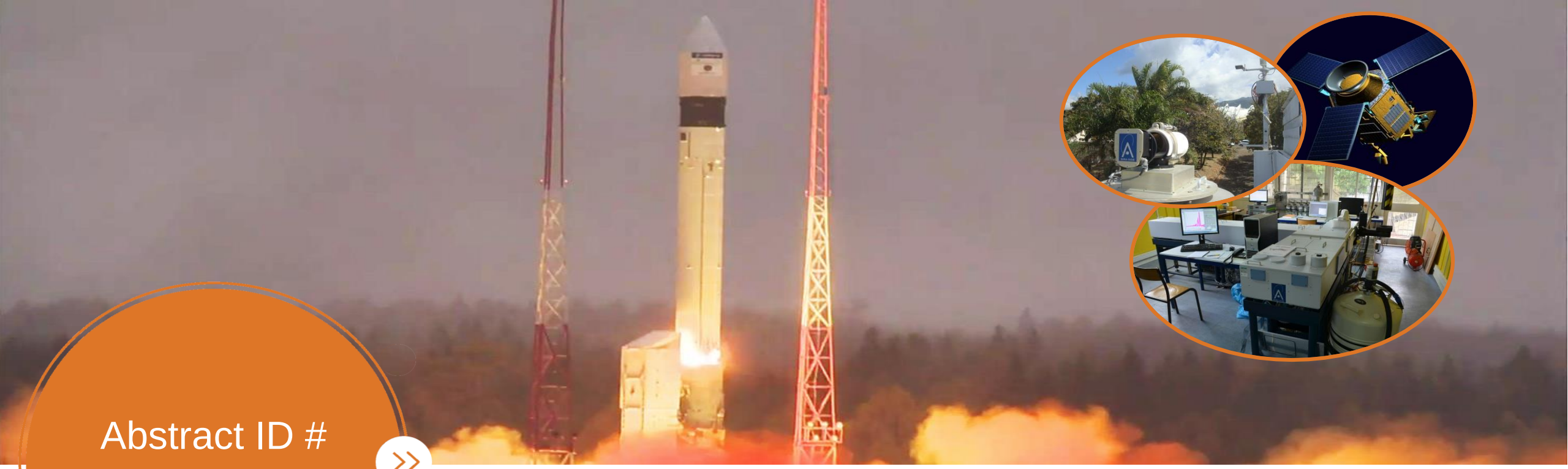

Abstract ID # 742 & 760

# Lessons learned from 2.5 years of Sentinel-5P methane validation using global TCCON and NDACC-IRWG data (Abstract # 742)

# Final intercomparison results of the FRM4GHG project showing the accuracy and precision achieved by the low-resolution FTIR spectrometers in comparison to TCCON and their application for GHG observations (Abstract # 760)

**Presenter: Mahesh Kumar Sha***

with contributions from the TCCON team, NDACC team, FRM4GHG team, SRON team and S5P MPC-VDAF

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ROYAL BELGIAN INSTITUTE FOR SPACE AERONOMY

# Sentinel-5 Precursor

**Sentinel-5 Precursor (S-5 P)** is the first of the ESA atmospheric composition of Sentinels contributing to the European Commission Copernicus Programme to improve our understanding of the planet and the environment.
S-5 P has been successfully launched on **13th October 2017**. Near-polar sun-synchronous orbit at an altitude of 824 km with an ascending node equatorial crossing at 13:30. Orbit cycle is 16 days (14 orbits per day, 227 orbits per cycle). Mission duration is 7 years.

**TROPOsheric Monitoring Instrument (TROPOMI)** onboard S-5 P is a grating spectrometer covering 8 bands (UV – short-wave IR), common telescope for UVN and SWIR, pushbroom configuration and wide swath (108° → **2600 km on surface**). The primary products measured are Ozone, $NO_2$, CO, $CH_2O$, $CH_4$, $SO_2$, Aerosol, Clouds and UV-Index. The application of the data measured will be on ozone layer monitoring, climate monitoring, air quality monitoring and forecast, volcanic plume detection and UV index forecast.

TROPOMI uses the absorption information from the Oxygen-A Band (757–774 nm) and the SWIR spectral channel (2305–2385 nm) to retrieve the $CH_4$ global abundance in the Earth's atmosphere. $CH_4$ products has a **spatial sampling of 7x7 km2 (launch – Aug 6 2019)**. Since **August 6 2019 (orbit 9388)** the along track resolution was increased from **7 km to 5.5 km**.

**Table 1** – Sentinel-5P TROPOMI mandatory atmospheric composition data products addressed in this talk

| Parameter | Data Product | Vertical resolution | Systematic Uncertainty Requirement | Random Uncertainty Requirement |
|---|---|---|---|---|
| $CH_4$ | Total $CH_4$ | Total column | 1.5% | 1% |

# Groundbased networks used for the validation study

- **The Total Carbon Column Observing Network (TCCON)**
  - 23 stations in the northern hemisphere, 5 stations in the southern hemisphere
  - High accuracy / precision (0.2% / 0.5% for $CH_4$ and 2% / 1% for CO)
- **The Infrared Working Group (IRWG) of the NDACC**
  - 17 stations in the northern hemisphere, 4 stations in the southern hemisphere
  - Accuracy / precision (3% / 1.5% for $CH_4$ and 3% / 1% for CO)

**Table 2.** List of FTIR stations that are associated to NDACC-IRWG and contributed to the present work by providing public and rapid delivery data. The location of the stations and the teams involved are indicated for the respective stations.

