

S5P MPC VDAF and TCCON4SP CH₄ validation results

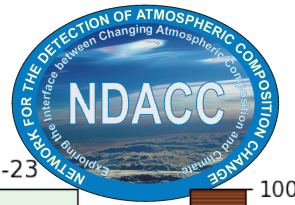
B. Langerock and M. K. Sha

bavo.langerock@aeronomie.be

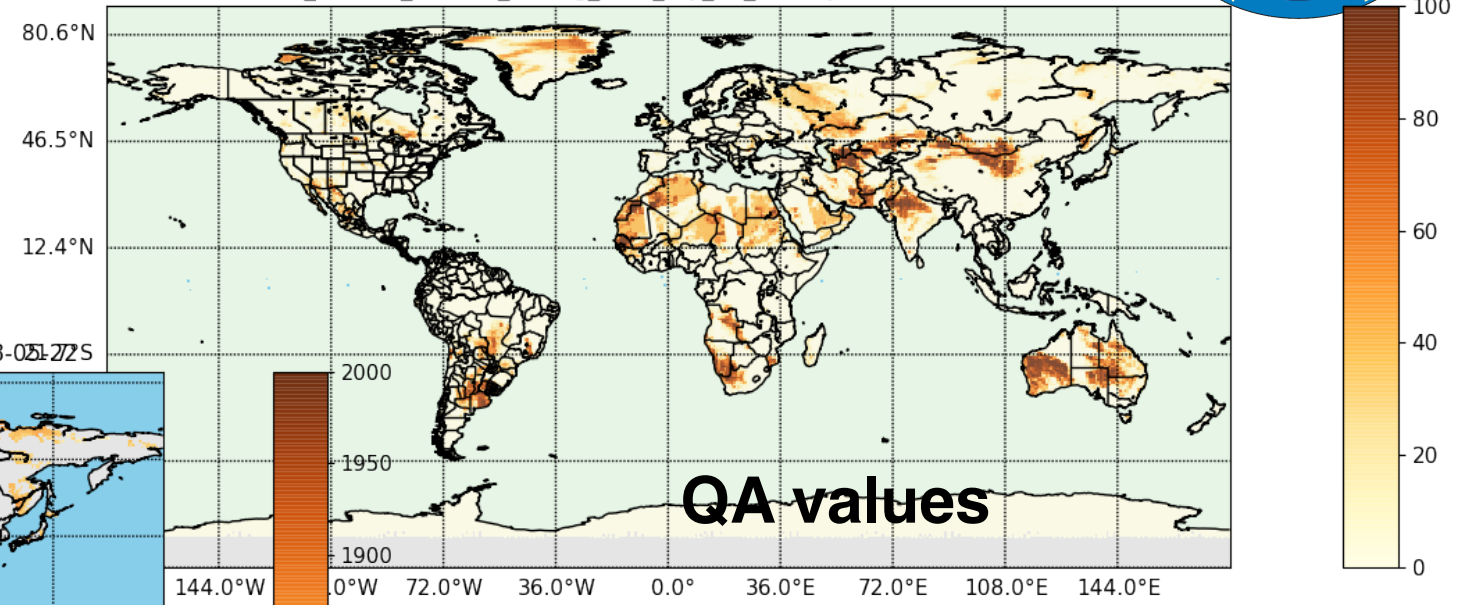
mahesh.sha@aeronomie.be



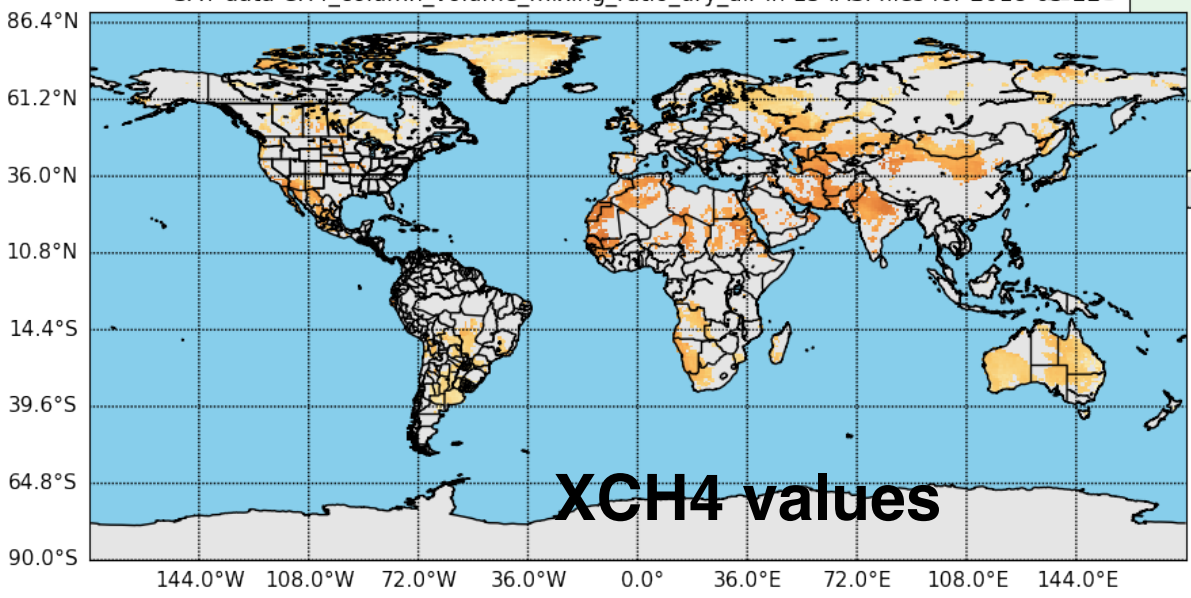
L2_CH4 (B. Langerock and M. K. Sha)



