Abstract ID # 108

Measurements of greenhouse gases from ground-based remote sensing and in-situ instruments and their application for satellite validation

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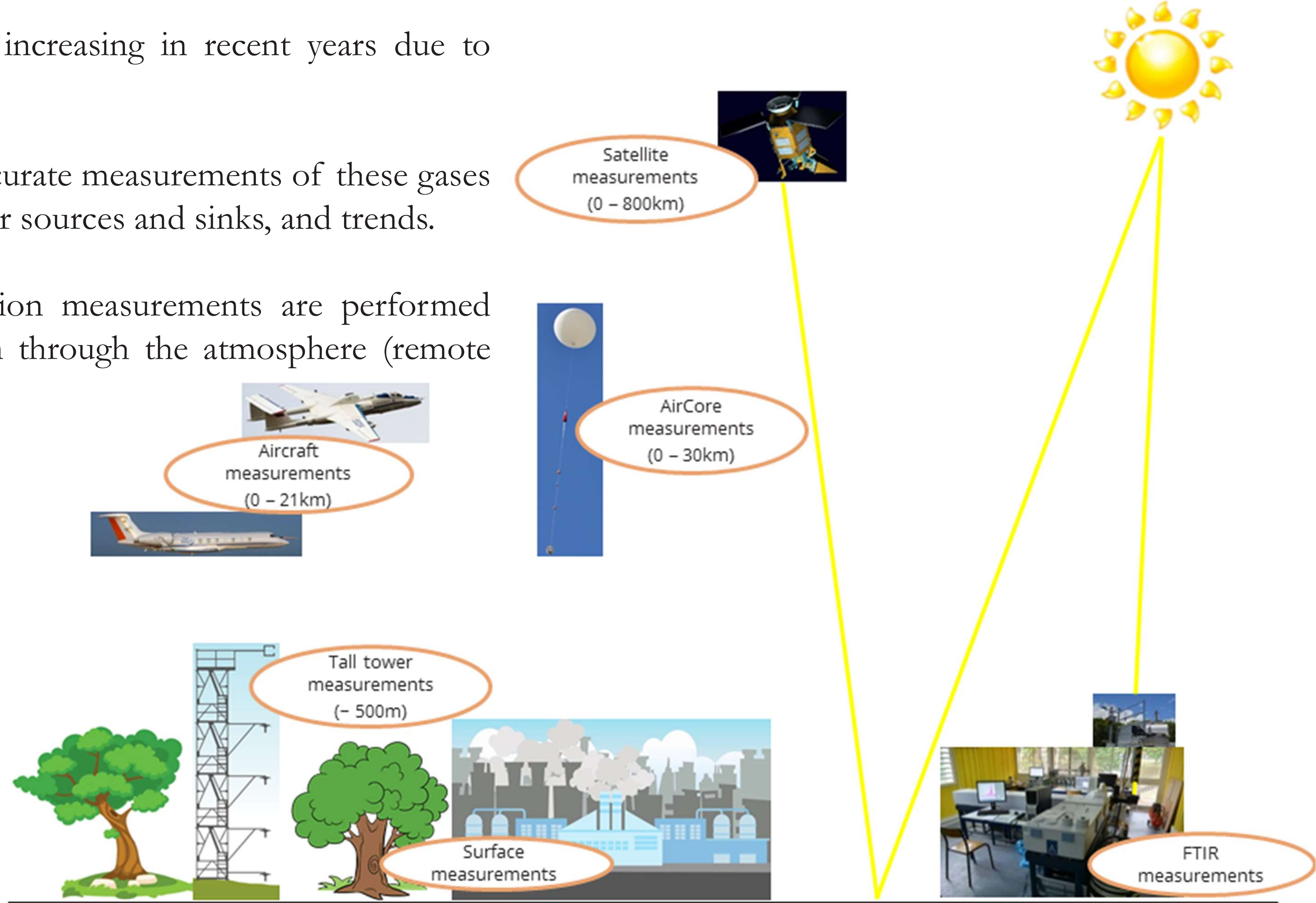
Atmospheric greenhouse gas measurements

Atmospheric GHGs have been steadily increasing in recent years due to anthropogenic activities

Continuous monitoring of precise and accurate measurements of these gases is of utmost importance to determine their sources and sinks, and trends.

Atmospheric greenhouse gas concentration measurements are performed locally (in-situ) and as integrated column through the atmosphere (remote sensing)



GHG measuring satellites

GHG measuring satellites with high sensitivity at the Earth's surface providing global information:

Pioneering space-based greenhouse gas sensors:

- SCIAMACHY onboard ESA's ENVISAT (2002 – 2012)
- GOSAT & GOSAT-2 (Japan); OCO-2 & OCO-3 (NASA); TanSat AGCS, Feng Yun-3D GAS and GaoFen-5 GMI (China); Copernicus Sentinel-5 Precursor and commercial GHGSat

Future missions under development and planning:

- MicroCarb (CNES); MERLIN (CNES/DLR); GeoCarb (NASA); GOSAT-GW (Japan); Copernicus CO2M, ESA/EUMETSAT Sentinel-5, …

Significant improvements in measurement and retrieval techniques over the last 18 years

Future improvements are expected to further improve the data quality and space-borne data become more important for carbon cycle research

As global GHG data from satellites become more abundant, high quality reference measurements are needed to detect and quantify spatial biases and / or temporal drifts in the sensor.

ENVISAT (2002 – 2012)

Footprint 1800 km^2

Sentinel-5 Precursor (2017 –)

Pixel resolution of 5.5 x 7 km^2

Swath of 2600 km across track

GHG measurement network

- Ground-based in-situ measurement network (surface air sampling, tower ~500 m)
  - Derived fluxes are accurate but are affected by surface exchange and vertical transport – highly variable but poorly simulated in global models
  - Limited / no column measurements which limits its use for satellite validation

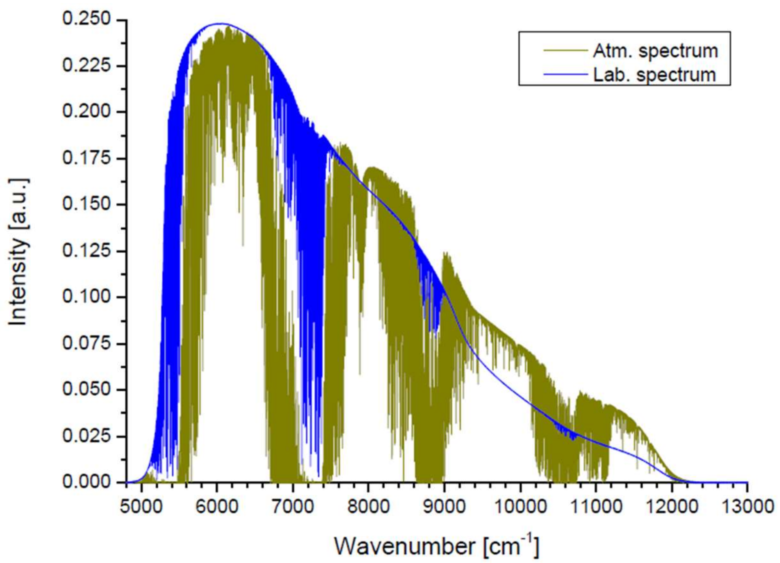
- In-situ aircraft (0 – 20 km) / AirCore (0 – 35 km) measurements
  - Derived fluxes are accurate, measurements are possible at several altitudes, but very sparse

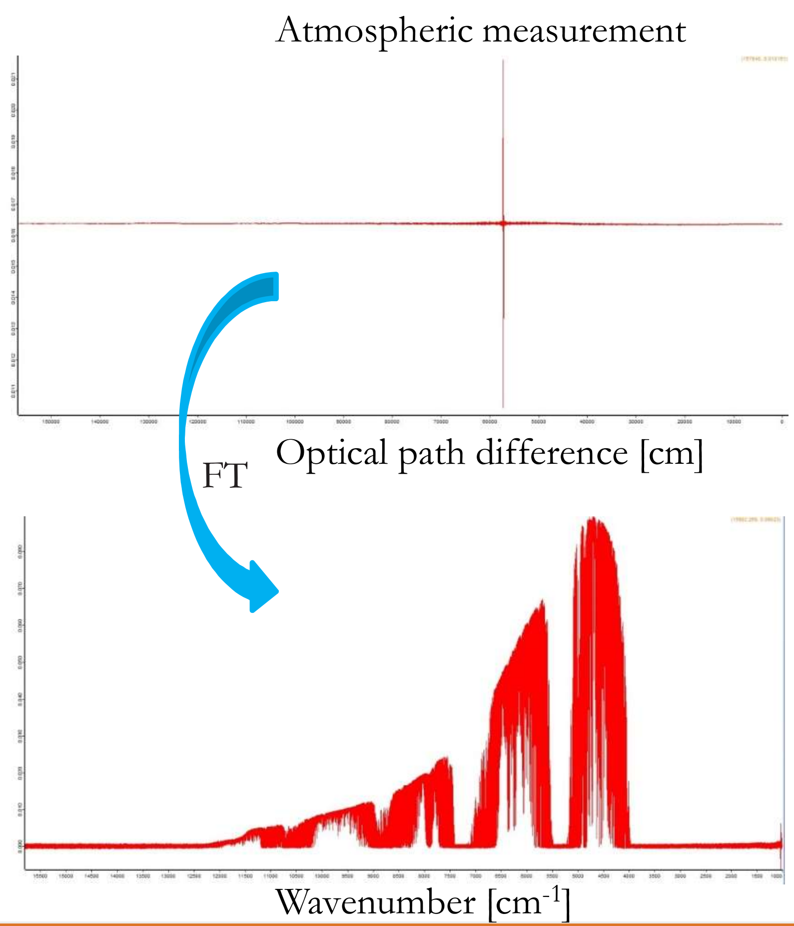
- Ground-based remote sensing measurement networks (NDACC-IRWG, TCCON, COCCON, …)
  - Column measurements of GHGs in the mid-IR (NDACC-IRWG) and near-IR (TCCON, COCCON) using FTS instruments, measurement sites world wide spanning from Arctic to Antarctic locations
  - Carbon cycle science and validation of satellite instruments
  - High precision and inter-calibration accuracy – TCCON, COCCON
  - Column measurements of GHGs in the near-IR using portable, low cost FTS (e.g., EM27/SUN, Vertex70/80, IRcube, …)

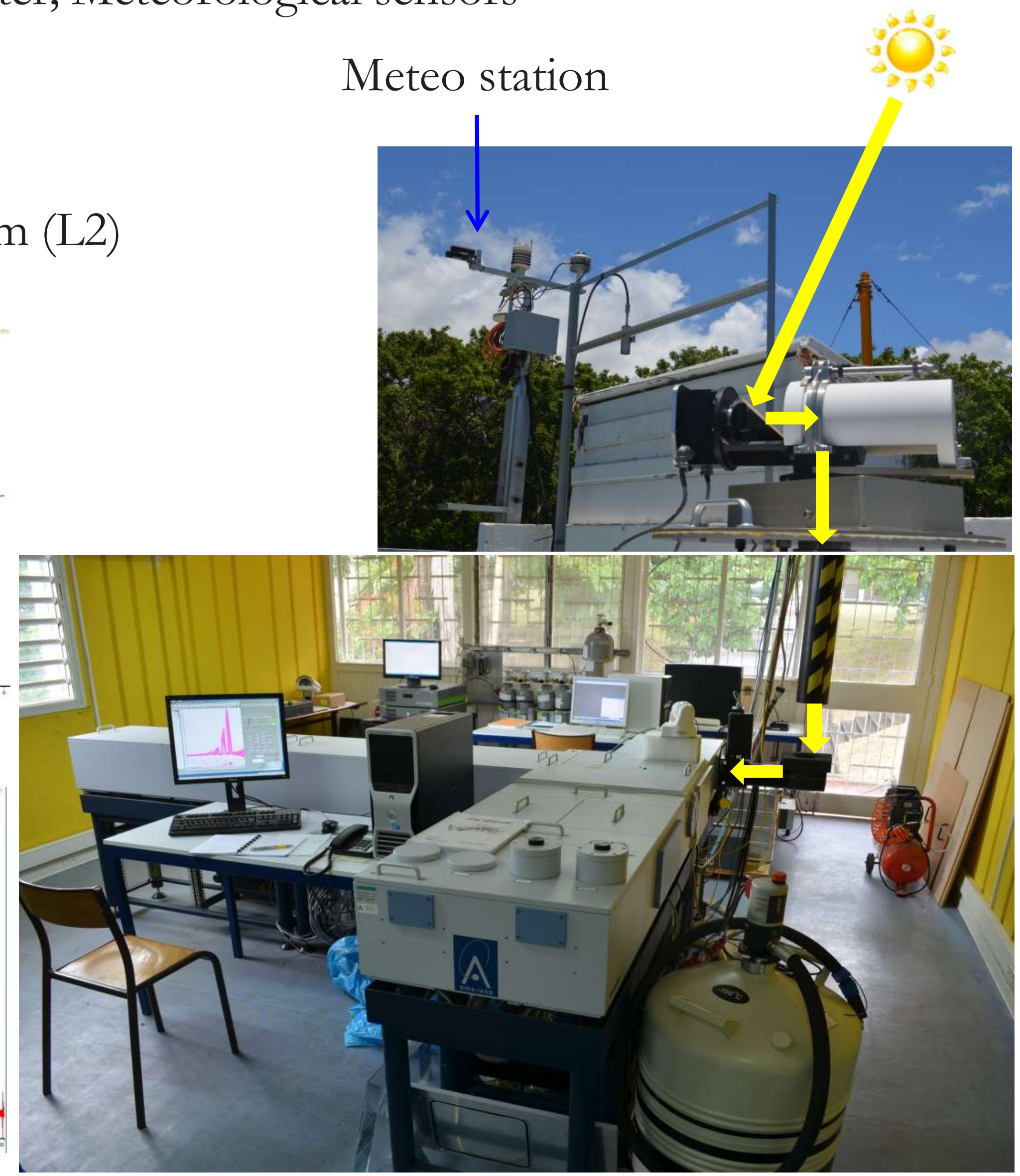
Solar absorption measurements using FTIR spectrometry

Sun as the source; Sun tracker + Fourier transform infrared (FTIR) spectrometer; Meteorological sensors

Recorded signal is interferogram (L0)
Interferogram transformed via FT into spectrum (L1)
Spectrum is used to retrieve information of the gases using a retrieval algorithm (L2)