| Station | Latitude | Longitude | Altitude (km a.s.l.) | Active dates | Teams |
|---|---|---|---|---|---|
| Eureka | 80.05° N | 86.42° W | 0.61 | Nov 2017 - Present | U. of Toronto |
| Ny-Ålesund | 78.90° N | 11.90° E | 0.02 | Nov 2017 - Present | U. of Bremen |
| Thule | 76.52° N | 68.77° W | 0.22 | Nov 2017 - Present | NCAR |
| Kiruna | 67.84° N | 20.40° E | 0.42 | Nov 2017 - Present | KIT-ASF; IRF Kiruna |
| Sodankylä | 67.37° N | 26.63° E | 0.19 | Nov 2017 - Present | FMI; BIRA-IASB |
| St-Petersburg | 59.88° N | 29.83° E | 0.02 | Nov 2017 - Present | SPbU |
| Bremen | 53.10° N | 8.85° E | 0.03 | Nov 2017 - Present | U. of Bremen |
| Garmisch | 47.48° N | 11.06° E | 0.74 | Nov 2017 - Present | KIT-IFU |
| Zugspitze | 47.42° N | 10.98° E | 2.96 | Nov 2017 - Present | KIT-IFU |
| Jungfraujoch | 46.55° N | 7.98° E | 3.58 | Nov 2017 - Present | U. of Liège |
| Toronto | 43.60° N | 79.36° W | 0.17 | Nov 2017 - Present | U. of Toronto |
| Rikubetsu | 43.46° N | 143.77° E | 0.38 | Nov 2017 - Present | Nagoya U.; NIES |
| Boulder | 40.04° N | 105.24° W | 1.61 | Nov 2017 - Present | NCAR |
| Izana | 28.30° N | 16.50° W | 2.37 | Nov 2017 - Present | AEMET; KIT-ASF |
| Mauna Loa | 19.54° N | 155.57° W | 3.40 | Nov 2017 - Present | NCAR |
| Altzomoni | 19.12° N | 98.66° W | 3.98 | Nov 2017 - Present | UNAM |
| Paramaribo | 5.81° N | 55.21° W | 0.03 | Nov 2017 - Present | U. of Bremen |
| Maïdo | 21.08° S | 55.38° E | 2.16 | Nov 2017 - Present | BIRA-IASB |
| Wollongong | 34.41° S | 150.88° E | 0.03 | Nov 2017 - Present | U. of Wollongong |
| Lauder | 45.04° S | 169.68° E | 0.61 | Nov 2017 - Present | NIWA |
| Arrival Heights | 77.82° S | 166.65° E | 0.20 | Nov 2017 - Present | NIWA |

**Table 1.** List of FTIR stations that are associated to TCCON and contributed to the present work by providing public and rapid delivery data. The station marked with a star (*) is not yet associated to TCCON but records data following the network recommendations. Active dates corresponds to the dates for which the measurements were provided from the satellite launch till the present work

| Station | Latitude | Longitude | Altitude (km a.s.l.) | Active dates | Data reference |
|---|---|---|---|---|---|
| Eureka | 80.05° N | 86.42° W | 0.61 | Nov 2017 - Present | Strong et al. (2019) |
| Ny-Ålesund | 78.90° N | 11.90° E | 0.02 | Nov 2017 - Present | Notholt et al. (2014b) |
| Sodankylä | 67.37° N | 26.63° E | 0.19 | Nov 2017 - Present | Kivi et al. (2014) |
| Easttroutlake | 54.35° N | 104.99° W | 0.50 | Nov 2017 - Present | Wunch et al. (2018) |
| Bialystock | 53.23° N | 23.05° E | 0.18 | Nov 2017 - Oct 2018 | Deutscher et al. (2019) |
| Bremen | 53.10° N | 8.85° E | 0.03 | Nov 2017 - Present | Notholt et al. (2014a) |
| Karlsruhe | 49.10° N | 8.44° E | 0.12 | Nov 2017 - Present | Hase et al. (2015) |
| Paris | 48.85° N | 2.36° E | 0.06 | Nov 2017 - Present | Té et al. (2014) |
| Orleans | 47.97° N | 2.11° E | 0.13 | Nov 2017 - Present | Warneke et al. (2019) |
| Garmisch | 47.48° N | 11.06° E | 0.74 | Nov 2017 - Present | Sussmann and Rettinger (2018a) |
| Zugspitze | 47.42° N | 10.98° E | 2.96 | Nov 2017 - Present | Sussmann and Rettinger (2018b) |
| Parkfalls | 45.95° N | 90.27° W | 0.44 | Nov 2017 - Present | Wennberg et al. (2017) |
| Rikubetsu | 43.46° N | 143.77° E | 0.38 | Nov 2017 - Present | Morino et al. (2018c) |
| Xianghe* | 39.75° N | 116.96° E | 0.05 | Nov 2017 - Present | Yang et al. (2019) |
| Lamont | 36.60° N | 97.49° W | 0.32 | Nov 2017 - Present | Wennberg et al. (2016b) |
| Tsukuba | 36.05° N | 140.12° E | 0.03 | Nov 2017 - Present | Morino et al. (2018a) |
| Nicosia* | 35.14° N | 33.38° E | 0.19 | Aug 2019 - Present | Petri et al. (2019) |
| Edwards | 34.96° N | 117.88° W | 0.70 | Nov 2017 - Present | Iraci et al. (2016) |
| JPL | 34.20° N | 118.18° W | 0.39 | Nov 2017 - May 2018 | Wennberg et al. (2016a) |
| Pasadena | 34.14° N | 118.13° W | 0.23 | Nov 2017 - Present | Wennberg et al. (2015) |
| Saga | 33.24° N | 130.29° E | 0.01 | Nov 2017 - Present | Kawakami et al. (2014) |
| Izana | 28.30° N | 16.50° W | 2.37 | Nov 2017 - Present | Blumenstock et al. (2017) |
| Burgos | 18.53° N | 120.65° E | 0.04 | Nov 2017 - Present | Morino et al. (2018b) |
| Ascension | 7.92° S | 14.33° W | 0.01 | Nov 2017 - Present | Feist et al. (2014) |
| Darwin | 12.46° S | 130.93° E | 0.04 | Nov 2017 - Present | Griffith et al. (2014a) |
| Reunion | 20.90° S | 55.49° E | 0.09 | Nov 2017 - Present | De Mazière et al. (2017) |
| Wollongong | 34.41° S | 150.88° E | 0.03 | Nov 2017 - Present | Griffith et al. (2014b) |
| Lauder | 45.04° S | 169.68° E | 0.61 | Nov 2017 - Present | Sherlock et al. (2014, 2019) |