SAT data CH4_column_volume_mixing_ratio_dry_air_validity in 15 IASI files for 2018-05-23

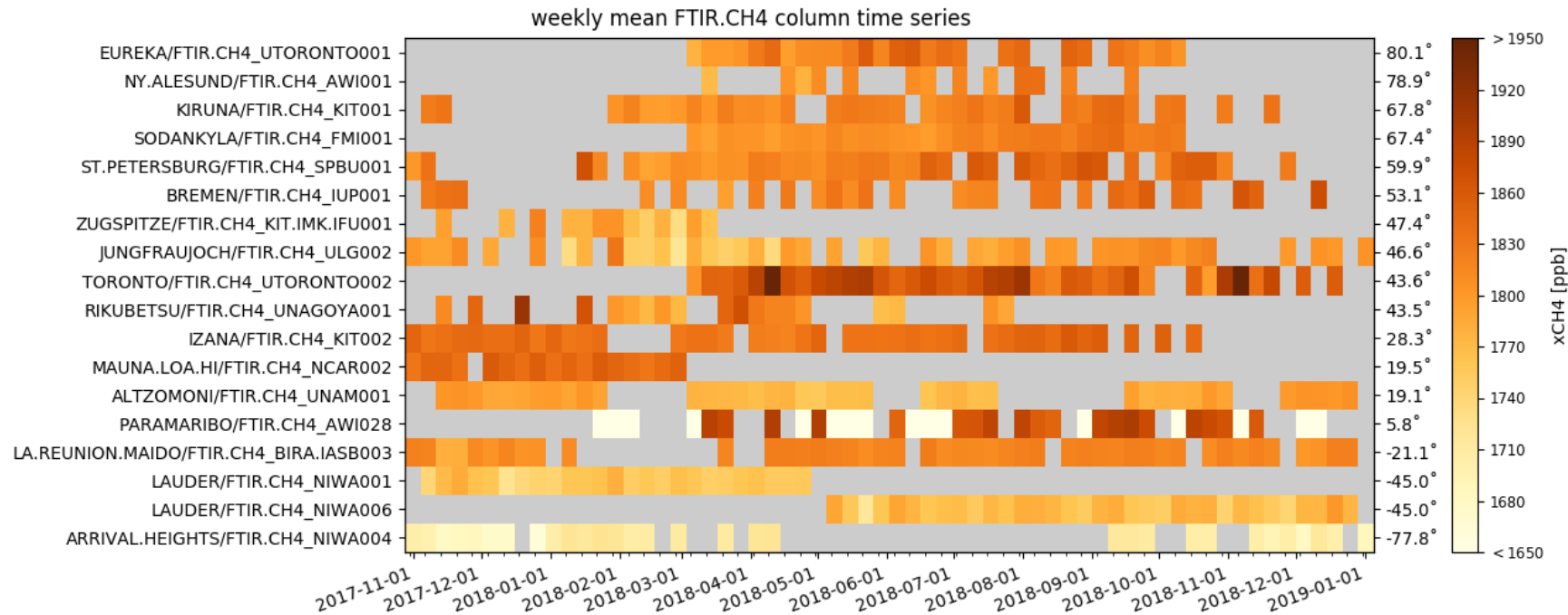
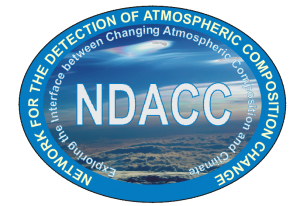


SAT data CH4_column_volume_mixing_ratio_dry_air in 15 IASI files for 2018-05-23



S5P qa value: strict filtering->no island stations
For NDACC only NH with rather high lat remaining, in SH only Lauder (NZ)