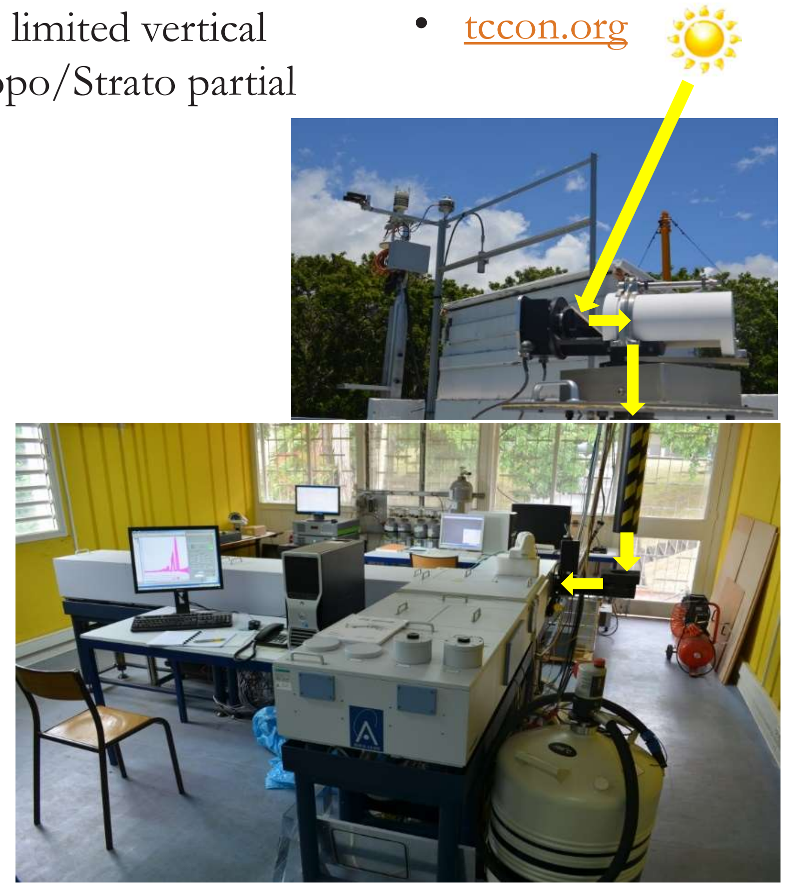


NDACC-IRWG

- Infrared Working Group (IRWG) of the Network for the Detection of Atmospheric Composition Change (NDACC)
- Bruker 120HR/125HR
- Resolution 0.0036cm^{-1}
- Profile retrievals (with limited vertical resolution, at least Tropo/Strato partial columns)
- ndacc.org

TCCON

- Total Carbon Column Observing Network
- Bruker 125HR
- Resolution 0.02cm^{-1}
- Profile scaling retrievals
- tccon.org



COCCON

- Collaborative Carbon Column Observing Network
- Bruker EM27/SUN
- Resolution 0.5cm^{-1}
- Profile scaling retrievals
- http://www.imk-asf.kit.edu/english/COCCON.php

NDACC-IRWG

- Bruker 120HR/125HR
- Resolution 0.0036cm^{-1}
- Profile retrievals (with limited vertical resolution, typical Tropo/Strato partial columns)
- Targets: O3, CH4, N2O, (CO2, HCHO, SF6, CFC, HCFC, H2O, HDO not official)
  CO, HNO3, HCL, HF, HCN, C2H6, CLONO2 (C2H2, PAN, OCS, CH3OH, NH3, HCOOH, NO2 not official)
- Retrieval software: SFIT or PROFFIT
- Measurements every ±10’
- Spectral range: SWIR, MIR and thermal IR
- 21 stations worldwide
- no central processing, QA/QC for selected targets in CAMS operational validation

TCCON

- Bruker 125HR
- Resolution 0.02cm^{-1}
- Profile scaling retrievals (profile retrievals are in development)
- Targets: CO2, CH4, N2O, H2O, HDO, CO, HF
- Retrieval software GGG
- Measurements every ~ 3’
- Spectral range: SWIR
- 28 stations worldwide
- central QA/QC

COCCON

- Bruker EM27/SUN
- Resolution 0.5cm^{-1}
- Profile scaling retrievals
- Targets: CO2, CH4, CO
- Retrieval software PROFFAST
- Measurements every ~ 1’
- Spectral range: SWIR
- > 60 instruments worldwide (some fixed sites but mostly for campaign operations)
- central calibration & processing facility at KIT

NDACC-IRWG

- Operational usage in: CAMS validation, EUMETSAT IASI validation, ESA TROPOMI validation (RD delivery through CAMS27)

https://global-evaluation.atmosphere.copernicus.eu
http://cdop.aeronomie.be/validation/valid-results
https://mpc-vdaf-server.tropomi.eu

- Recent and ongoing harmonization efforts in QA4ECV, GAIA-CLIM, CAMS27, C3S-311a-Lot3. Upcoming SFIT/PROFFIT: improve harmonization of uncertainties evaluation, improve spectroscopy
- Selected NDACC stations to join ACTRIS EU research infrastructure: with central processing facility, training, QA/QC, …
- CO_2 retrieval strategy under development (UBremen & BIRA)

TCCON

- Operational usage in: CAMS validation, ESA TROPOMI validation (limited RD delivery), OCO-2/3 & GOSAT/2 cal/val, …
- GGG2020 will improve prior profiles (shape and possible bias), verify CO calibration factor, improve spectroscopy, reduce remaining airmass and H_2O dependences, reduce scatter in CO product, improve diagnostics for instrumental issues
- Negotiations are ongoing for selected TCCON stations to join ICOS EU research infrastructure, with central processing facility
- Profile retrievals under development. Tropospheric partial columns can be derived indirectly

COCCON

- Operational usage in: ESA TROPOMI validation (started in 2020), OCO-2/3, GOSAT/2, …
- Planned update foreseen for PROFFAST, redefined spectroscopic descriptions + improved linelists
- EM27/SUN as travelling standard for within TCCON, COCCON can complement TCCON, support by ESA for COCCON-PROCEEDS and follow-up crucial for current capabilities of COCCON
- Towards extension of COCCON with Vertex70 and IRcube (2 other low resolution FTIR instruments – with higher spectral resolution and additional species) – ESA FRM4GHG project https://frm4ghg.aeronomie.be

Ongoing comparisons NDACC/TCCON in recent papers: https://doi.org/10.5194/amt-12-5979-2019 (CO), https://doi.org/10.5194/amt-12-1393-2019 (N_2O), CH_4 Profile retrievals from TCCON spectra: https://doi.org/10.5194/amt-12-6125-2019, FRM4GHG paper – low resolution FTIR comparison to TCCON: https://doi.org/10.5194/amt-2019-371

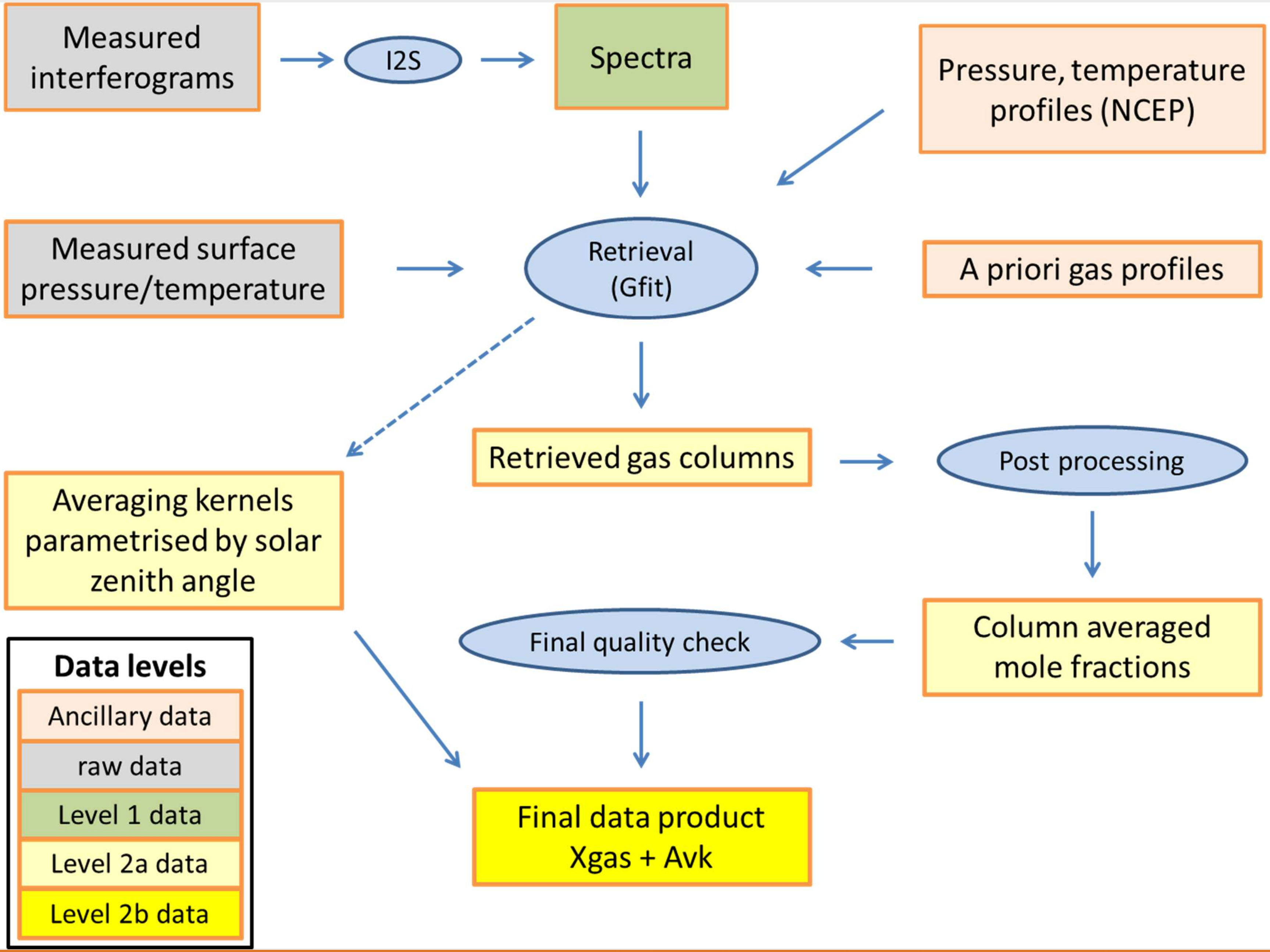
TCCON processing chain

Xgas = column averaged dry air mole fraction of the gas

$$\text{Xgas} = \frac{\text{gas}_{\text{column,dry}}}{O_{2,\text{column,dry}}} \times 0.2095$$

where 0.2095 is the dry air O_2 mole fraction.

T. Warneke, M. K. Sha, M. De Mazière, L. Rivier, J. Tarniewicz, Scientific and technical concept for the integration of ground-based greenhouse gas remote sensing into ICOS and resulting costs, https://www.icos-cp.eu/sites/default/files/2020-04/D1.5.%20Scientific-technical%20concept%20for%20the%20integration%20of%20European%20TCCON%20sites%20into%20ICOS%20and%20resulting%20costs.pdf, RINGO (European Union's Horizon 2020 research and innovation programme under grant agreement No 730944) Deliverable D1.5, 2019.



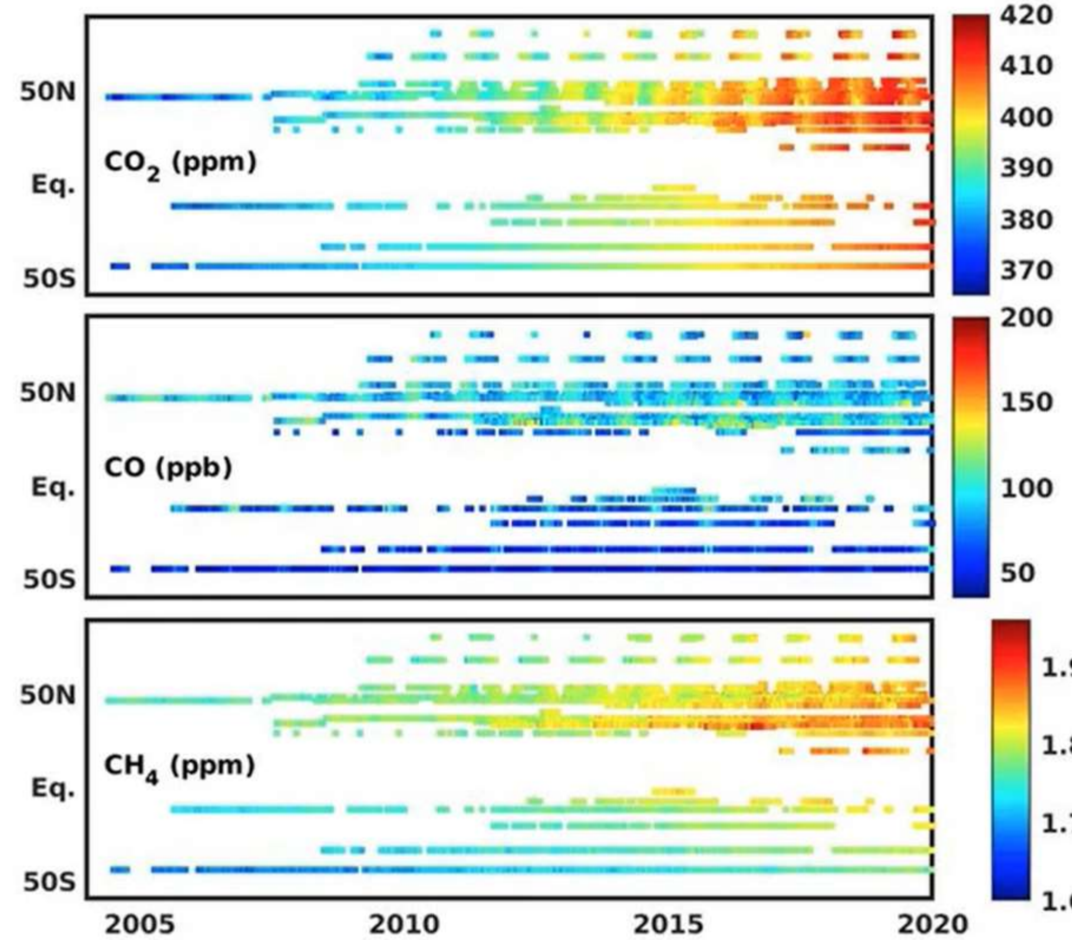
Ground-based FTIR remote sensing – TCCON