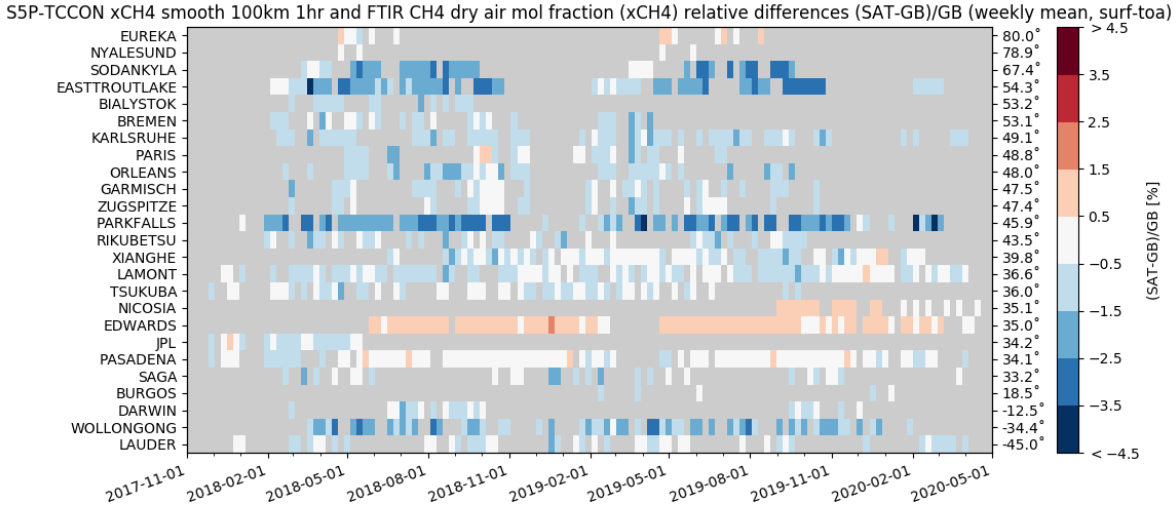
# Coincidence criteria used for the validation study

- Period of study started with the first available data (**17 November 2017 till 1 May 2020**)
- **TCCON data** provided by 28 stations (fast data delivery and standard data) ➔ **Many Thanks!**
- **NDACC data** provided by 19 stations (rapid data delivery – CAMS27 contract cams27.aeronomie.be) ➔ **Many Thanks!**
- **S-5P data** from the Copernicus data hub and the Mission Performance Centre (**MPC**) provided by the Payload Data Ground Segment (**PDGS**) at DLR
  S-5P $CH_4$ versions **RPRO & OFFL** – latest version of the files taken for the validation
- S-5P $XCH_4$ provides **pixels above land** ➔ Many NDACC stations and **some** TCCON **stations are islands** and **do not co-locate** to any satellite pixel
- Coincidence criteria for $CH_4$: Time delta = **1h (TCCON) & 3h (NDACC)**; Geo-distance delta (radius) = **100 km**, qa_value**>0.5**. **Standard $XCH_4$ product** and **bias-corrected $XCH_4$ product**. From the coincident and filtered satellite measurements an average of all pixels is taken for each TCCON and NDACC measurement
- S-5P $CH_4$ priori is used as **common prior** (Rodgers, 2003), **altitude correction** is done for each satellite pixel to the ground-based station height

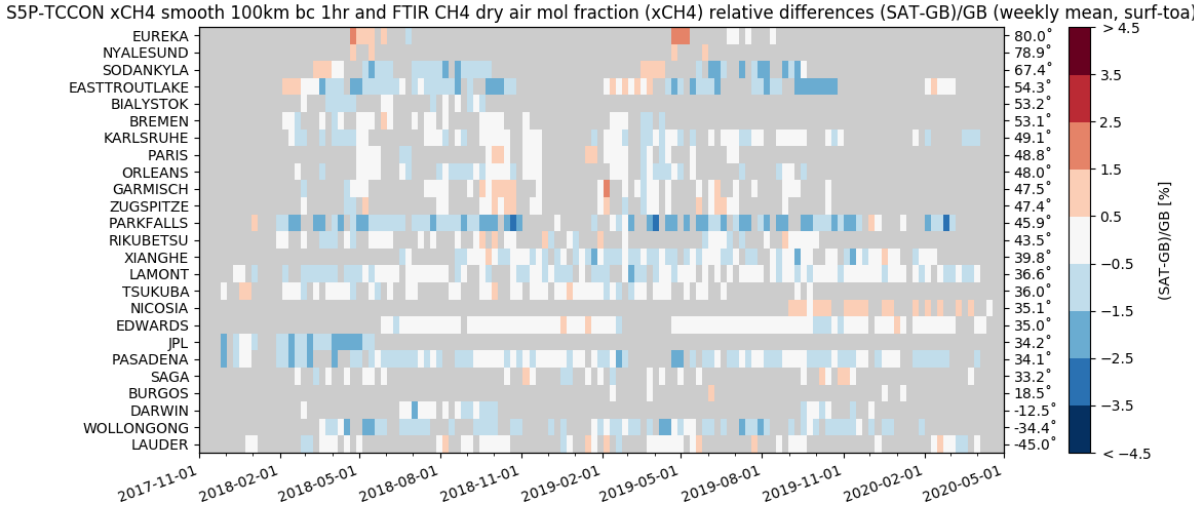
- Validation using TCCON & NDACC $CH_4$ data are part of the **VDAF** study (mpc-vdaf.tropomi.eu)