L2_CH4 (B. Langerock and M. K. Sha)



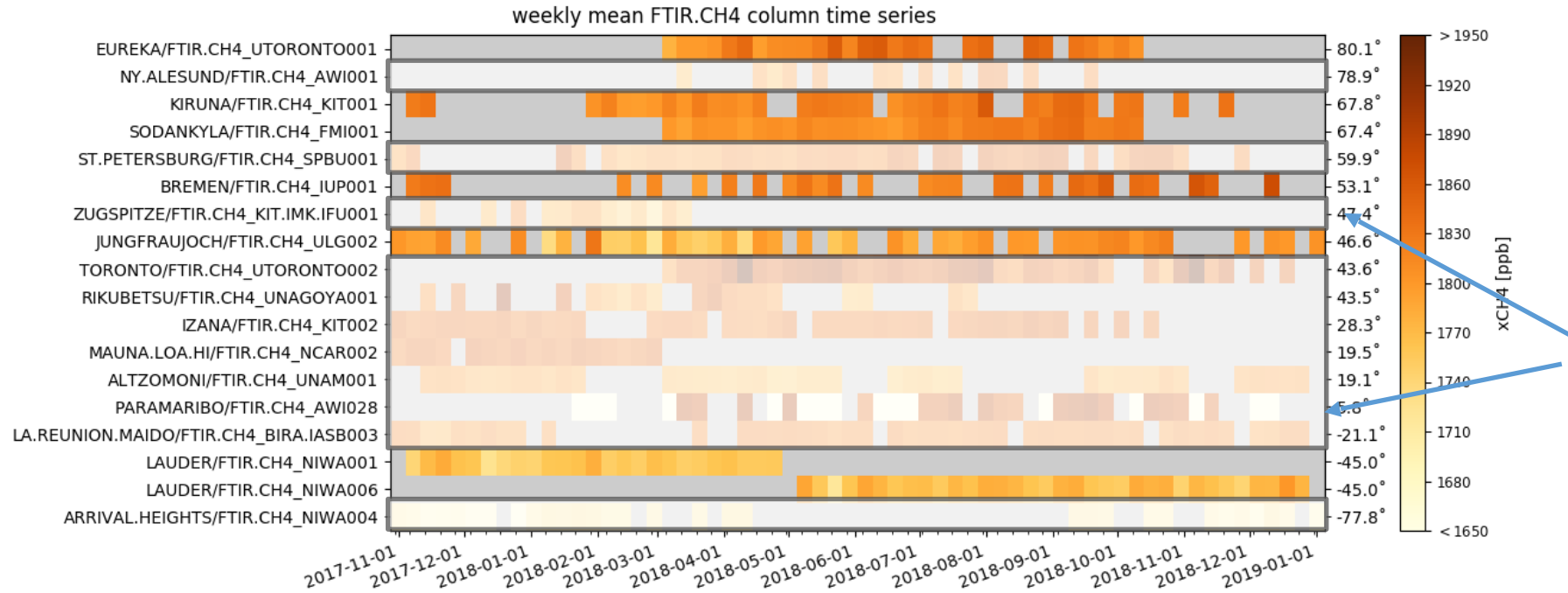
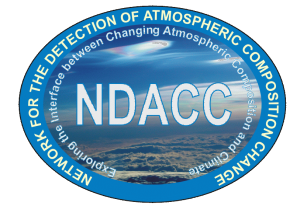
NDACC FTIR characteristics

- Less stations: CH4 is not reported by all PI's ...
- Typical uncertainty is 4%. This is due to a too conservative spectroscopic uncertainty component
- S5P Prior is substituted in NDACC FTIR profile
- high lat stations have no measurements during local winter

S5P setup

- FTIR smoothed with SAT AVK
- $\Delta t=6h, 3h$ and $1h$
- 50km radius and 100km radius
- QA filtering: qa_value>0.5
- Normal xCH₄ product and bias-corrected xCH₄ product
- Data processor version: 01.02.02 (RPRO & OFFL)

L2_CH4 (B. Langerock and M. K. Sha)



Paramaribo is left out:
issue with surface pressure
Zugspitze not up to date
Toronto: too high variability in signal
Island stations
AH, St Peter, Ny.Ale: no co-locations