Total Carbon Column Observing Network – TCCON

- Every instrument runs in as similar configuration as possible
- Regular ILS measurements with HCl/N2O cell to monitor instrument's alignment
- Spectral fitting and data processing homogenized using GFIT code
- Calibration to the World Meteorological Organization (WMO) reference standards using vertically resolved in-situ measurements

TCCON provides complementary information to the in-situ measurements
TCCON is the reference network for calibration and validation of GHG satellites
Validation using TCCON links the satellite data to the in-situ standards of the WMO
TCCON supports modelling efforts by providing verification datasets and assimilation dataset – e.g., model from the Copernicus Atmospheric Monitoring Service (CAMS)

Contribute to the carbon cycle community by providing high quality data with support for their interpretation



Source: Debra Wunch

Sentine-5 Precursor XCH4 validation results

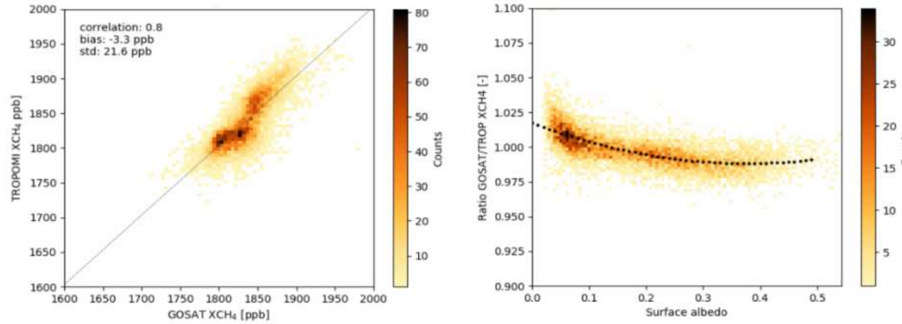
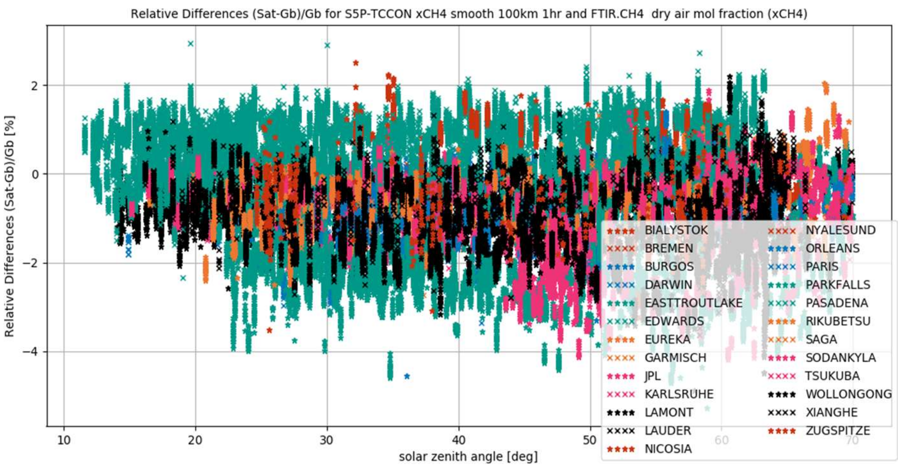
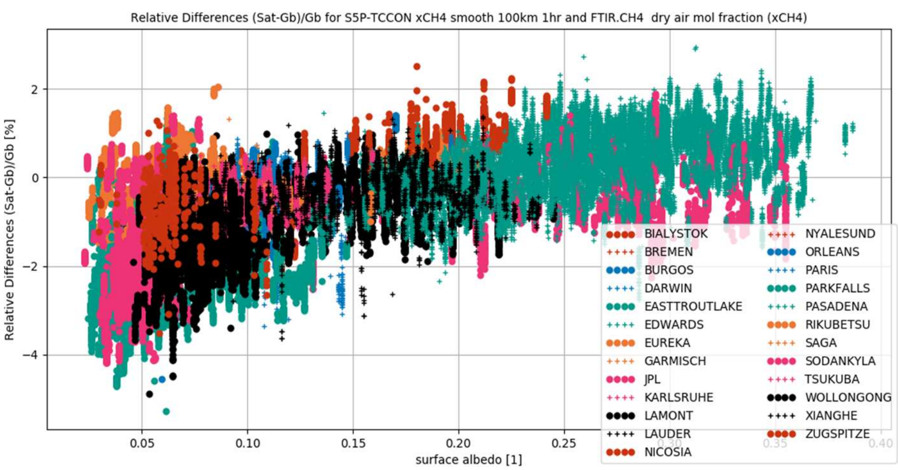


Figure 5: Left panel: correlation plot of TROPOMI and GOSAT CH_4 measurements. Right panel: ratio of GOSAT and TROPOMI CH_4 as a function of surface albedo. The black dashed line represents the second order polynomial fit from which the correction coefficients in Eq. 54 have been derived.

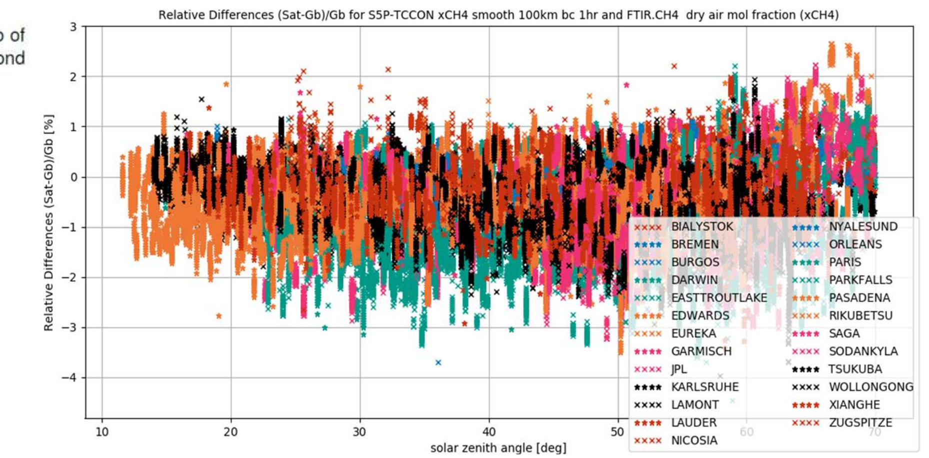
Reference: ATBD for Sentinel-5 Precursor Methane Retrieval