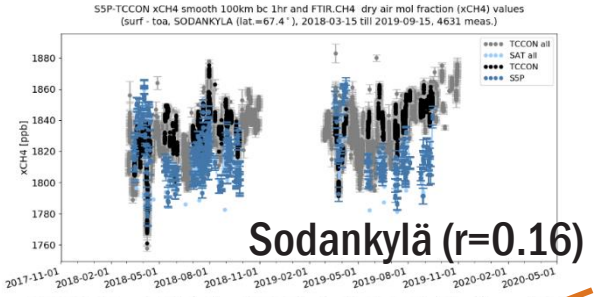
# S-5P validation results – $XCH_4$

## S-5P Standard product

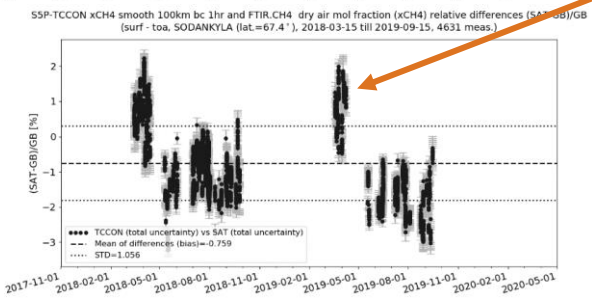



## S-5P Bias corrected product

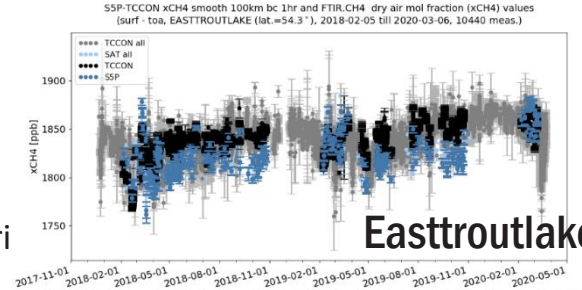


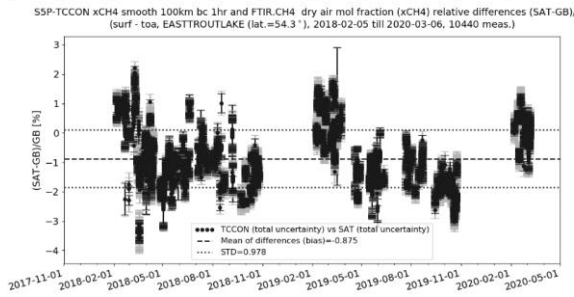

**Sodankylä (r=0.16)**



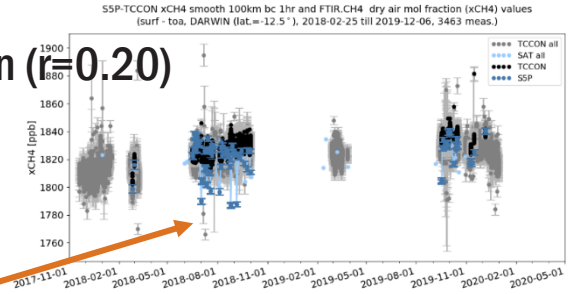

High bias during spring time (large difference of a priori to true atm. state and their influence on the instrument sensitivities)



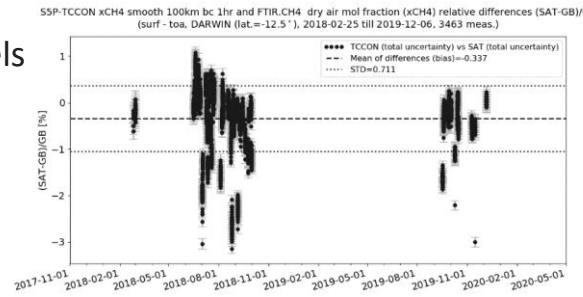

**Easttroutlake (r=0.57)**



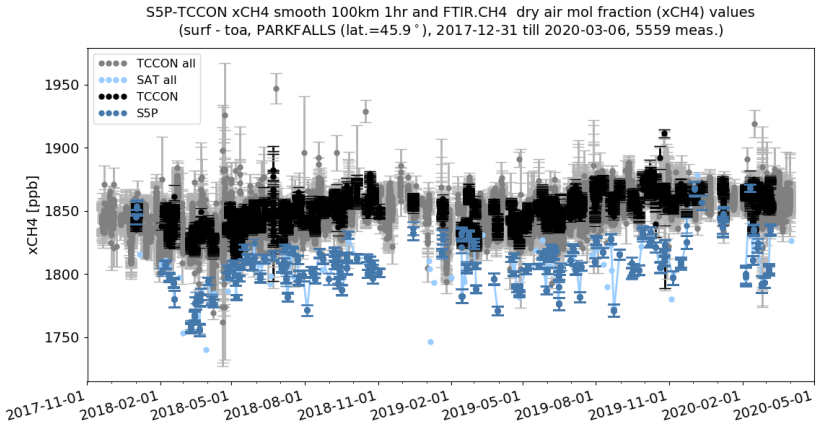

**Darwin (r=0.20)**

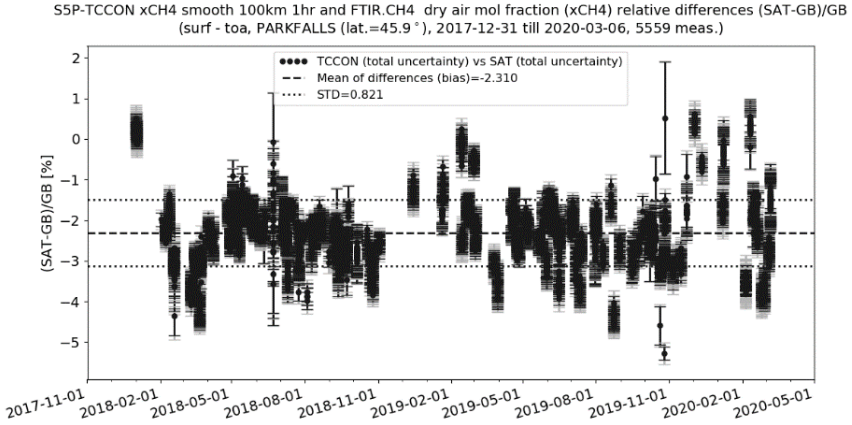



Low satellite pixels



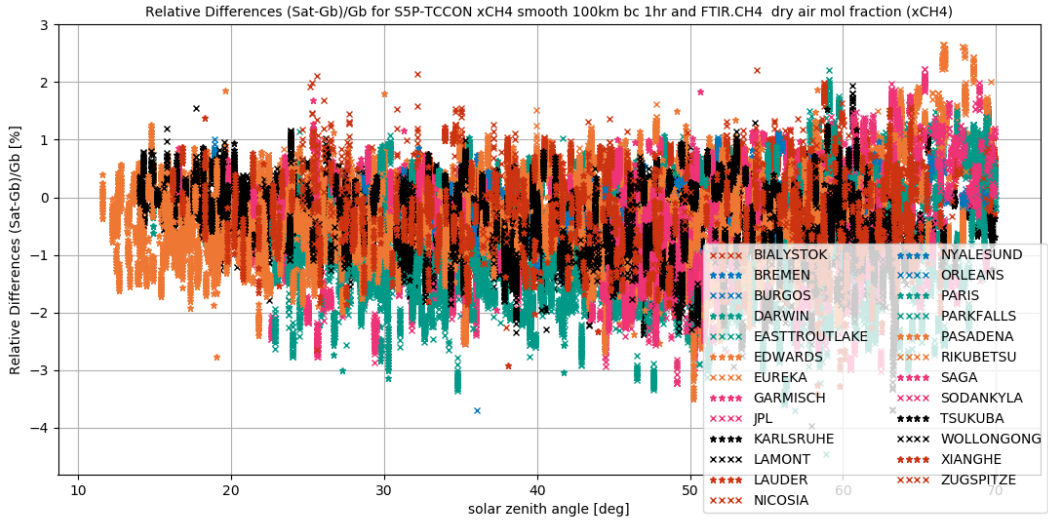
# S-5P validation results – bias corrected $XCH_4$