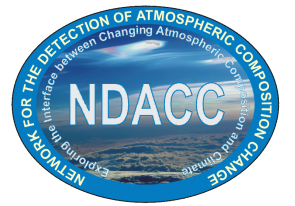
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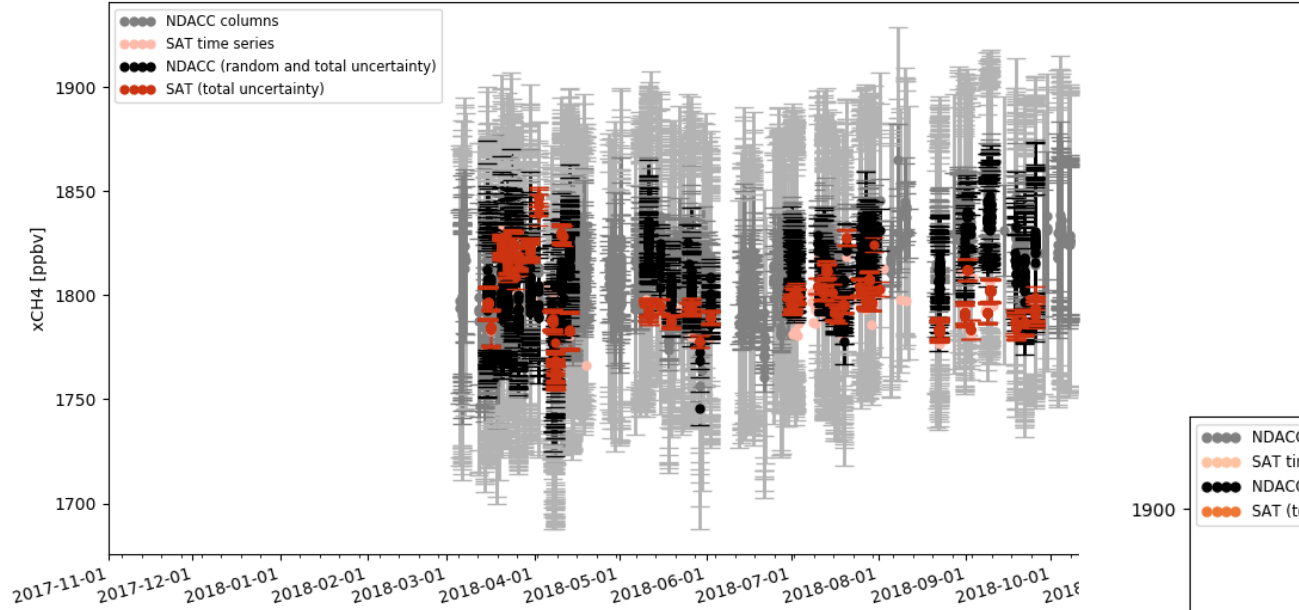
S5P setup

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- Data processor version: 01.02.02 (RPRO & OFFL)

L2_CH4 (B. Langerock and M. K. Sha)