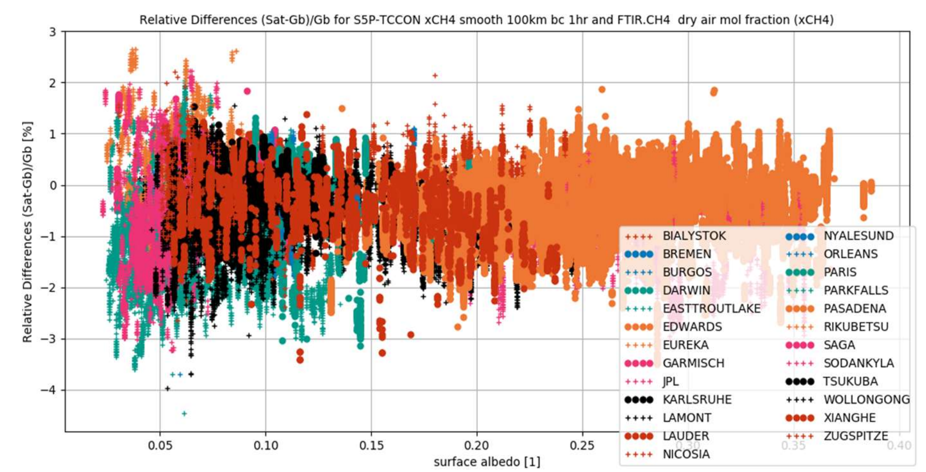
S-5p Standard product



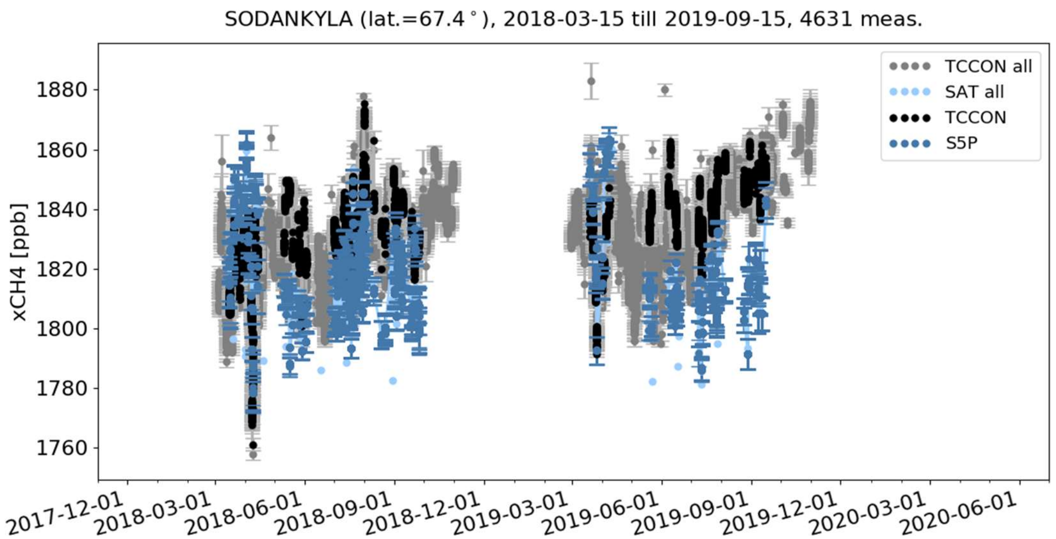


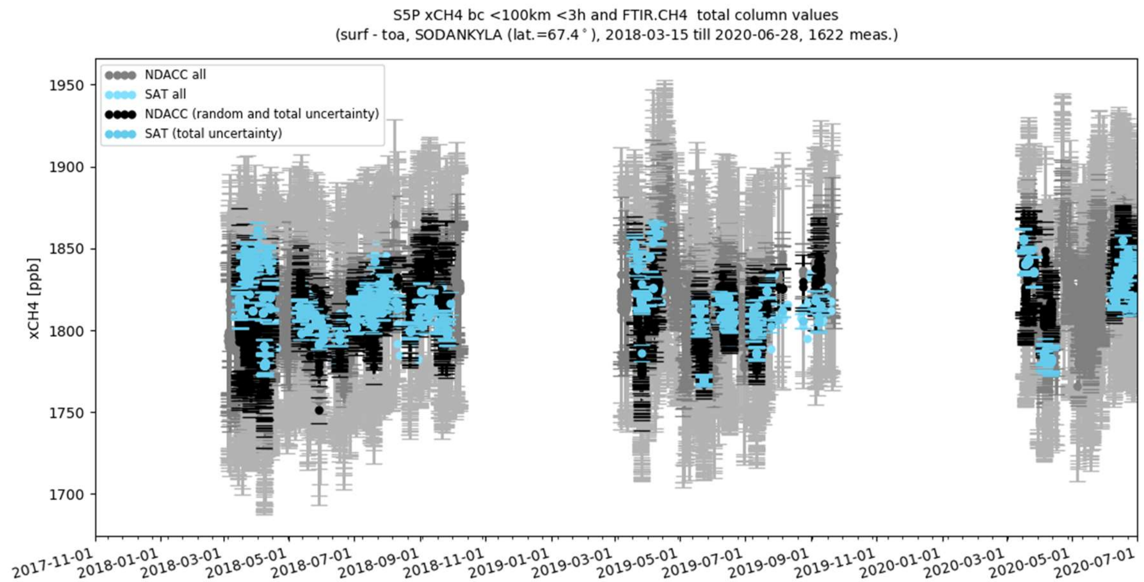
S-5p Bias corrected product

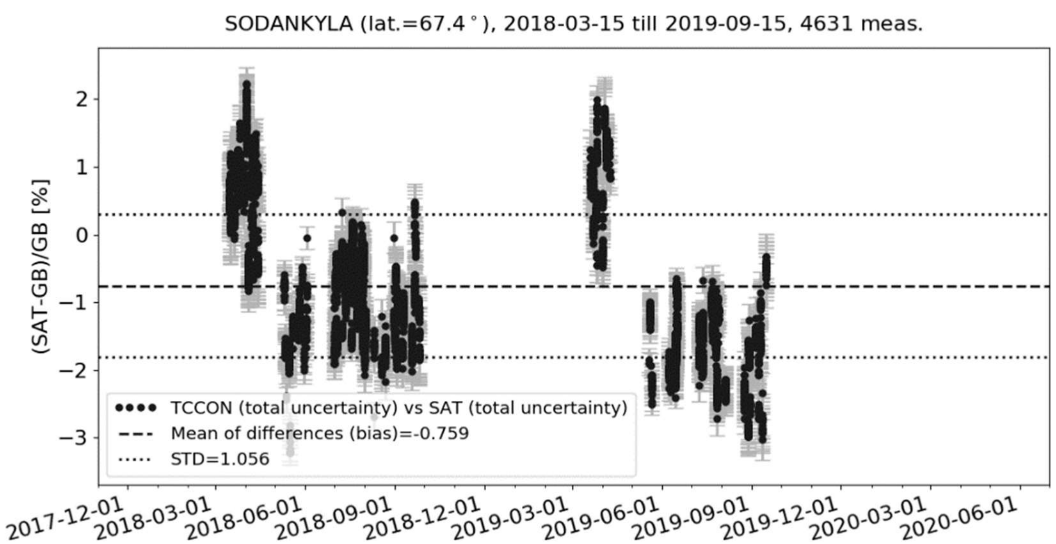


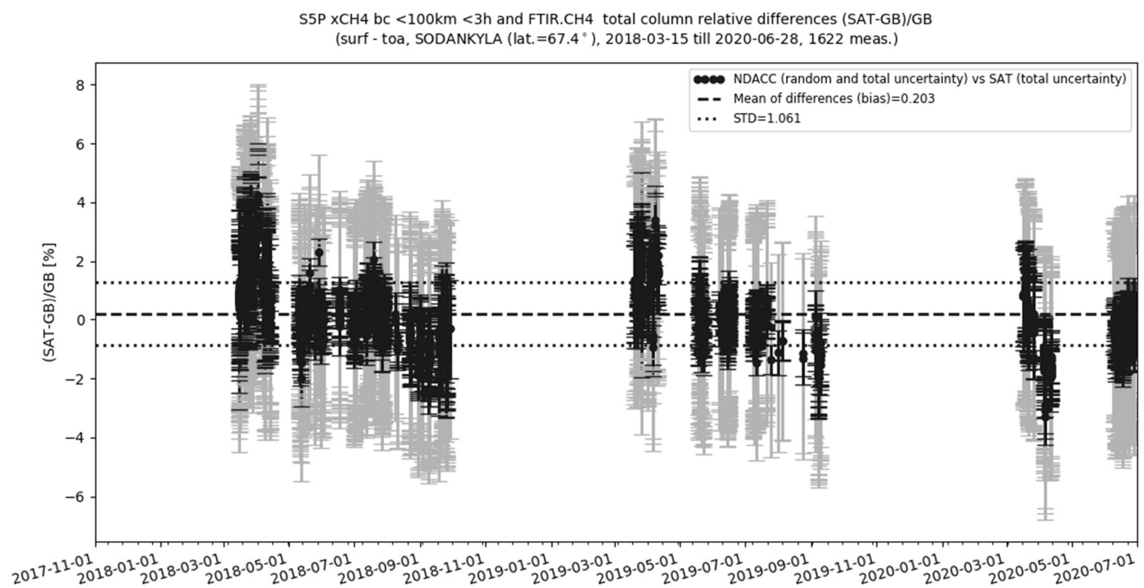


S-5p XCH4 validation using TCCON and NDACC









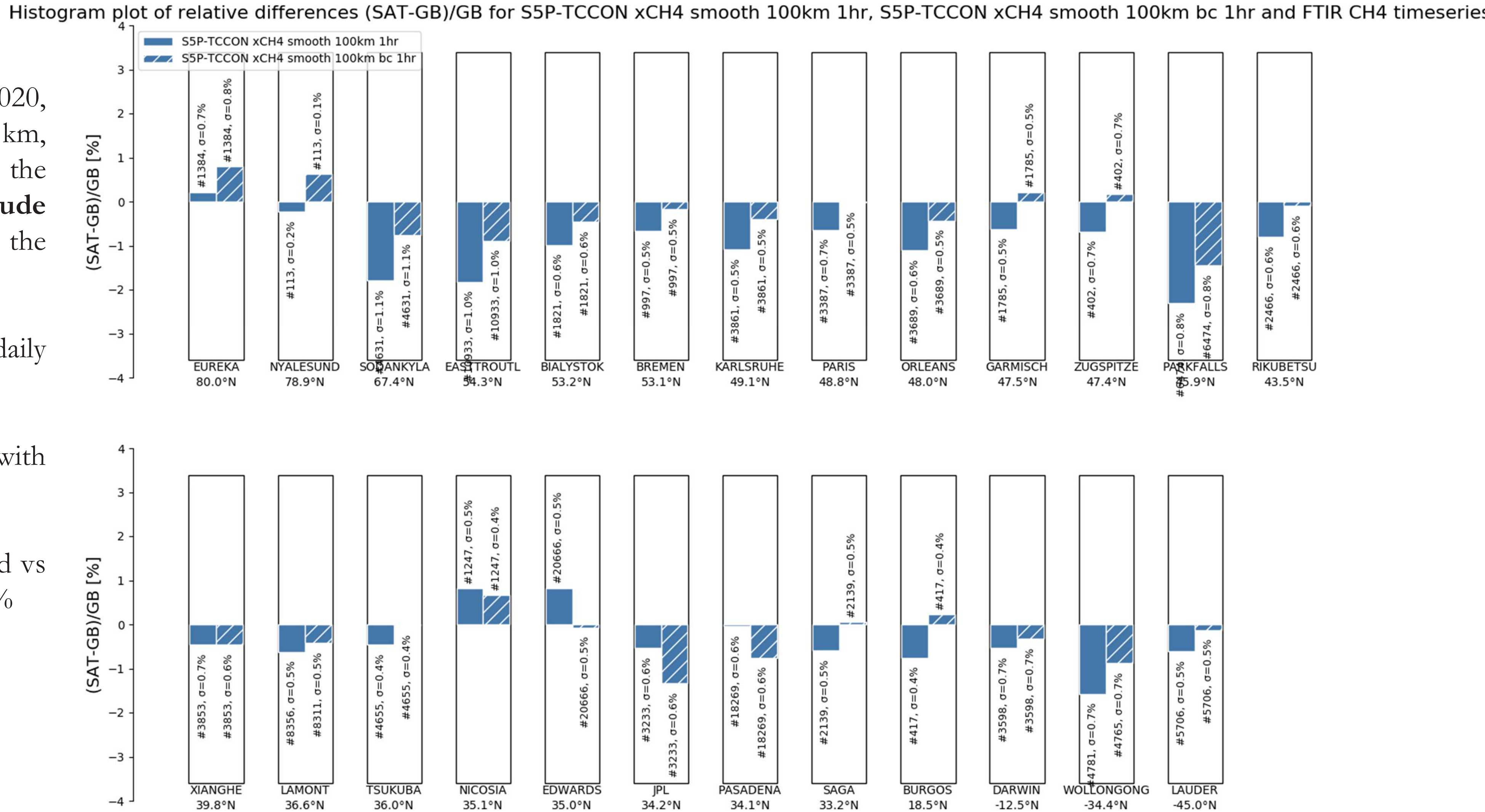
Bias corrected vs standard S-5p XCH4 product validation using TCCON

Validation period: 15/11/2017 – 01/07/2020, Time delta = 1hr, Geo-distance = 100 km, **smooth** case = S-5p CH4 a priori is used as the common a priori (Rodgers, 2003), **altitude correction** is done for each satellite pixel to the ground-based station height.

Relative difference (SAT-GB)/GB in % for daily mean of CH4

Low-albedo sites show higher differences with larger scatter

Mean difference in bias between bias corrected vs standard XCH4 product case = 0.43% ± 0.54%
Median = 0.60%



Bias corrected XCH4 product: mean bias -0.25% ± 0.56%; median = -0.21%; mean sd = 0.58% validation w.r.t TCCON
Standard XCH4 product: mean bias -0.68% ± 0.71%; median = -0.63%; mean sd = 0.60% validation w.r.t TCCON

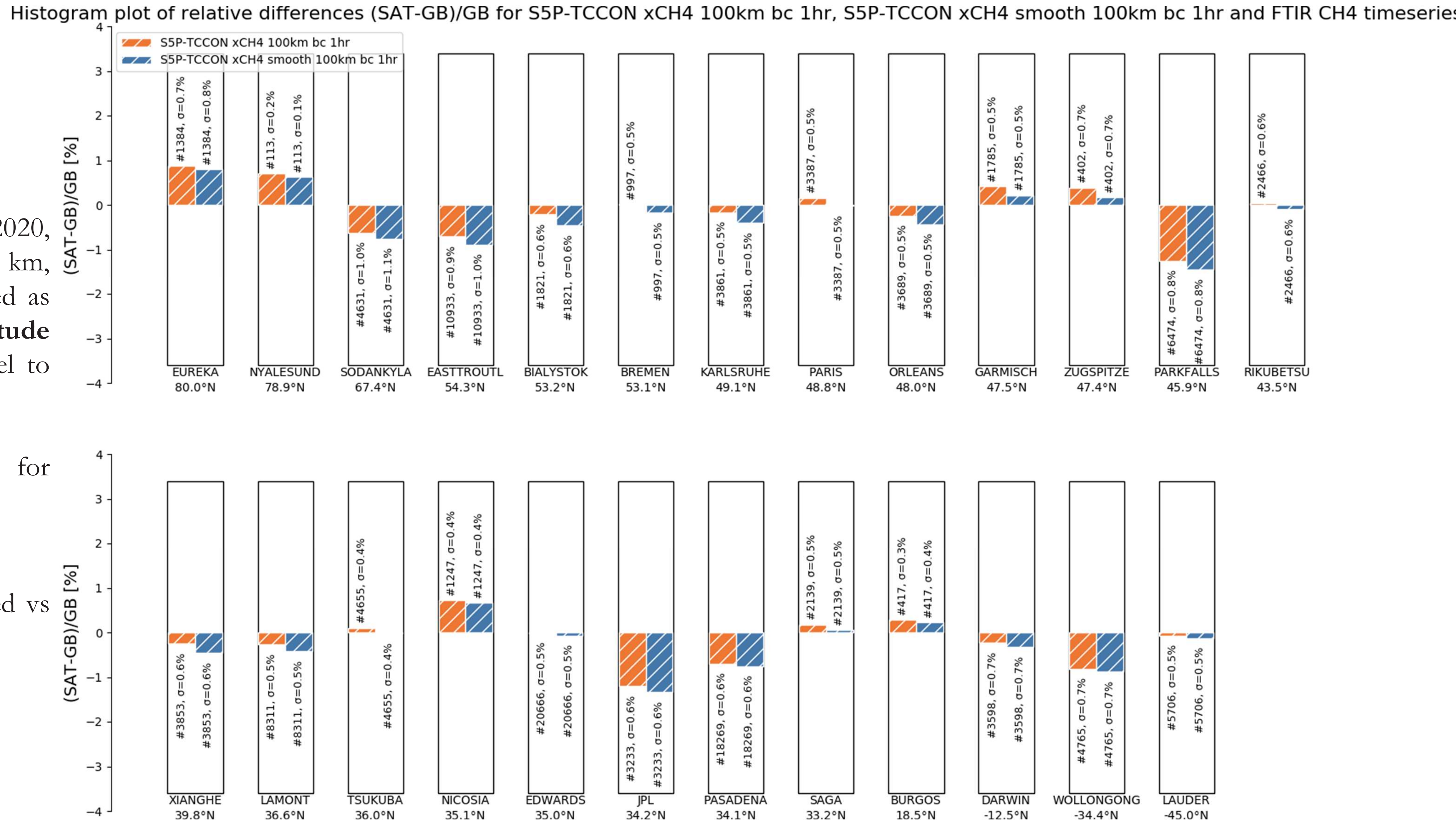
Compliant with mission requirement accuracy (1.5%) and precision (1%)

Smoothing effect – a priori substitution – S-5p XCH4 vs TCCON

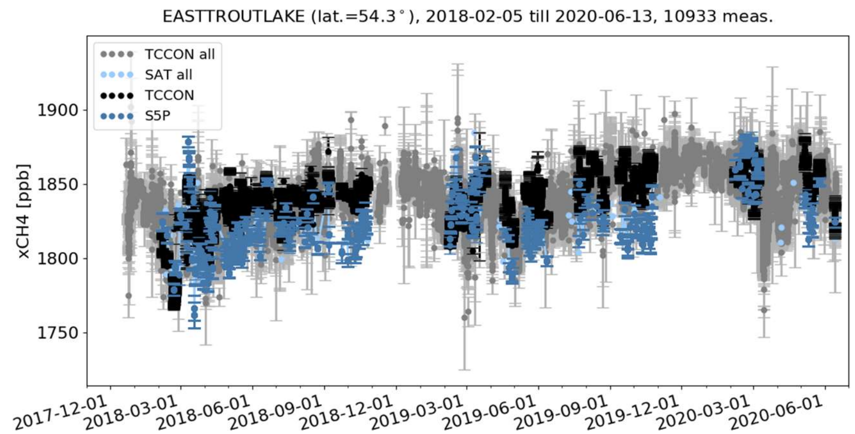
Validation period: 15/11/2017 – 01/07/2020, Time delta = 1hr, Geo-distance = 100 km, **smooth** case = S-5p CH4 a priori is used as the common a priori (Rodgers, 2003), **altitude correction** is done for each satellite pixel to the ground-based station height.

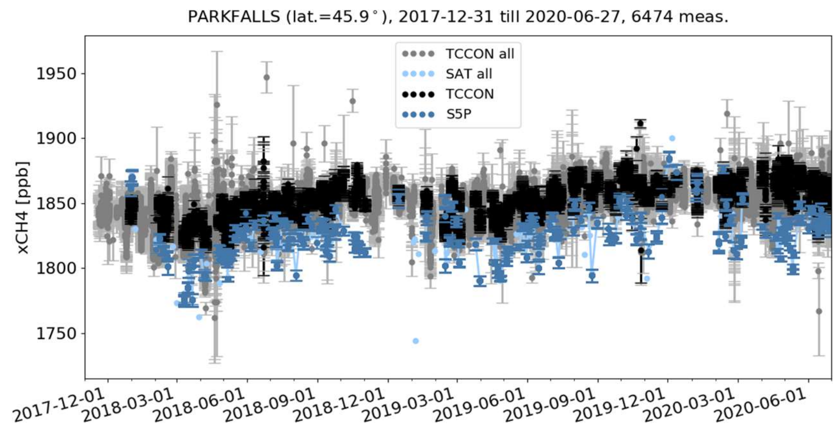
Relative difference (SAT-GB)/GB in % for daily mean of CH4

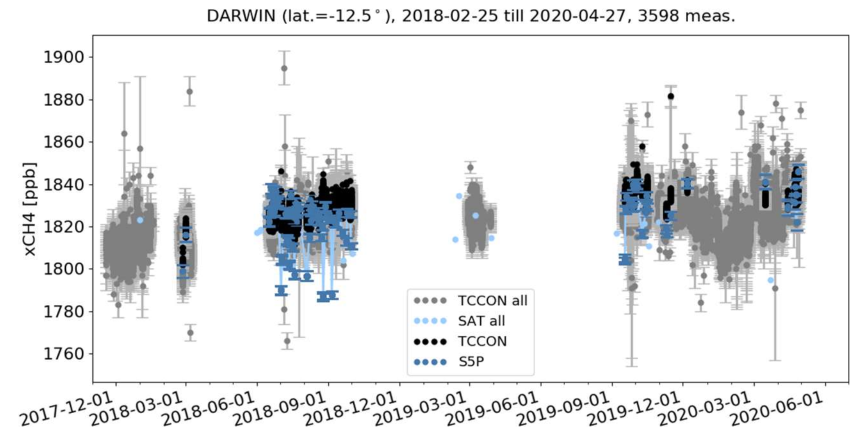
Mean difference in bias between smoothed vs no smoothed case = -0.14% ± 0.06%
Median = -0.14%