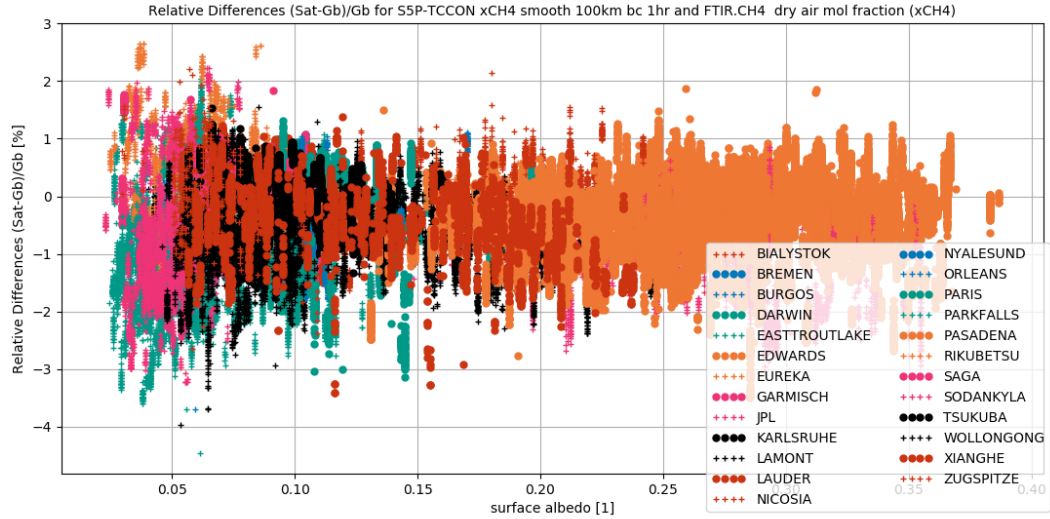




Potential seasonal cycle in the residual bias

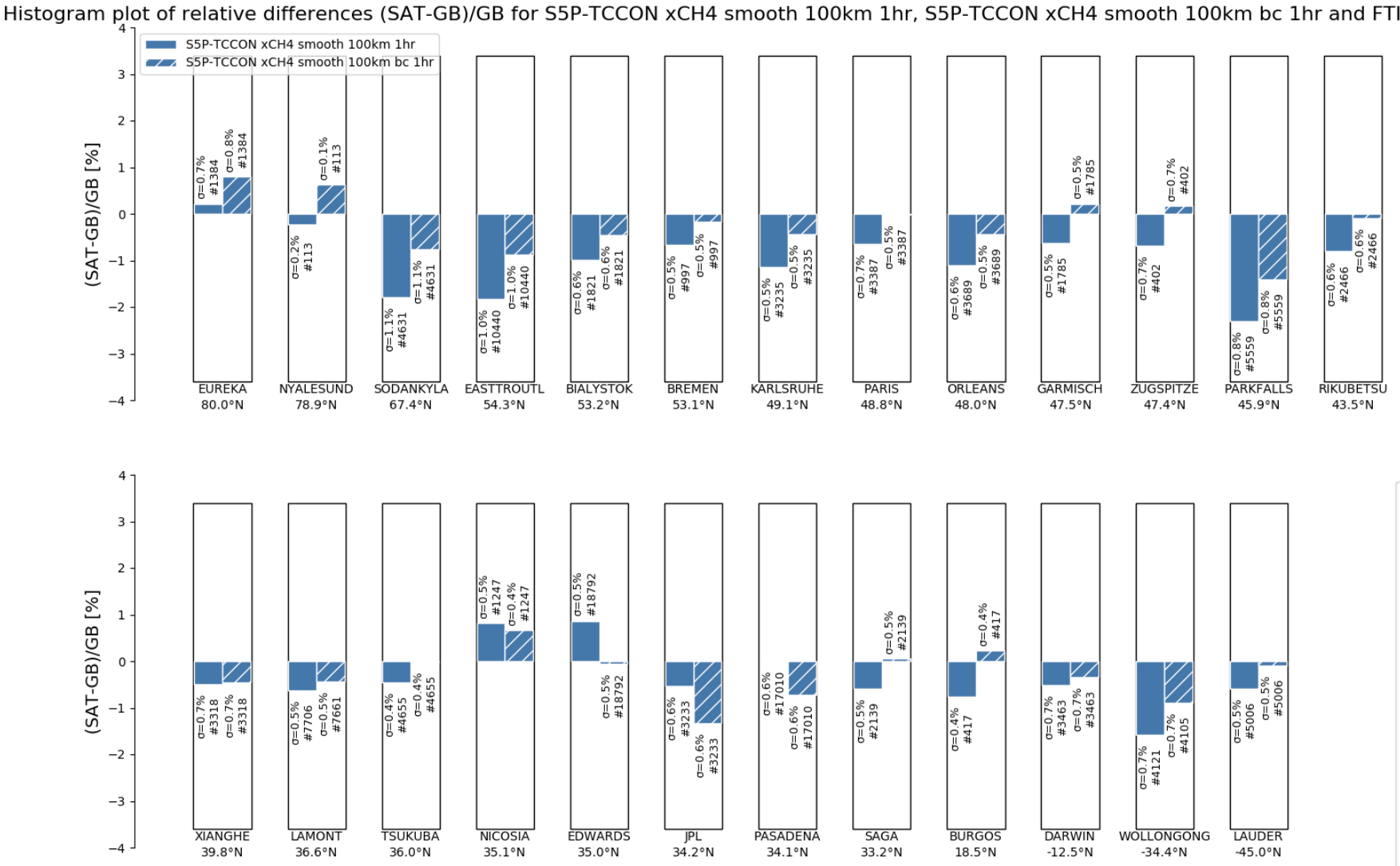
High scatter for high solar zenith angle