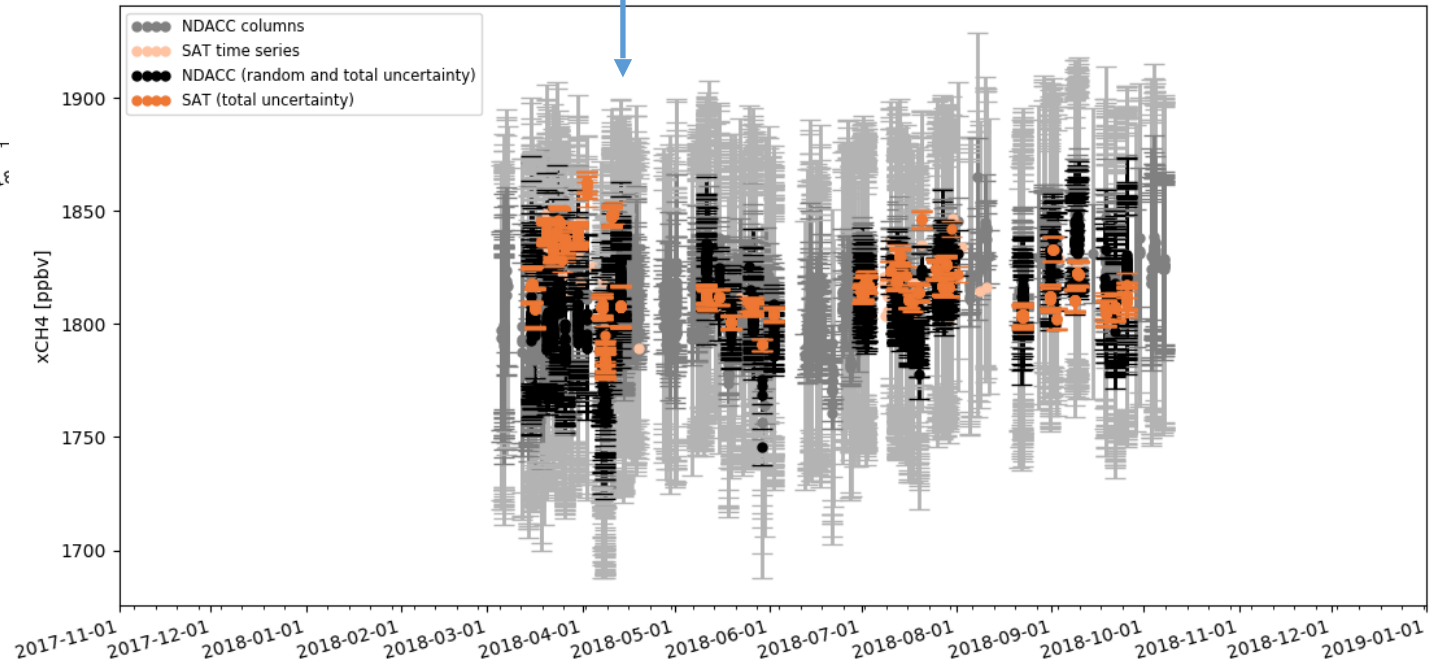


S5P xCH4 and FTIR.CH4 total column values
(surf - toa, SODANKYLA (lat.=67.4°), 2018-03-15 till 2018-09-25, 829 meas.)



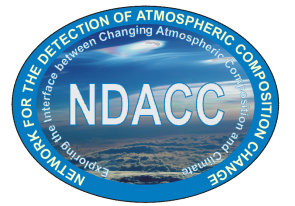
bias corrected

S5P xCH4 bias corrected and FTIR.CH4 total column values
(surf - toa, SODANKYLA (lat.=67.4°), 2018-03-15 till 2018-09-25, 829 meas.)

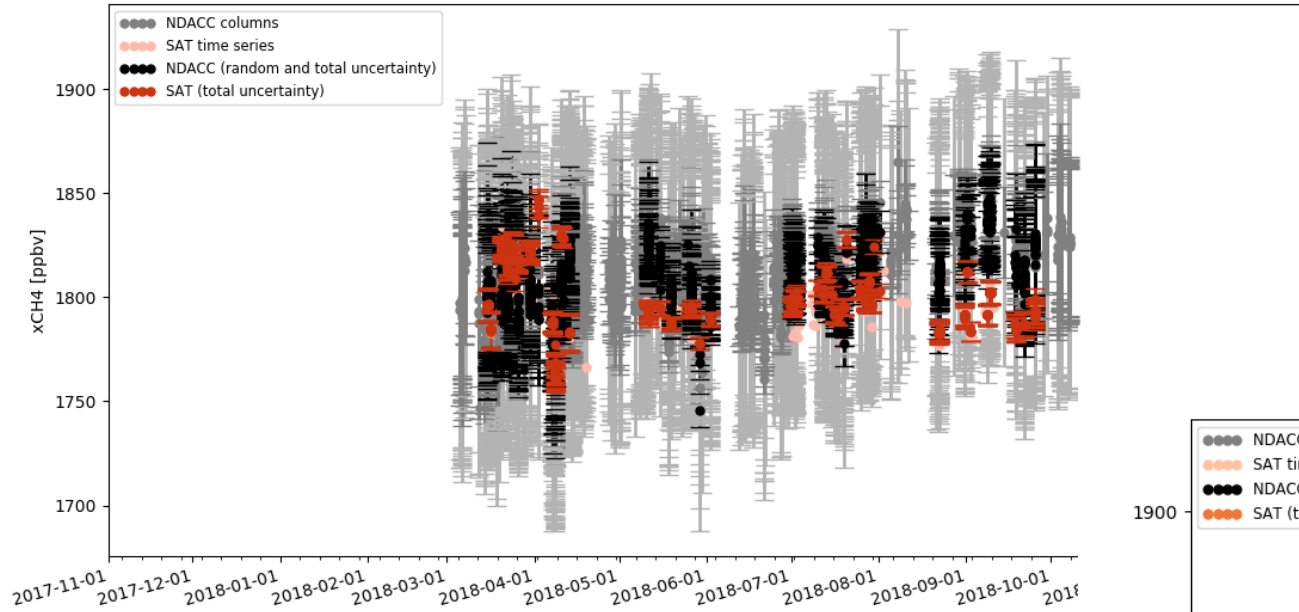


- Bias corrected S5P XCH4 data show better match improved overall bias relative to NDACC
- **Spring >> § Summer == § Autumn <<**
- rel diff has high variation ($\Delta t < 6h$) compared to ($\Delta t < 1h$) -> diurnal variation: stats for daily mean

L2_CH4 (B. Langerock and M. K. Sha)