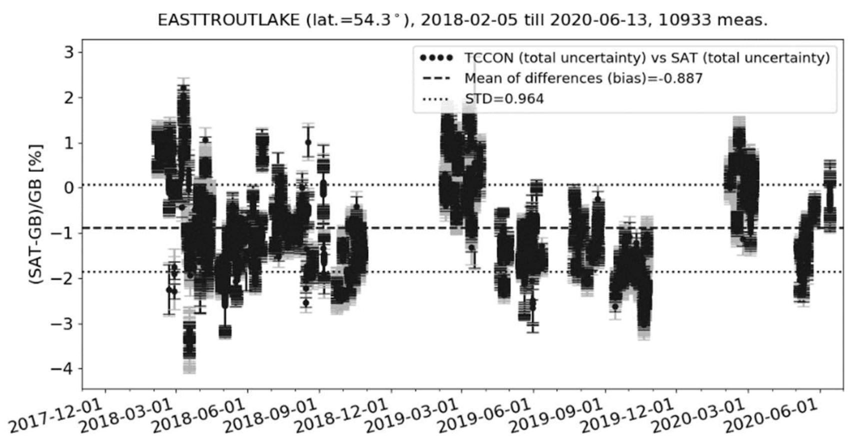


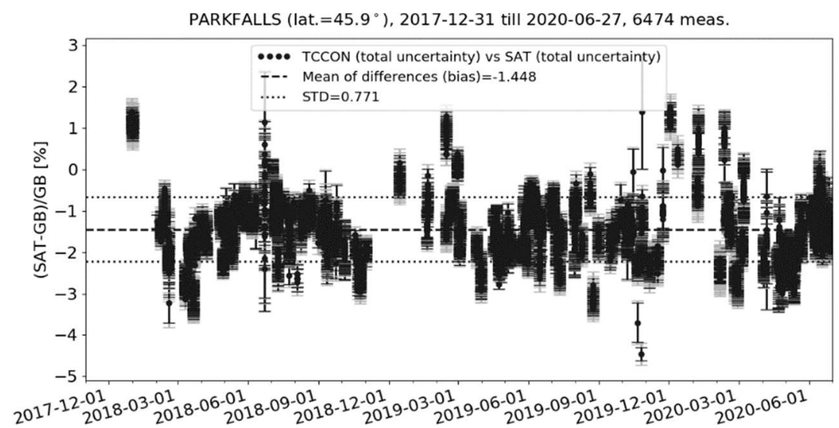
S-5p vs TCCON validation results – XCH4

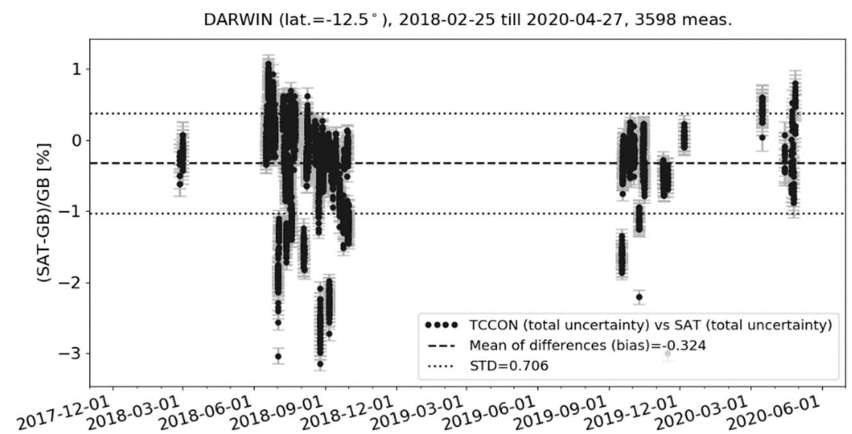












- High bias during spring time (large difference of a priori to true atmospheric state and their influence on the instrument sensitivities)
- Potential seasonal cycle in the residual bias

- Identification of low satellite pixels

Smoothing effect – a priori substitution – S-5p XCO vs TCCON

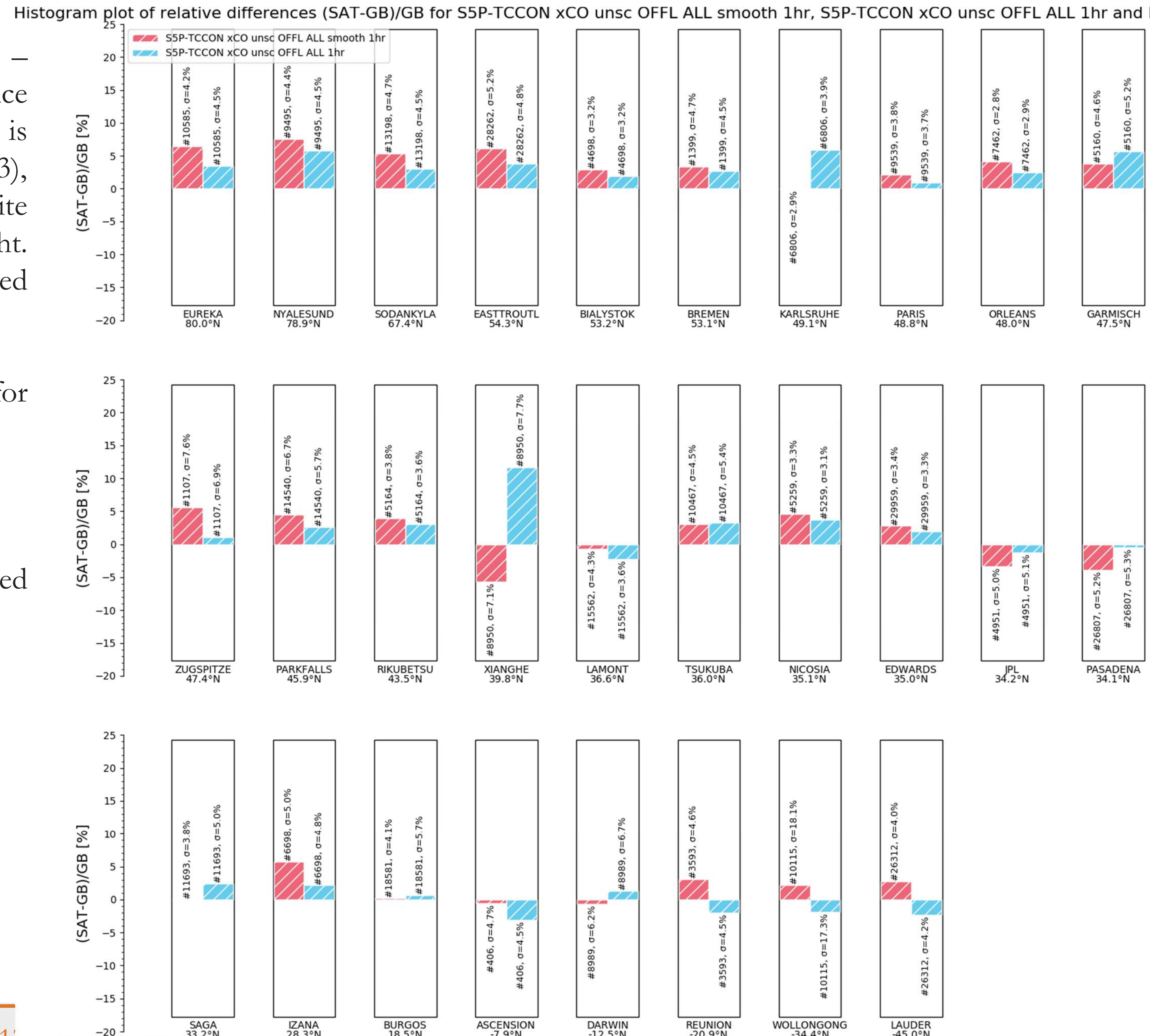
Validation period: 15/11/2017 – 01/07/2020, Time delta = 1hr, Geo-distance = 50 km, **smooth** case = S-5p CO a priori is used as the common a priori (Rodgers, 2003), **altitude correction** is done for each satellite pixel to the ground-based station height. Here unscaled TCCON XCO is calculated without using the in-situ calibration factor.

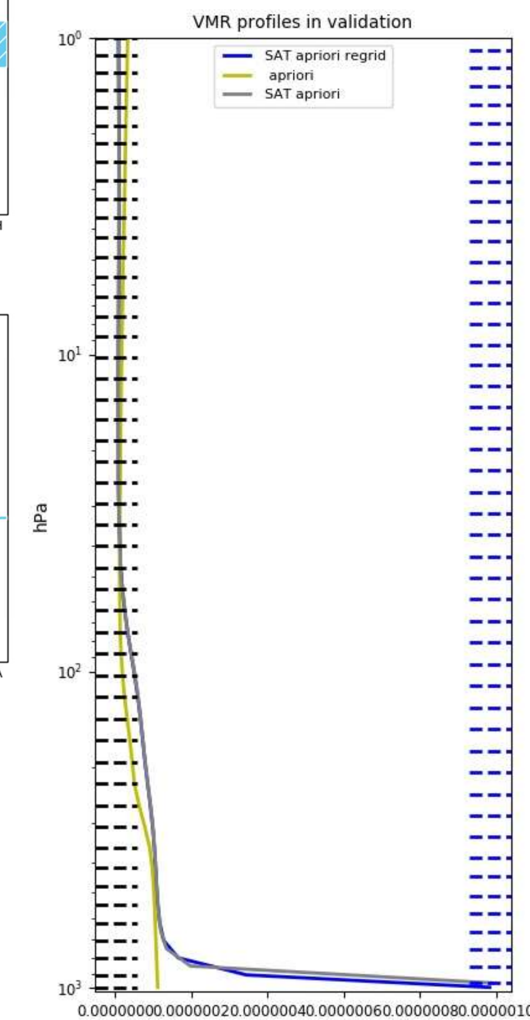
Relative difference (SAT-GB)/GB in % for daily mean of CO

Polluted sites show the strongest change

Mean difference in bias between smoothed vs no smoothed case = 0.32 % ± 4.26 %
Median = 0.94%

Compliant with mission requirement accuracy (15%) and precision (<10%)





Validation requirements for S-5p CH4 and CO products

Specific validation requirements have been identified by the S-5p level-2 developers and the validation team members

spatial validation requirements, e.g.,

global, over land, tropics, urban, polluted conditions, background conditions

temporal validation requirements, e.g.,

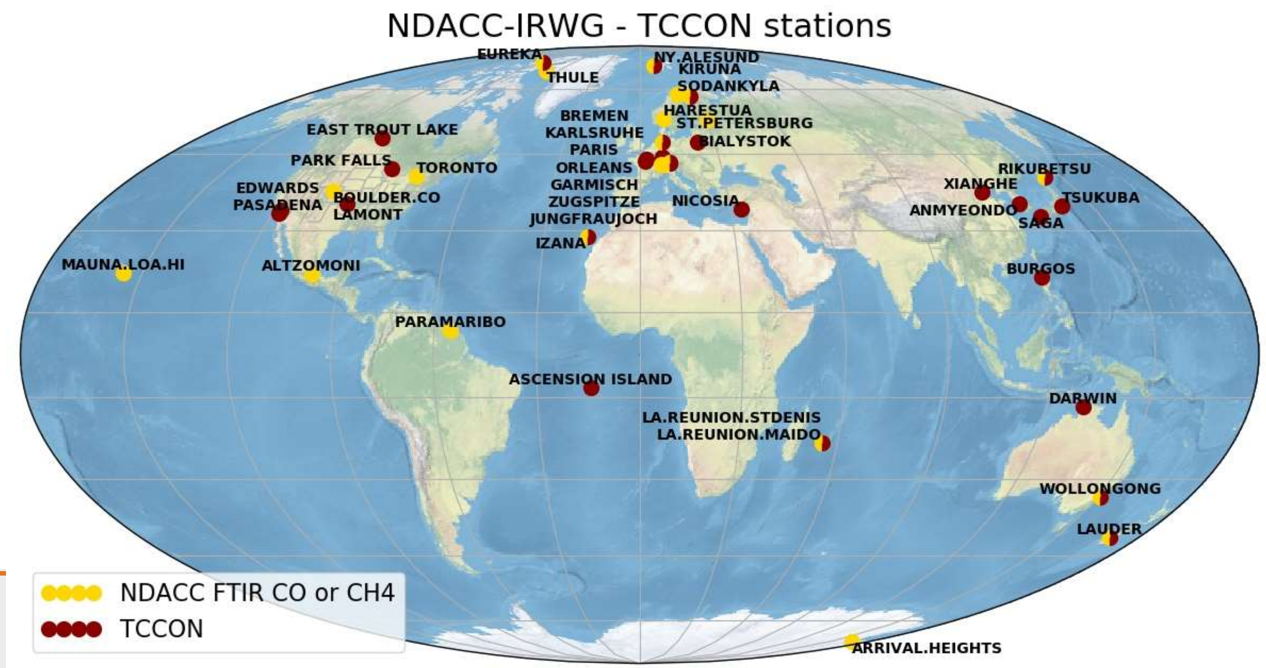
long time series, seasonal cycle

special validation requirements, e.g.,

artic regions, emission regions, humid & dry atmospheric conditions, high & low albedo conditions

specific validation requirements, e.g.,

observation of localized sources to deduce detection limit for small scale variations, detection of possible spurious variations as a function of the observed line-of-sight, detection of possible problems under less than ideal meteorological conditions



ESA funded FRM4GHG campaign

Fiducial Reference Measurements for Ground-Based Infrared Greenhouse Gas Observations (FRM4GHG) is a **European Space Agency (ESA) funded project** focusing on the **intercomparison** of instruments and the **harmonization** of retrievals and products from collocated new and established GHG observation **ground-based infrared instrumentations** to get Fiducial Reference Measurements (FRMs) for Greenhouse Gases (GHGs). These datasets will also be used for the **validation of satellite missions** targeting: carbon dioxide (CO2); methane (CH4); carbon monoxide (CO); other climate relevant trace gases (e.g. formaldehyde (HCHO))

Lead by: Justus Notholt (University of Bremen) and Martine De Mazière (BIRA-IASB)
https://frm4ghg.aeronomie.be/

Sha, M. K., De Mazière, M., Notholt, J., Blumenstock, T., Chen, H., Dehn, A., Griffith, D. W. T., Hase, F., Heikkinen, P., Hermans, C., Hoffmann, A., Huebner, M., Jones, N., Kivi, R., Langerock, B., Petri, C., Scolas, F., Tu, Q., and Weidmann, D.: Intercomparison of low and high resolution infrared spectrometers for ground-based solar remote sensing measurements of total column concentrations of CO_2, CH_4 and CO, Atmos. Meas. Tech. Discuss., https://doi.org/10.5194/amt-2019-371, 2019.