High scatter for low surface albedo

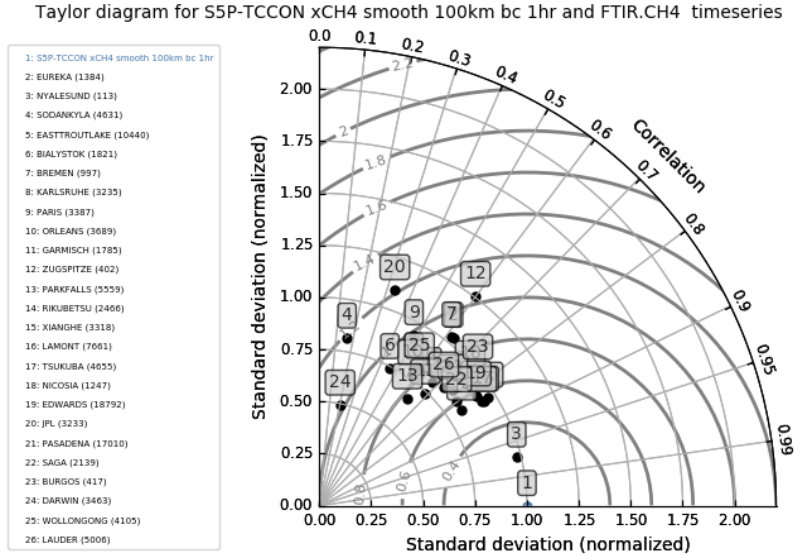


# S-5P validation results – $XCH_4$



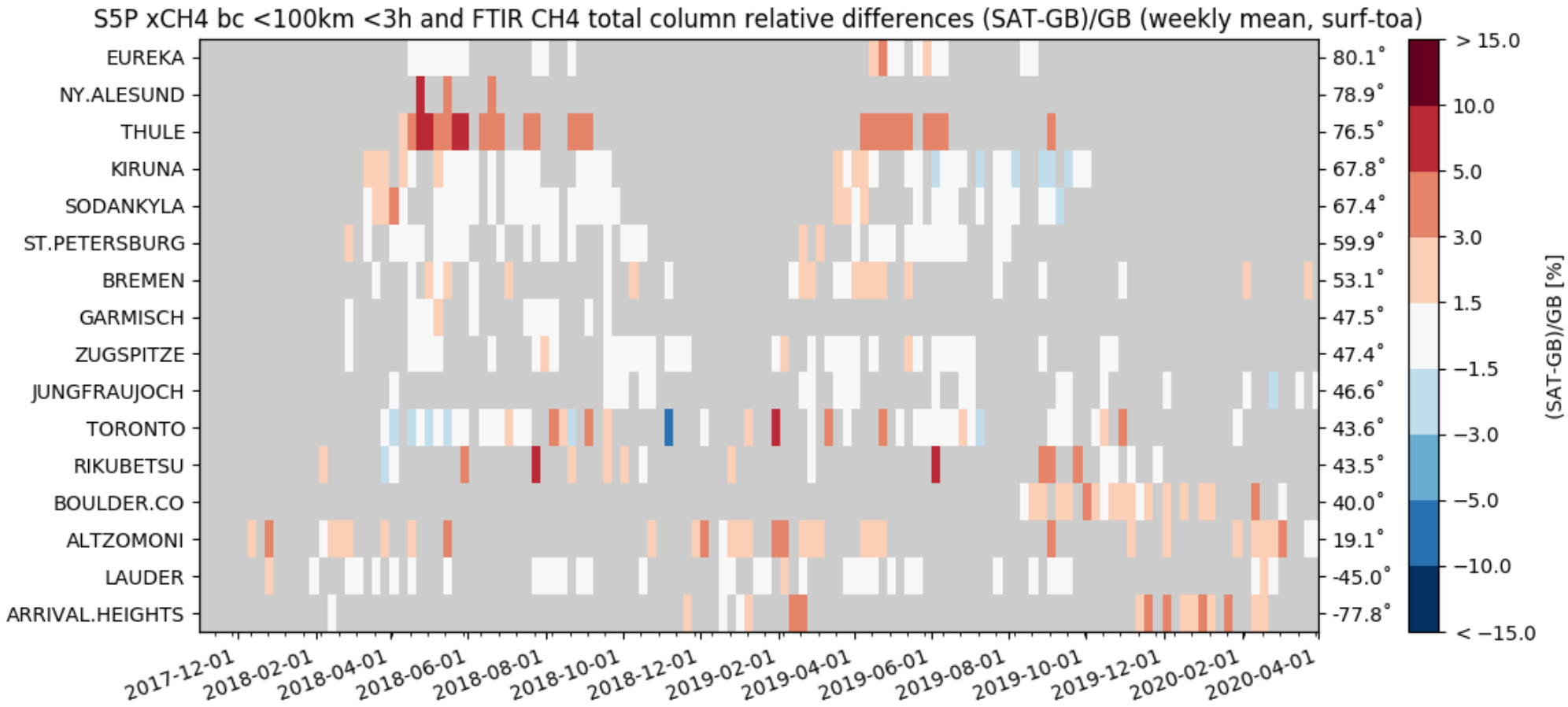

**Bias corrected S-5P $XCH_4$**
**Mean bias: -0.25%, Standard deviation: 0.58%, R = 0.65**

**Standard S-5P S-5P $XCH_4$**
**Mean bias: -0.68%, Standard deviation: 0.60%, R = 0.65**




**Solid blue: S-5P Standard product** **Dashed blue: S-5P Bias corrected product**

# S-5P bias corrected $XCH_4$ product validation results with NDACC-IRWG




Very few coincidences for several sites. Statistics not yet robust enough.

**Objective** – perform an intercomparison of simultaneously measured **total column amounts of $CO_2$, $CH_4$ and CO** using different **portable low-cost spectrometric instruments** under different atmospheric conditions in **comparison to the TCCON instrument**. Assess these instruments regarding their capability to **complement the existing TCCON network**.

**Description** – perform side-by-side measurements using these low-resolution instruments next to a TCCON instrument.
**Location** – TCCON site at **Sodankylä (Finland), Wollongong & Darwin (Australia)**; **AirCore launches** at the Sodankylä site to complement the total column measurements.
**Duration** – 2017 – 2019 (direct solar absorption measurements under clear-sky conditions).

**Table 1.** List of instruments participating in the FRM4GHG campaign and their properties.

| Instrument | Institute | Spectral range | Resolution | Main species | Retrieval code |
|---|---|---|---|---|---|
| Bruker IFS 125HR (TCCON) | FMI | 1800 – 15000 $cm^{-1}$ | 0.004 $cm^{-1}$ | $XCO_2$, $XCH_4$, XCO @ 0.02 $cm^{-1}$ | GFIT 2014 |
| Bruker EM27/SUN (COCCON) | KIT | 4000 – 9000 $cm^{-1}$ | 0.5 $cm^{-1}$ | $XCO_2$, $XCH_4$, XCO | PROFFAST |
| Bruker IRcube | Uni Wollongong | 4500 – 15000 $cm^{-1}$ | 0.5 $cm^{-1}$ | $XCO_2$, $XCH_4$ | GFIT 2014 |
| Bruker Vertex70 | Uni Bremen & BIRA-IASB | 2500 – 15000 $cm^{-1}$ | 0.16 $cm^{-1}$ | $XCO_2$, $XCH_4$, XCO XHCHO @ 0.2 $cm^{-1}$ | GFIT 2014 |
| Bruker IFS 125HR (HR125LR) | FMI & KIT | 1800 – 15000 $cm^{-1}$ | 0.004 $cm^{-1}$ | $XCO_2$, $XCH_4$, XCO @ 0.5 $cm^{-1}$ | PROFFAST |
| LHR (Laser Heterodyne Radiometer) | RAL | 954 – 960 $cm^{-1}$ 1233.5 $cm^{-1}$ | 0.002 and 0.02 $cm^{-1}$ | $CO_2$, $H_2O$ $CH_4$, $H_2O$ | 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 | |