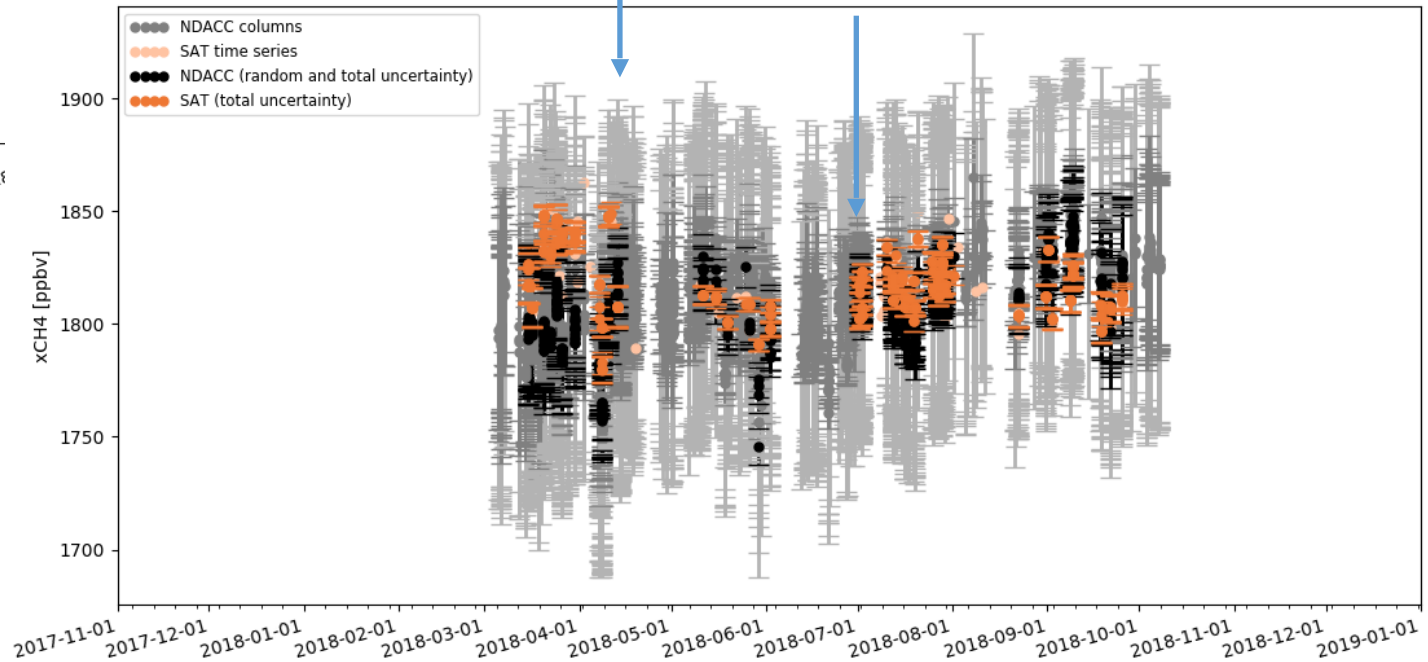


S5P xCH4 and FTIR.CH4 total column values
(surf - toa, SODANKYLA (lat.=67.4°), 2018-03-15 till 2018-09-25, 829 meas.)



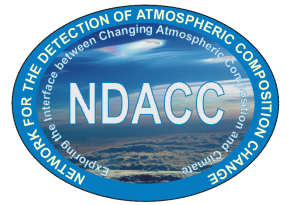
bias corrected

S5P xCH4 bc <50km 1h and FTIR.CH4 total column values
(surf - toa, SODANKYLA (lat.=67.4°), 2018-03-15 till 2018-09-25, 404 meas.)