FRM4GHG instruments setup at Sodankylä (67.37 N, 26.63 E)

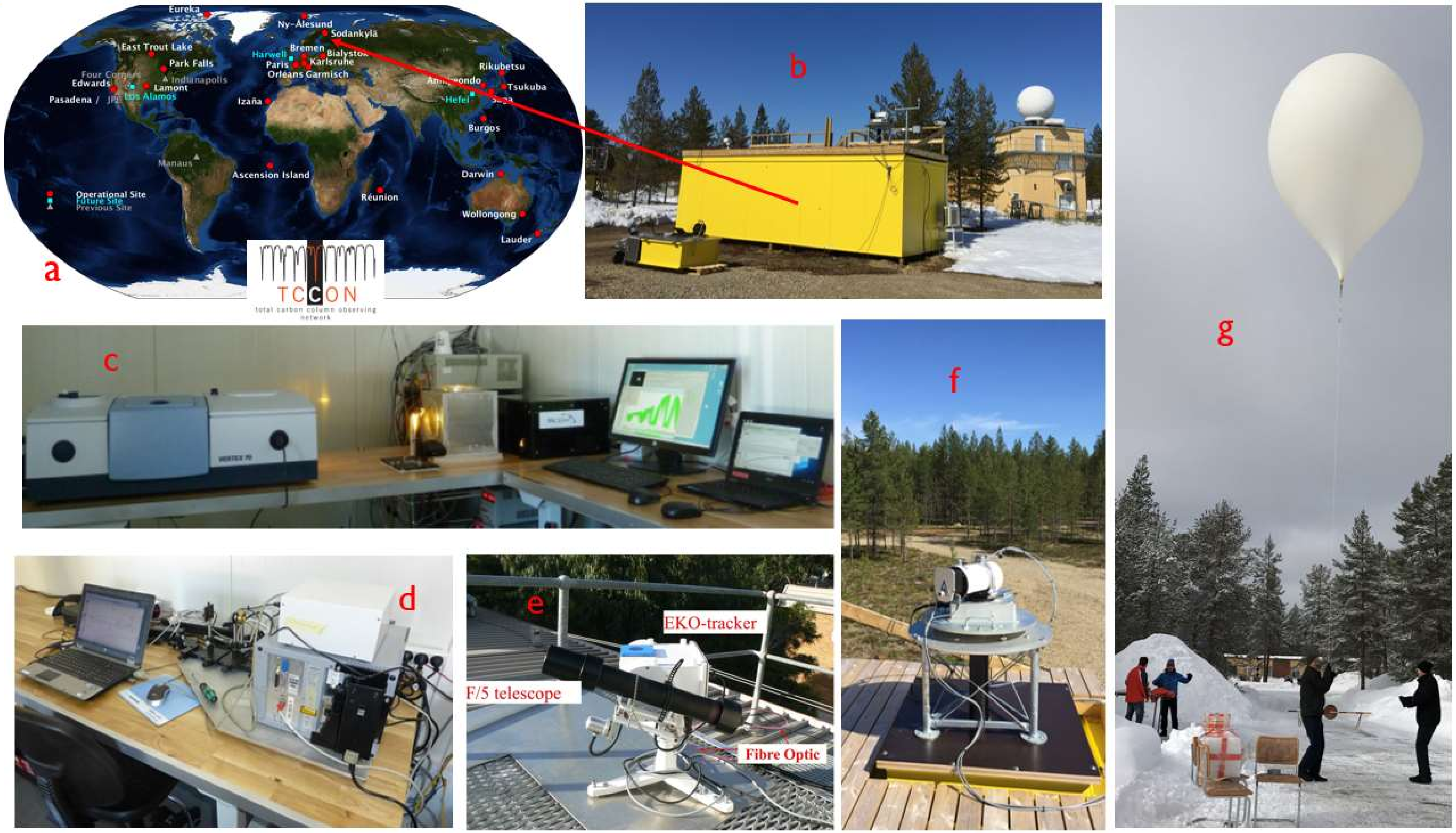


Fig. 1: (a) TCCON sites, (b) FRM4GHG container and EM27/SUN in front, (c-left) Vertex70 and (c-right) LHR, (d) IRCube, (e) suntracker for IRCube, (f) suntracker for Vertex70 and LHR, (g) Aircore launch at Sodankylä site.

All instruments performed measurements during 2017 – 2019 at Sodankylä.

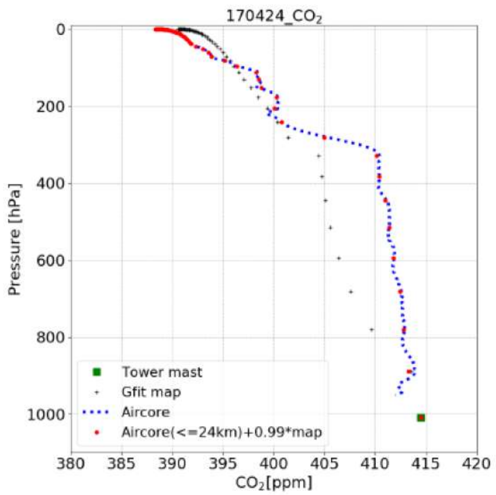
In 2019 IRcube performed measurements at two other TCCON sites (Wollongong and Darwin – Australia) instead of Sodankylä.

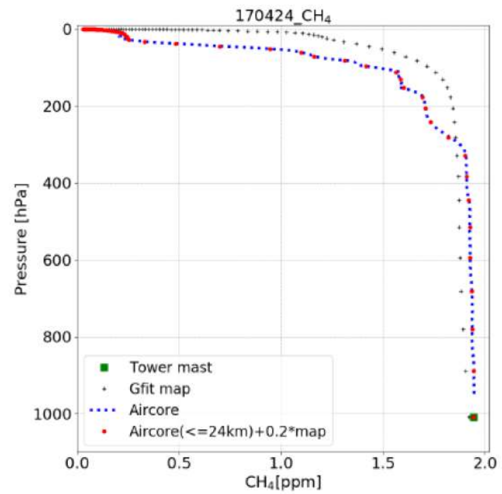
FRM4GHG campaign configuration

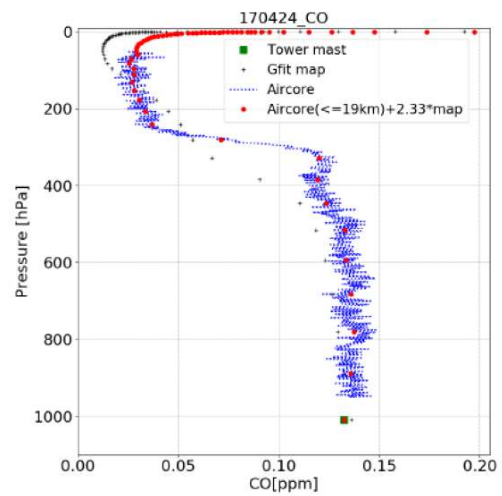
Table 1. List of instruments, their measurement properties and retrieval strategy for the FRM4GHG campaign.

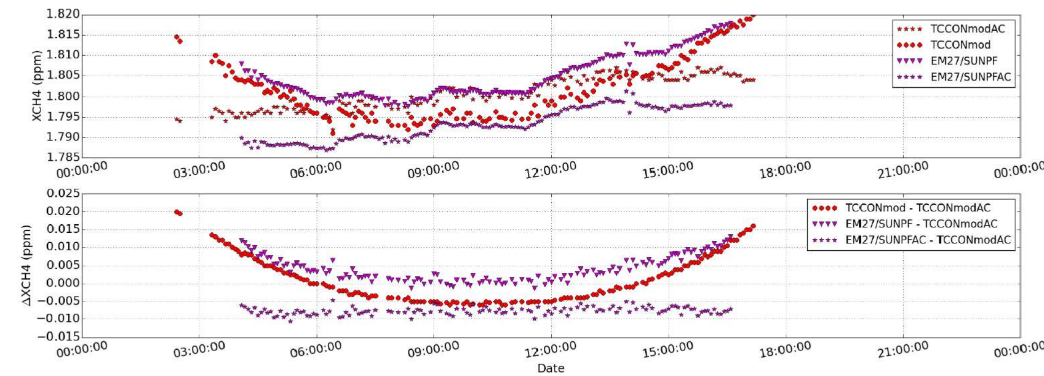
Instrument	Institute	Spectral range (cm^{-1})	Resolution (cm^{-1})	Measurement time (approx., min)	Sample scans	Main species	Dataset	Retrieval code
Bruker IFS 125HR (TCCON)	FMI	1800–15000	0.004	2.6	4	XCO_2, XCH_4, XCO @ 0.02 cm^{-1}	TCCON	GFIT 2014
Bruker Vertex70	Uni Bremen & BIRA-IASB	2500–15000	0.16	2.5	18	XCO_2, XCH_4, XCO @ 0.2 cm^{-1}	VERTEX70	GFIT 2014
Bruker IRcube	Uni Wollongong	4500–15000	0.5	1.7	33	XCO_2, XCH_4	IRCUBE	GFIT 2014
Bruker EM27/SUN (COCCON)	KIT	4000–9000	0.5	1	10	XCO_2, XCH_4, XCO	EM27/SUN	PROFFAST
Bruker IFS 125HR (HR125LR)	FMI & KIT	1800–15000	0.004	1	10	XCO_2, XCH_4, XCO @ 0.5 cm^{-1}	HR125LR	PROFFAST
LHR	RAL	954–960 1233.5	0.002 and 0.02	0.5	1	CO_2, H_2O @ 0.02 cm^{-1} CH_4, H_2O @ 0.02 cm^{-1}	LHR	own code, optimal estimation
AirCore	Uni Groningen & FMI	In-situ sampling	13.4 mbar (Amb.P. > 232 mbar) 3.9 mbar (Amb.P. < 232 mbar)			CO_2, CH_4, CO vertical profiles calibrated to WMO standards	AirCore	