# FRM4GHG project results

http://frm4ghg.aeronomie.be/

| Species | Duration | XCO2 / ppm | XCH4 / ppm | XCO / ppb |
|---|---|---|---|---|
| Bias (mean standard ± deviation) and correlation coefficient (r) | | | | |
| EM27/SUN vs TCCON (Sodankylä) | 2017 – 2019 | -0.722±0.510 (0.995) | 0.001±0.004 (0.963) | 4.738±1.321 (0.994) |
| VERTEX70 (good) vs TCCON (Sodankylä) | 2017 – 2019 | -0.636±0.558 (0.996) | 0.009±0.003 (0.968) | 0.856±0.961 (0.995) |
| IRCUBE (good) vs TCCON (Darwin) | 2019 | -10.487±0.597 (0.73) | 0.002±0.003 (0.808) | - |
| LHR vs TCCON (Sodankylä) | 2019 | -0.979±10.424 (0.315) | 0.005±0.069 (0.160) | - |

The EM27/SUN ✓
The VERTEX70 ✓
The IRCUBE ✓
} fulfil the TCCON precision requirements

XCO2: < 0.25% ~ 1 ppm
XCH4: 0.5% ~ 0.009 ppm
XCO: < 4% ~ < 4 ppb

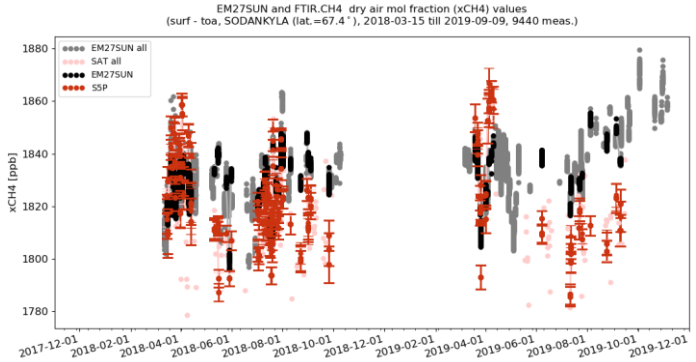
The calibration to the WMO will be performed by scaling the Xgas value to the TCCON.

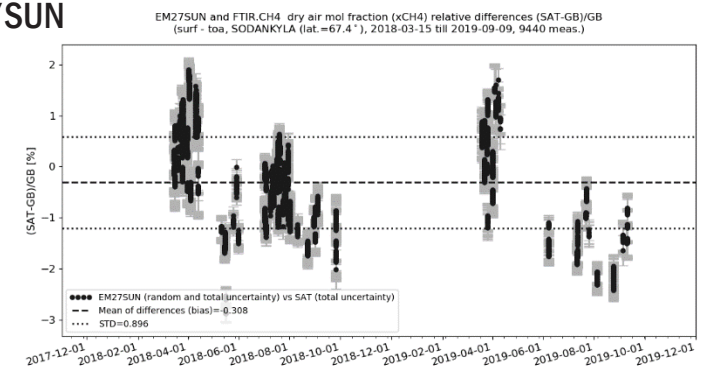
Details on the 2017 campaign results: Sha et al., 2019, https://doi.org/10.5194/amt-2019-371

Publication of the results of 2018 & 2019 is in preparation.

# S-5P bias corrected $XCH_4$ product validation using EM27/SUN @ SO

S-5P vs EM27/SUN

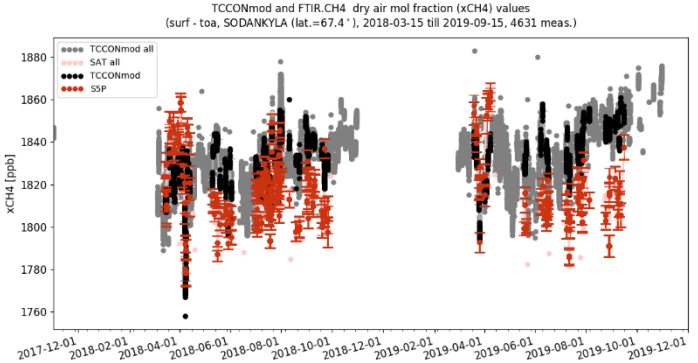


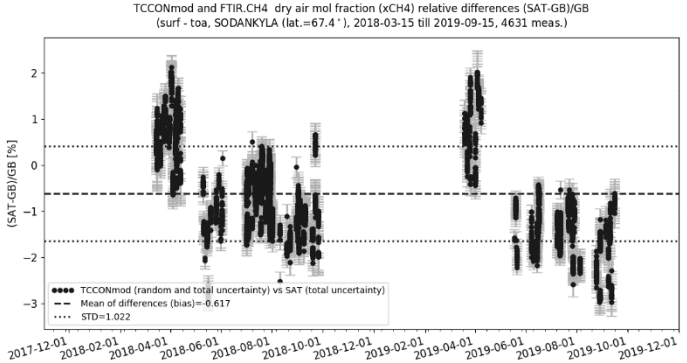



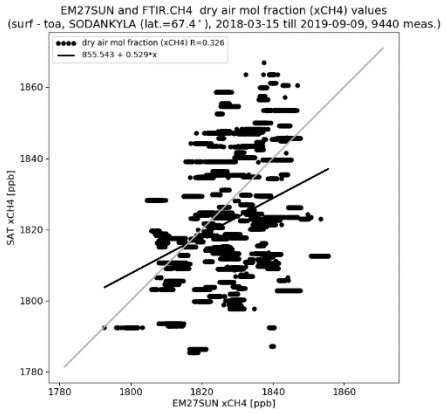

Period of study: 01 March 2018 – 31 December 2019.
S5P data from Mission Performance Centre (MPC) provided by the Payload Data Ground Segment (PDGS) at DLR.

Coincidence criteria for CH4: Time delta = 1 hour; Geo-distance delta = 100 km radius. QA filtering: qa_value > 50; bias corrected S5P-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.