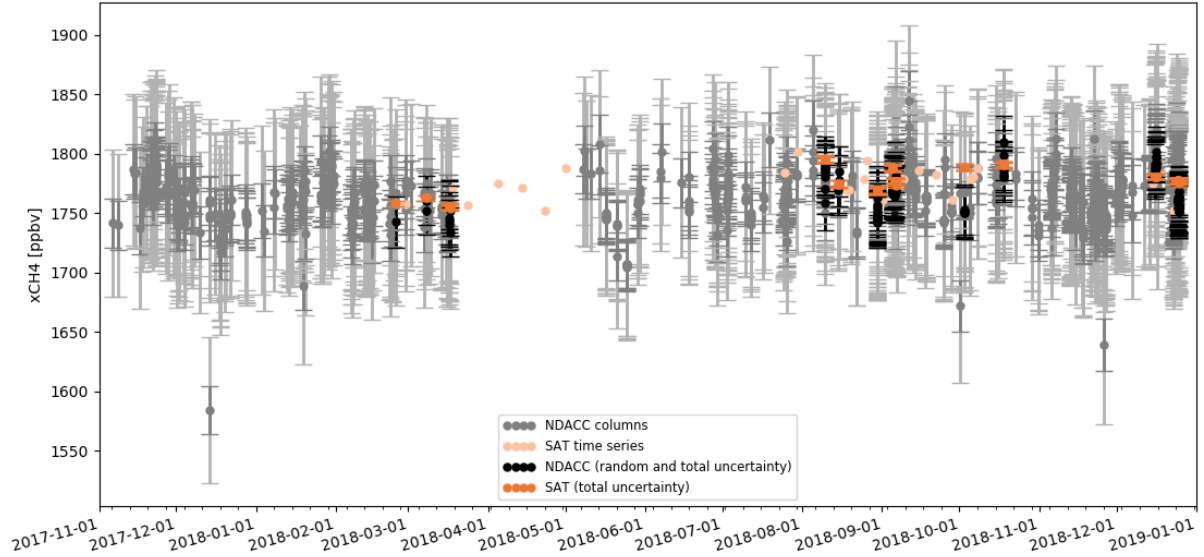


- Bias corrected S5P XCH4 data show better match improved overall bias relative to NDACC
- **Spring >> § Summer == § Autumn <<**
- rel diff has high variation ($\Delta t < 6h$) compared to ($\Delta t < 1h$) -> diurnal variation: stats for daily mean

L2_CH4 (B. Langerock and M. K. Sha)

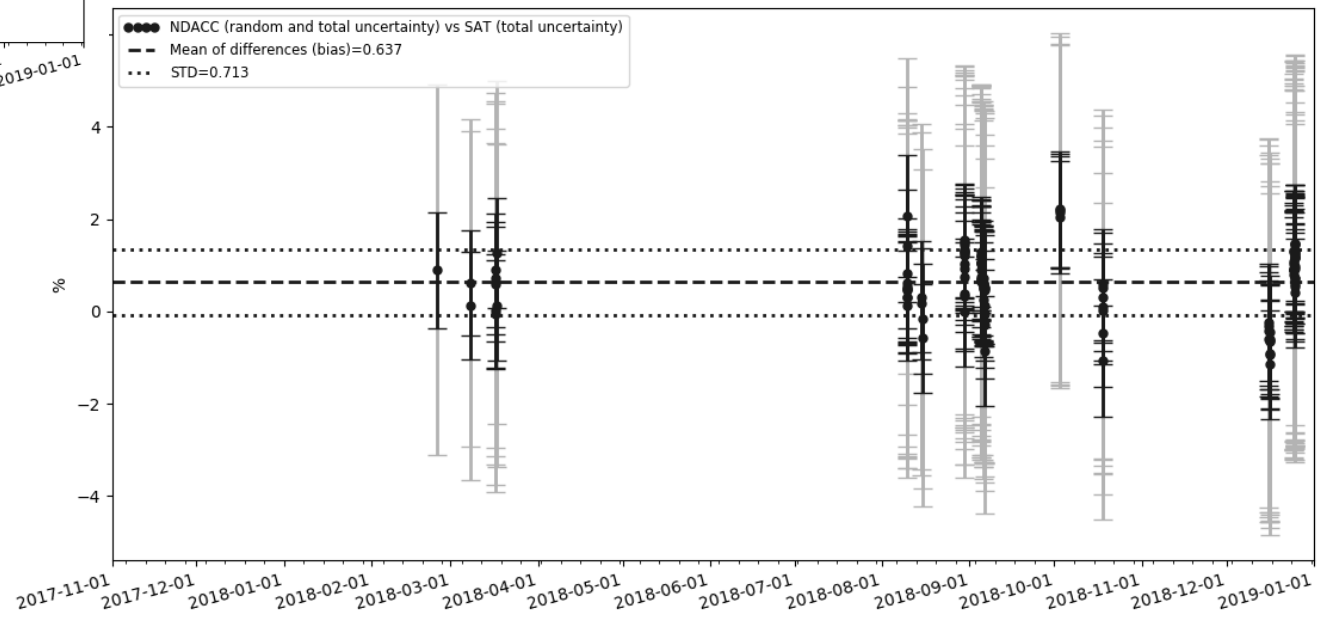


S5P xCH4 bias corrected and FTIR.CH4 total column values
(surf - toa, LAUDER (lat.=-45.0°), 2018-02-24 till 2018-12-25, 115 meas.)