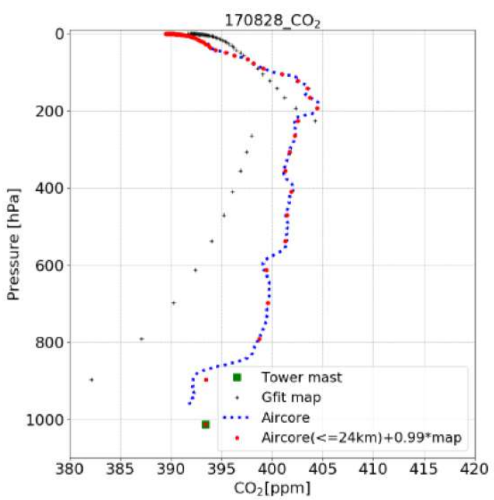
Advantage of in-situ measurements

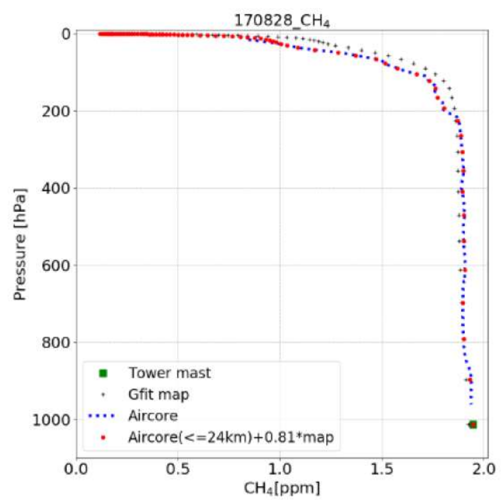


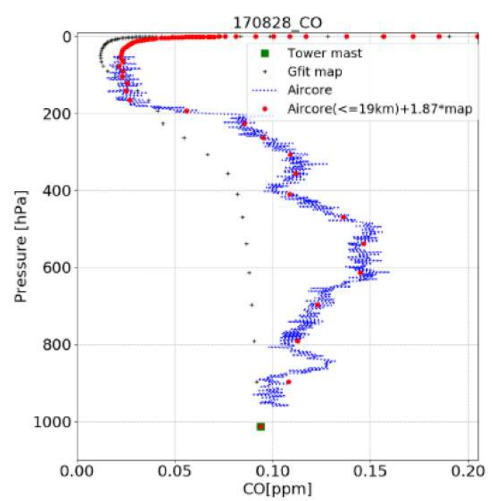






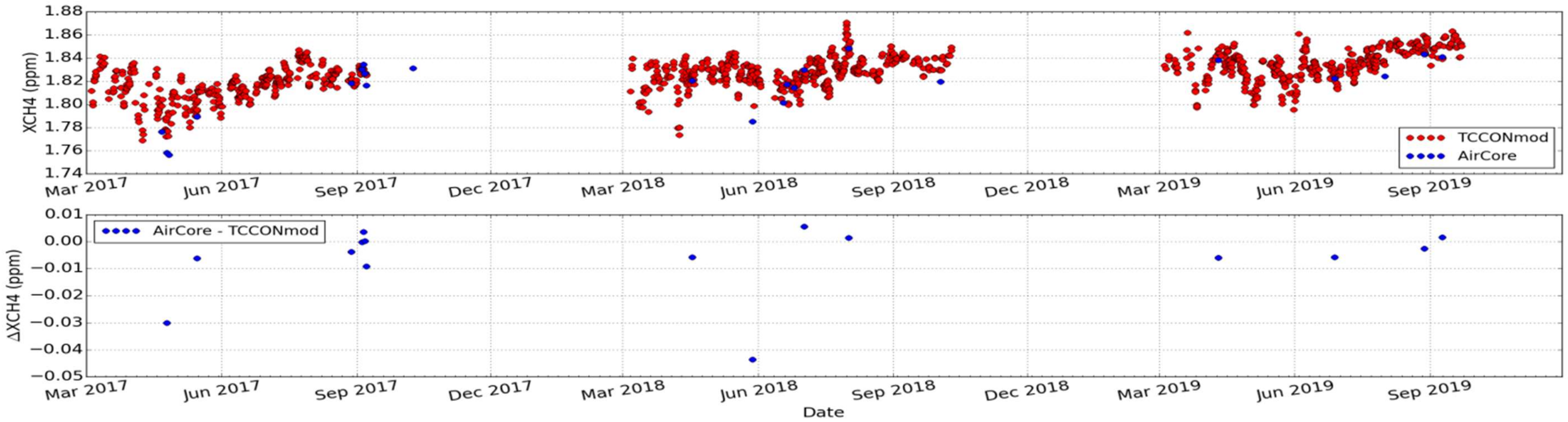


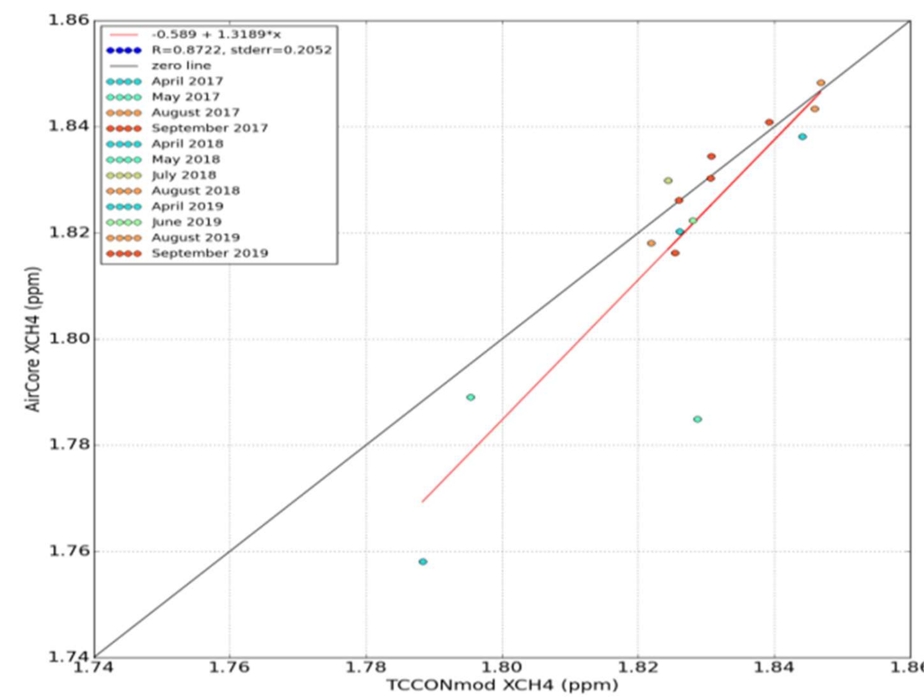




- In-situ measurements from the tower mast are used to fix the lower most point of the a priori profile
- AirCore provides the true representation of the sampled atmosphere till the cut-off altitude
- A priori above the highest AirCore measurements is extended by the scaled TCCON a priori

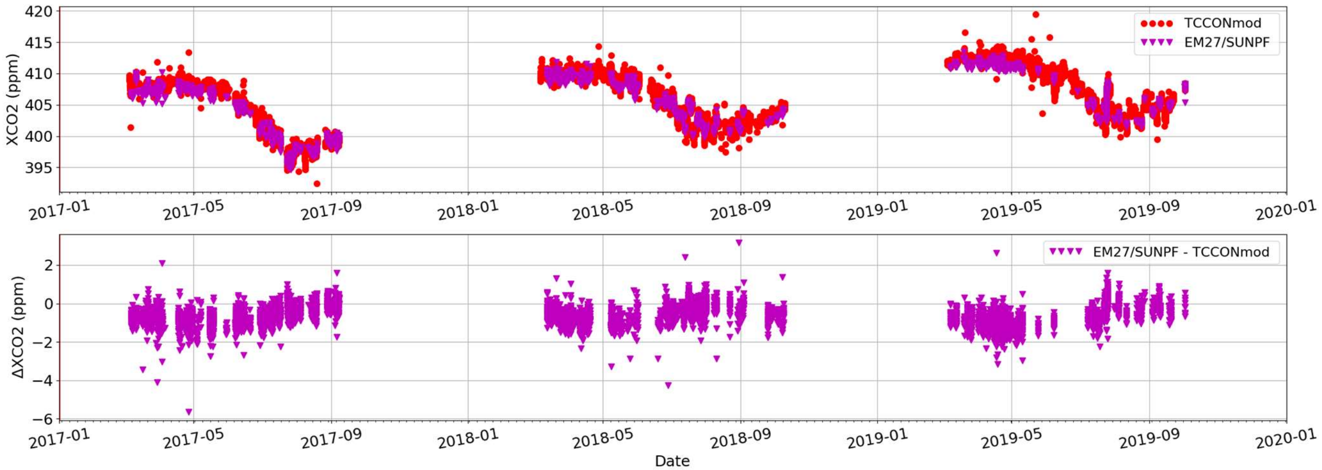
AirCore vs TCCON – XCH4



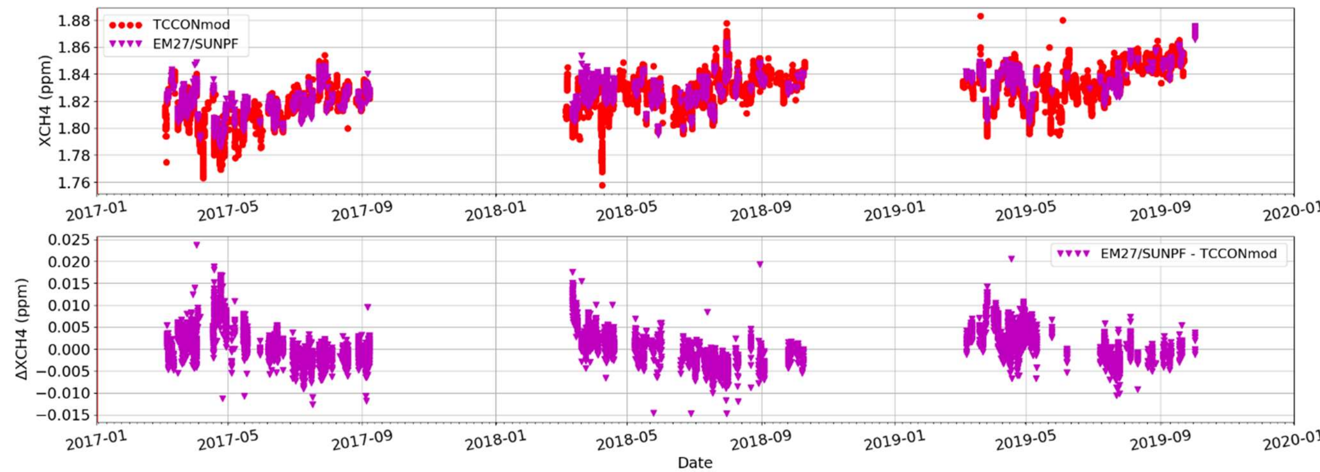


EM27/SUN (0.5 cm^{-1}) vs TCCON (0.02 cm^{-1}) at a high latitude location

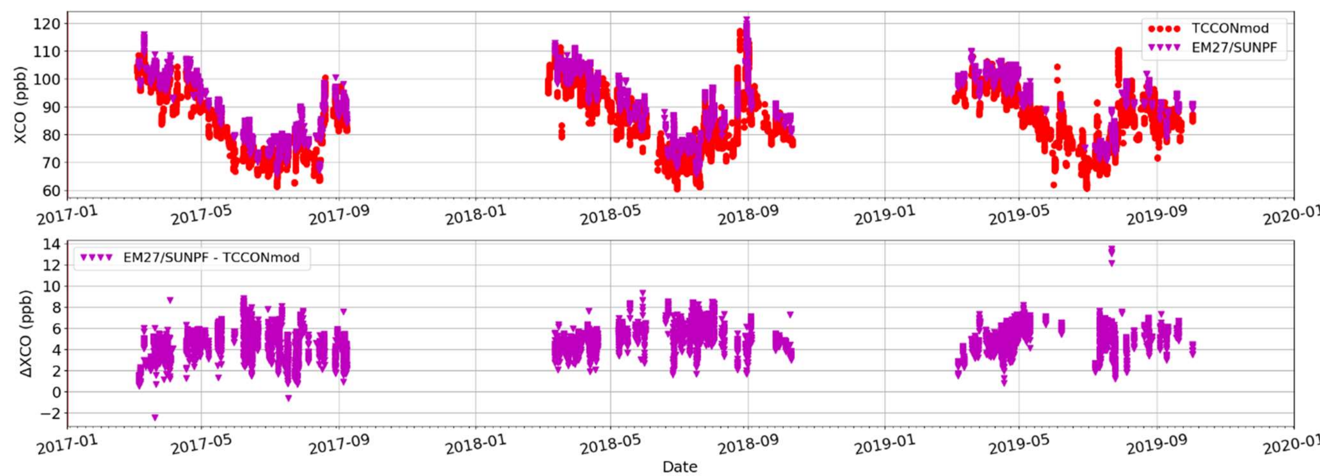
Seasonality seen in the bias (~ 1 ppm) ➔ significant ~ the accuracy requirement (0.25%) of TCCON.
The seasonality of the bias for other sites will depend on the variability of the profile shape during the year and their difference to the true profile.



Seasonality seen in the bias. About 10 ppb during spring polar vortex conditions – not usual for standard TCCON site, ~ 3 – 5 ppb bias during the summer – autumn period ➔ significant ~ the accuracy requirement (0.2%) of TCCON.



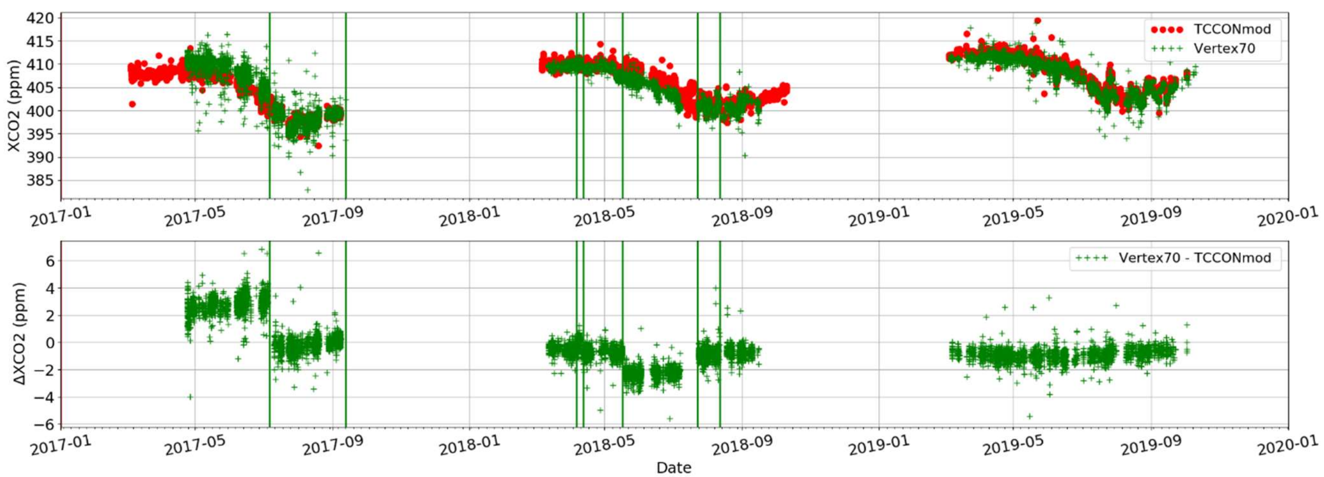
Seasonality seen in the bias. About 2 – 4 ppb bias ➔ significant ~ the accuracy requirement (2%) of TCCON.



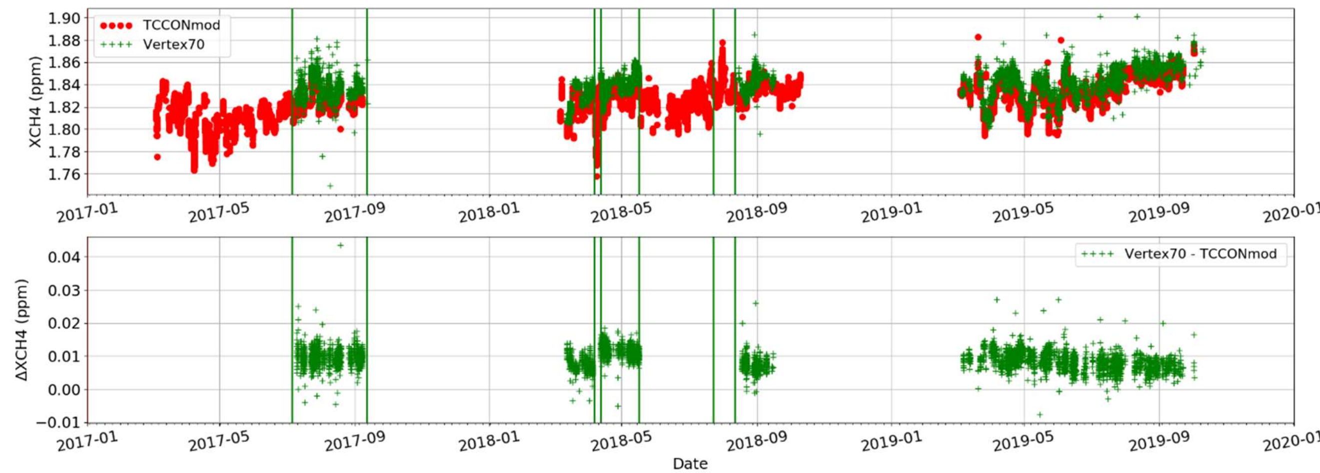
Vertex70 (0.2 cm^{-1}) vs TCCON (0.02 cm^{-1}) at a high latitude location

Vertex70 is a new instrument tested at the campaign. Vertical lines indicate instrument modifications for improvements.