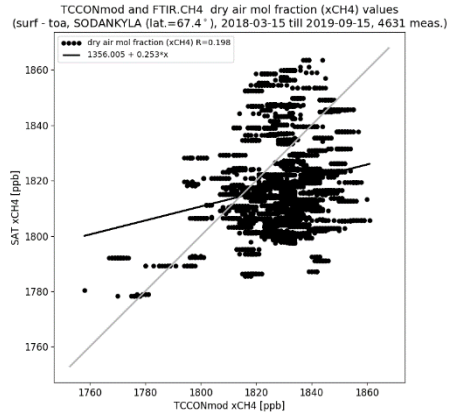
S-5P vs TCCON




| 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 |



# 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 $XCO_2$, $XCH_4$, XCO and $XH_2O$ scaling factors
- Central facility for EM27/SUN spectra
  - Central data handling and processing facility
  - Retrieval algorithm available (PROFFAST) and training possible
- **COCCON applications:**
- 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 $CO_2$, $CH_4$ and CO**. Work towards operationalisation of VERTEX70 and demonstration of stability of HCHO for satellite validation.

- **IRCUBE** shows good precision, **operated with a telescope and optical fibre cable** for tracking the sun. **Instrument can be further away from the telescope**. Work towards operationalisation of IRCUBE.

- **LHR** still **needs improvements** to improve precision. It has the possibility to provide **profile information of $CO_2$ and $CH_4$**.

# Conclusions

- S-5P methane validation study results covering whole TCCON and several NDACC-IRWG stations was shown
- Good coincidences for many sites but also very few coincidences for some sites
- Validation of TROPOMI $XCH_4$ with TCCON $XCH_4$:
  - Bias corrected product shows better results; high negative bias for some stations is due to the way the albedo correction is currently done; biases in the high latitude sites is due to the profile difference of $CH_4$; SZA dependence seen for the stations
  - Mean bias of -0.25% ± 0.56% (25 stations; median bias of -0.18 %)
    ➔ **systematic uncertainty (1.5%) compliant with mission requirement** ✓
  - Standard deviation for sites < 1%
    ➔ **random uncertainty (1%) compliant with mission requirement** ✓
  - Correlation coefficient is ~ 0.68 (median)
- Filtering on qa value > 0.5 for methane does not remove all pixels considered bad. Some pixels with too low and too high methane concentrations are still present.

- The FRM4GHG campaign data from the low-resolution spectrometers were used for S-5P CO and $CH_4$ validation. The results show good agreement with respect to the TCCON validation results.
- Low-resolution spectrometers (EM27/SUN, VEERTEX70 and IRCUBE) show excellent performance and are suitable for complementing TCCON.

# Notes

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**Thank you for your attention!**

**Questions / comments to mahesh.sha@aeronomie.be**

# Extra slides

# FRM4GHG campaign deployment in Sodankylä, Finland

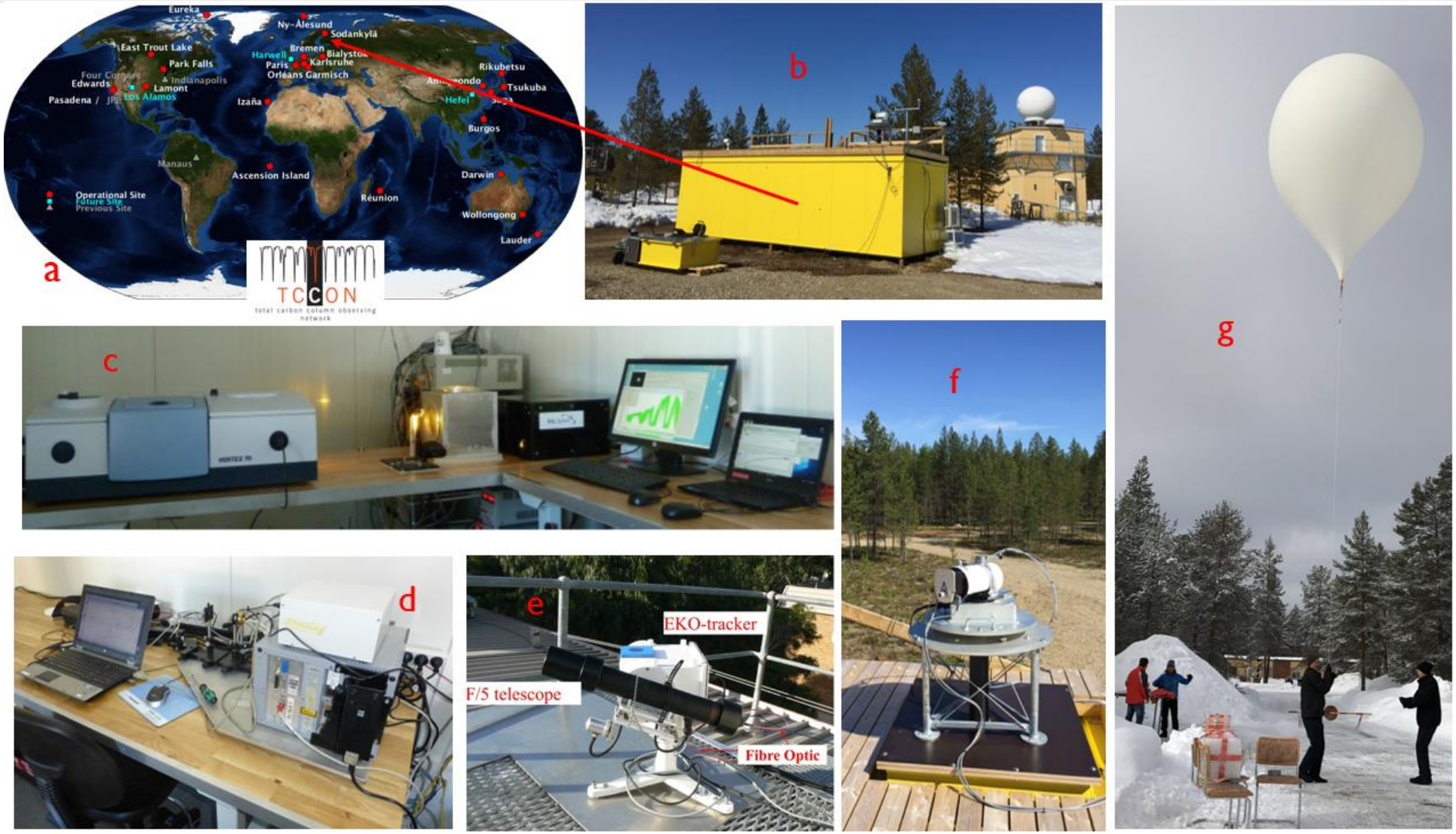


Fig. 1: (a) TCCON sites, (b) FRM4GHG container and EM27/SUN in front, (c-left) Vertex70 and (c-right) LHR, (d) IRCube, (e) suntracker for IRCube, (f) suntracker for Vertex70 and LHR, (g) Aircore launch at Sodankylä site.