCON data from Orléans (FR), Release GGG2020.R0 (Version R0) [Data set]. CaltechDATA. https://doi.org/10.14291/tccon.ggg2020.orleans01.R0

Weidmann, D., Brownsword, R., & Doniki, S. (2023). TCCON data from Harwell, Oxfordshire (UK), Release GGG2020.R0 (Version R0) [Data set]. CaltechDATA. https://doi.org/10.14291/tccon.ggg2020.harwell01.R0

Hasekamp, O., Lorente, A., Hu, H., Butz, A., de Brugh, J., and Landgraf, J. (2022). Algorithm Theoretical Baseline Document for Sentinel-5 Precursor Methane Retrieval. SRON-S5P-LEV2-RP-001, Issue 2.4.0

Laughner, J. L., et al..(2023) The Total Carbon Column Observing Network's GGG2020 Data Version, Earth Syst. Sci. Data Discuss. [preprint], https://doi.org/10.5194/essd-2023-331, in review

Lorente, A., Borsdorff, T., Landgraf, J., and the SRON L2 team (2022), SRON RemoTeC-S5P scientific XCH4 data product Product User Guide.

Schneising, O. (2022), Algorithm Theoretical Basis Document (ATBD) - TROPOMI WFM-DOAS (TROPOMI/WFMD) XCH_4. https://www.iup.uni-bremen.de/carbon_ghg/products/tropomi_wfmd/atbd_wfmd.pdf.

Schneising, O., et al., (2012), Atmospheric greenhouse gases retrieved from SCIAMACHY: comparison to ground-based FTS measurements and model results, Atmos. Chem. Phys., 12, 1527–1540, https://doi.org/10.5194/acp-12-1527-2012

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

Schneising, O., Buchwitz, M., Reuter, M., Bovensmann, H., Burrows, J. P., Borsdorff, T., Deutscher, N. M., Feist, D. G., Griffith, D. W. T., Hase, F., Hermans, C., Iraci, L. T., Kivi, R., Landgraf, J., Morino, I., Notholt, J., Petri, C., Pollard, D. F., Roche, S., Shiomi, K., Strong, K., Sussmann, R., Velazco, V. A., Warneke, T., and Wunch, D. (2019), A scientific algorithm to simultaneously retrieve carbon monoxide and methane from TROPOMI onboard Sentinel-5 Precursor, Atmos. Meas. Tech., 12, 6771–6802, https://doi.org/10.5194/amt-12-6771-2019.

Schneising, O., Buchwitz, M., Reuter, M., Vanselow, S., Bovensmann, H., and Burrows, J. P. (2020), Remote sensing of methane leakage from natural gas and petroleum systems revisited, Atmos. Chem. Phys., 20, 9169–9182, https://doi.org/10.5194/acp-20-9169-2020

Schneising, O., Buchwitz, M., Hachmeister, J., Vanselow, S., Reuter, M., Buschmann, M., Bovensmann, H., and Burrows, J. P. (2023). Advances in retrieving XCH_4 and XCO from Sentinel-5 Precursor: improvements in the scientific TROPOMI/WFMD algorithm, Atmos. Meas. Tech., 16, 669–694, https://doi.org/10.5194/amt-16-669-2023.

Tsuruta A, Kivimäki E, Lindqvist H, Karppinen T, Backman L, Hakkarainen J, Schneising O, Buchwitz M, Lan X, Kivi R, et al. (2023), CH_4 Fluxes Derived from Assimilation of TROPOMI XCH_4 in CarbonTracker Europe-CH_4: Evaluation of Seasonality and Spatial Distribution in the Northern High Latitudes. Remote Sensing. 15(6):1620. https://doi.org/10.3390/rs15061620

Wunch, D., G. C. Toon, J.-F. L. Blavier, R. A. Washenfelder, J. Notholt, B. J. Connor, D. W. T. Griffith, V. Sherlock, and P. O. Wennberg (2011), The Total Carbon Column Observing Network, Philos. Trans. R. Soc. A Math. Phys. Eng. Sci., 369(1943), 2087–2112, doi:10.1098/rsta.2010.0240.

Wunch, D., G. C. Toon, V. Sherlock, N. M. Deutscher, C. Liu, D. G. Feist, and P. O. Wennberg (2015), The Total Carbon Column Observing Network's GGG2014 Data Version, Pasadena, California.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395

https://eyeclima.eu

BRUSSELS, 11 12 2023

Funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union. Neither the European Union nor the granting authority can be held responsible for them.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101081395