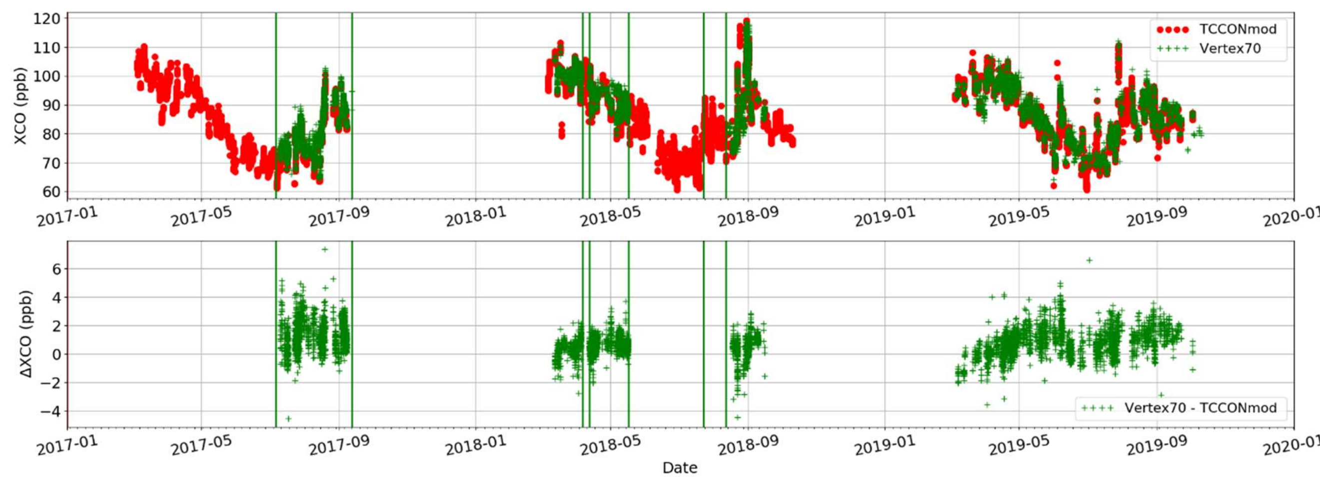
Seasonality seen in the bias (~ 1 ppm) ➔ significant ~ the accuracy requirement (0.25%) of TCCON.
The seasonality of the bias for other sites will depend on the variability of the profile shape during the year and their difference to the true profile.



Seasonality in the bias is not obvious – related to resolution (0.2 cm^{-1} rather than 0.5 cm^{-1}).

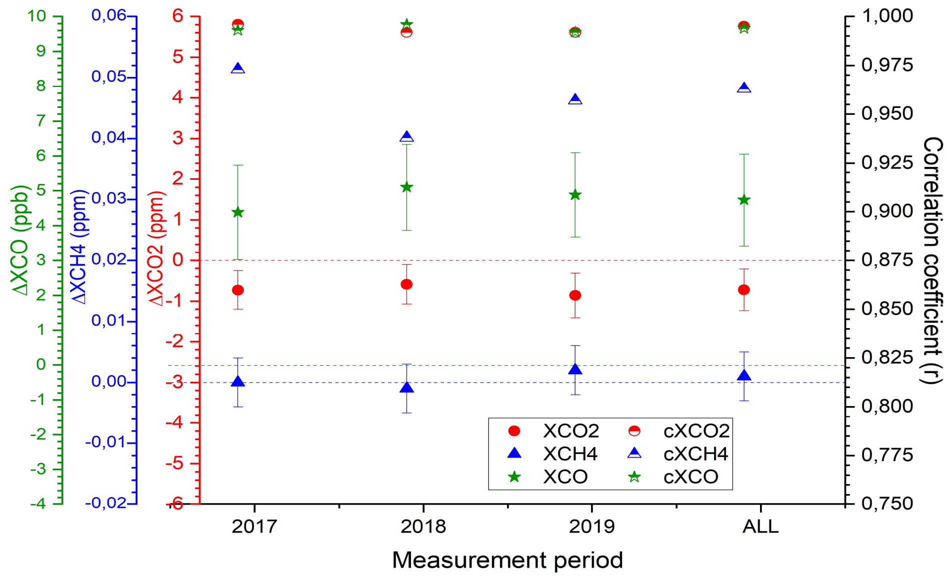


Seasonality seen in the bias. About 2 – 4 ppb bias ➔ significant ~ the accuracy requirement (2%) of TCCON.

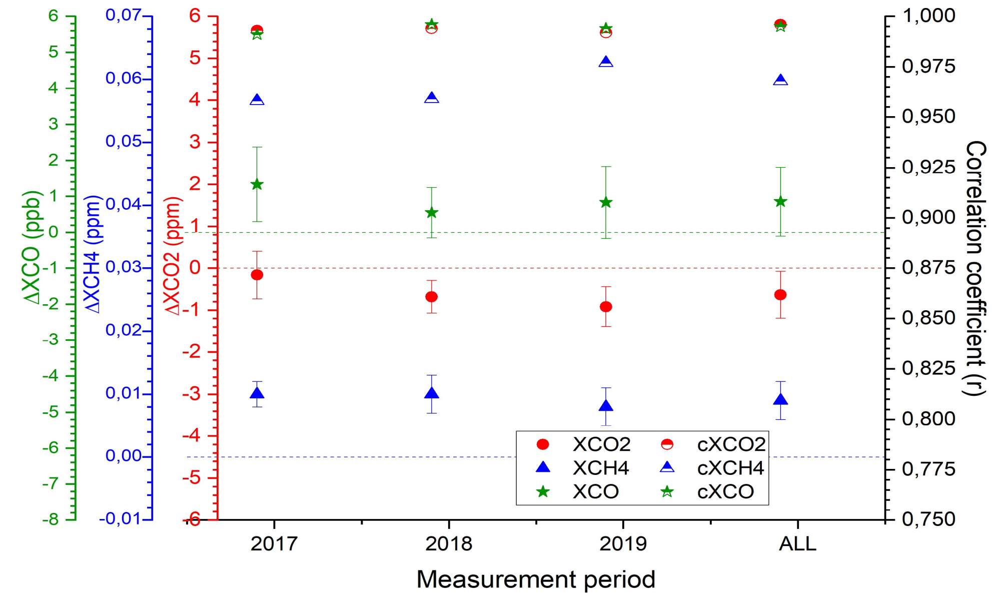


EM27/SUN and Vertex70 summary plots – FRM4GHG campaign

EM27/SUN vs TCCON



Vertex70 vs TCCON



Overall, stability looks very good over several years.

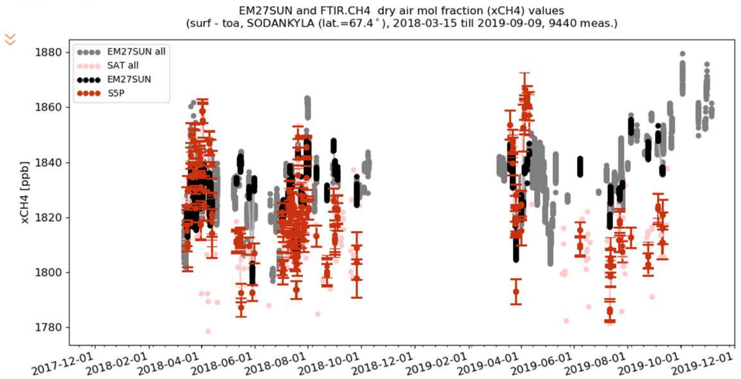
The bias values are very close to each other and the small differences seen from year-to-year are due to the data representative issue.

Annual cycle in comparison to TCCON is likely due to difference map – a priori vs true atmospheric state which generates differences in Xgas because sensitivities of TCCON and COCCON differ.

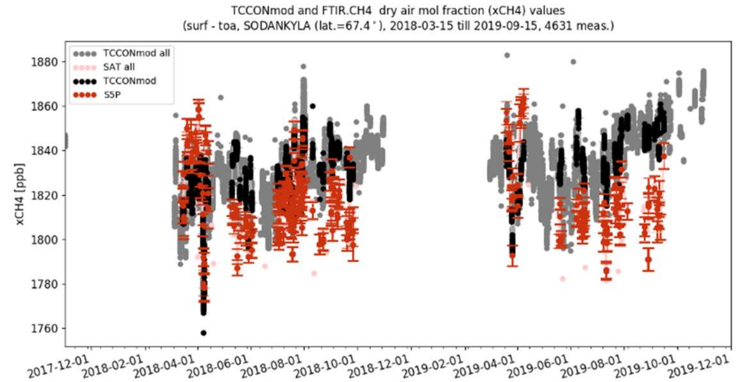
The values for 2019 are the most representative for a full year since no instrument modification done.

The bias values for 2017 and 2018 have data representative issue due to the instrument modifications. However, the bias change from year-to-year are within the seasonal variability seen in the comparison.

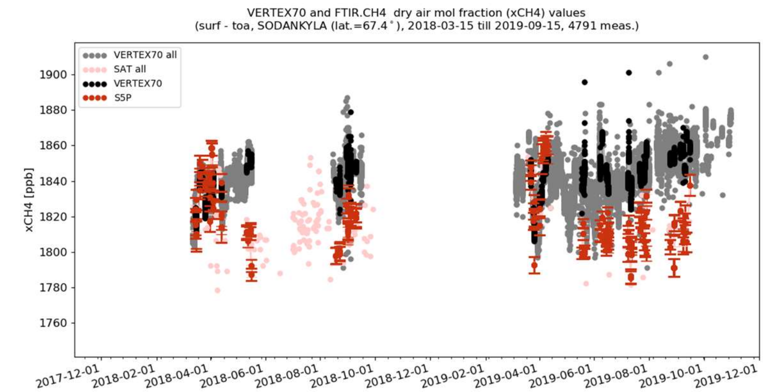
S-5p validation results using FRM4GHG datasets



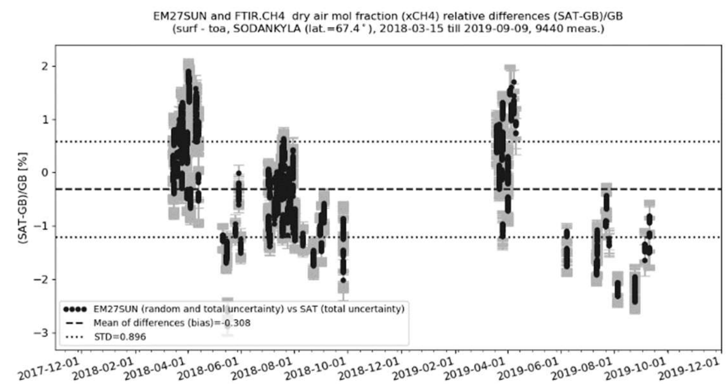
EM27/SUN

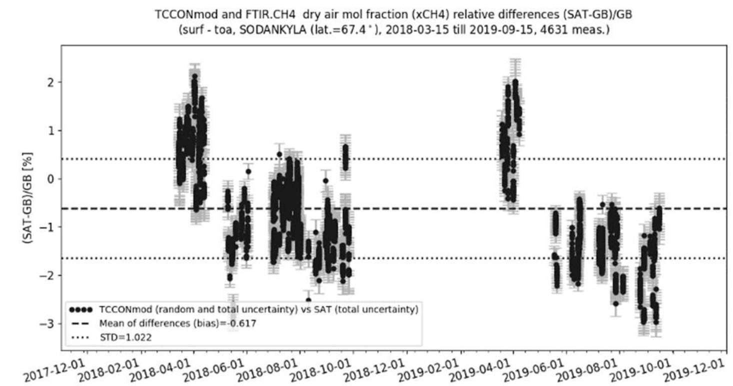


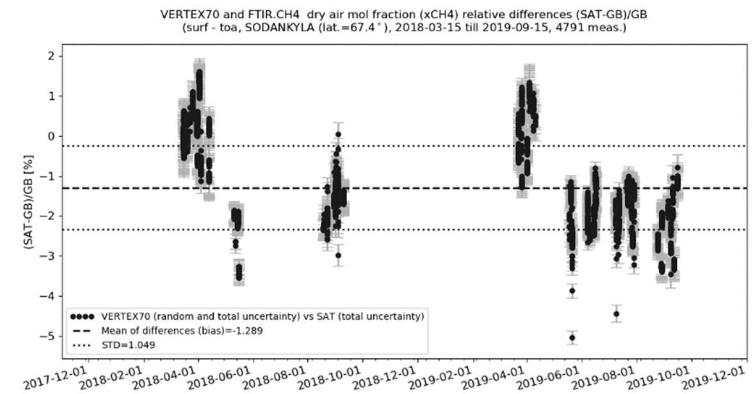
TCCON



Vertex70







Validation type	Bias %	STD %	R
EM27/SUN vs TCCON	0.05 (1 ppb)	0.22 (4 ppb)	0.943
S-5p vs EM27/SUN	-0.31	0.9	0.326
S-5p vs TCCON	-0.62	1.02	0.198

Period of study: 01/03/2018 – 31/12/2019
S-5p data from Mission Performance Centre (MPC) provided by the Payload Data Ground Segment (PDGS) at DLR

Coincidence criteria for CH4: Time delta = 1 hour; Geo-distance delta = 100 km radius. QA filtering: qa_value > 50; bias corrected S-5p CH4 product used for the study. From the coincident and filtered satellite measurements an average of all pixels is taken for each ground-based reference measurement

Lessons learned from the FRM4GHG campaign

- Assessment of low-resolution TCCON-complementing instruments for CO2, CH4, CO
- S-5p CH4 and CO validation using low-resolution instruments

➔ The EM27/SUN, the IRcube and the Vertex70 portable low-resolution FTS instruments are suitable to be used for campaign deployment or long-term measurements from any site and offer the ability to complement the TCCON and expand the global coverage of ground-based reference measurements of the target gases (CO_2, CH_4 and CO).

➔ An EM27/SUN as a traveling standard is planned for the next FRM4GHG project to allow a direct calibration bridge between the different TCCON sites by performing side-by-side measurements at several other TCCON sites.

Application of low-resolution spectrometers

- COCCON (Collaborative Carbon Column Observing Network) as framework for **EM27/SUN** spectrometer
- http://www.imk-asf.kit.edu/english/COCCON.php
- More than 60 devices operated worldwide
- Long term stability check at KIT. Frey et al., AMT, 2019,
- Check for new instruments at KIT (before delivery to customer)
  - Solar measurements together with reference EM27/SUN and co-located TCCON instrument
  - Alignment check and ILS measurements
  - Determination of XCO2, XCH4, XCO and XH2O scaling factors
- Central facility for EM27/SUN spectra
  - Central data handling and processing facility
  - Retrieval algorithm available (PROFFAST) and training possible
- **COCCON application:**
  - Measurement campaign with partner institutions
    - Paris, Berlin, Boulder, Tokyo, etc.
    - City emissions, fracking, dairy farms, coal mining, etc.
    - Vogel et al., ACP, 2019; Kille et al., GRL, 2019; Luther et al., AMTD, 2019; etc.

- **Vertex70** instrument tested shows good stability, second detector in the mid-infrared spectral range provides other species e.g. HCHO in addition to CO2, CH4 and CO. Work towards operationalization of Vertex70 and demonstration of stability of HCHO for satellite validation.

- **IRcube** shows good precision, operated with a telescope and optical fiber cable for tracking the sun. Instrument can be away from the telescope. Work towards operationalization of IRcube.

- **LHR** still needs improvements to improve precision. It has the possibility to provide profile information.

Thank you for your attention