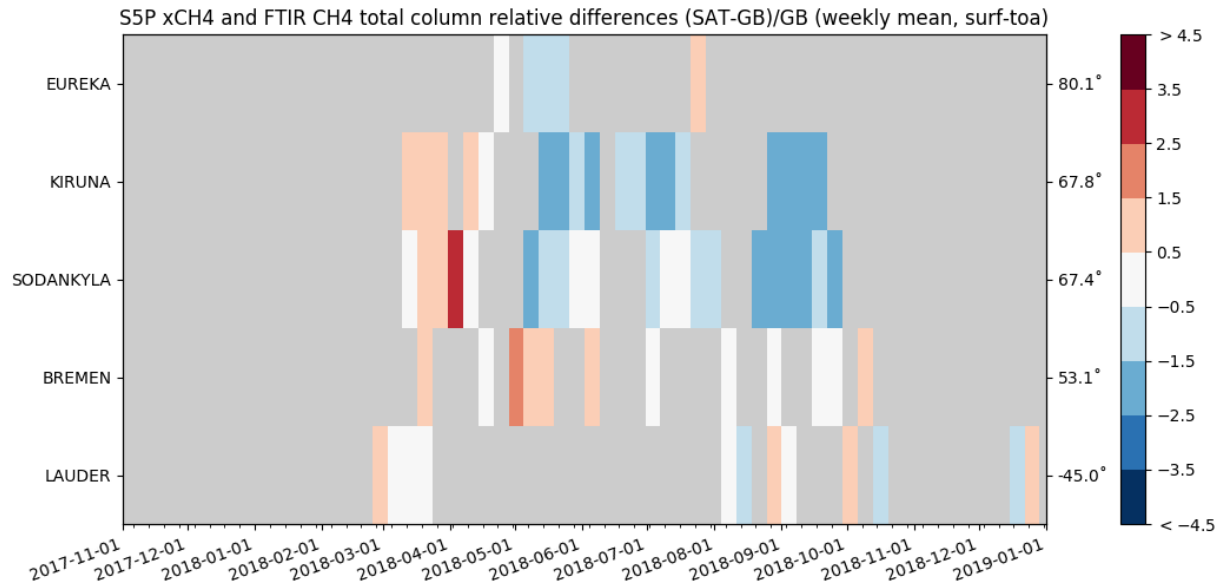
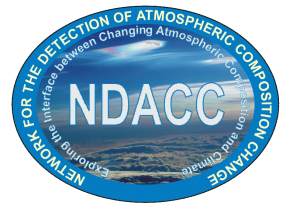


few co-locations
-> stats (bias/correlations)
should be treated with care

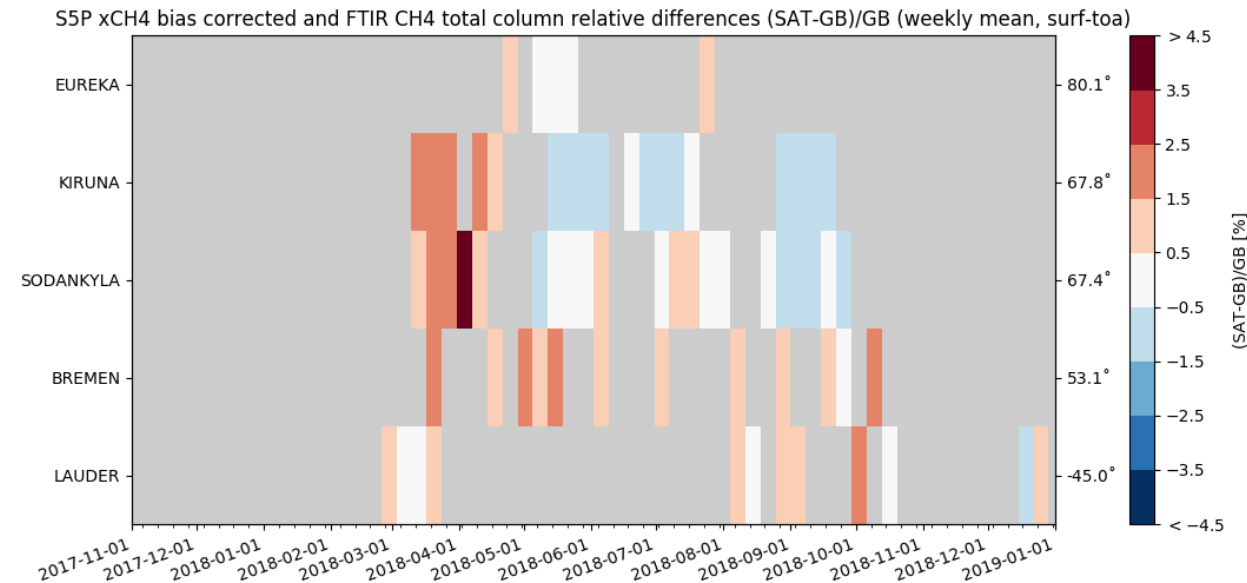
S5P xCH4 bias corrected and FTIR.CH4 total column relative differences (SAT-GB)/GB
(surf - toa, LAUDER (lat.=-45.0°), 2018-02-24 till 2018-12-25, 115 meas.)



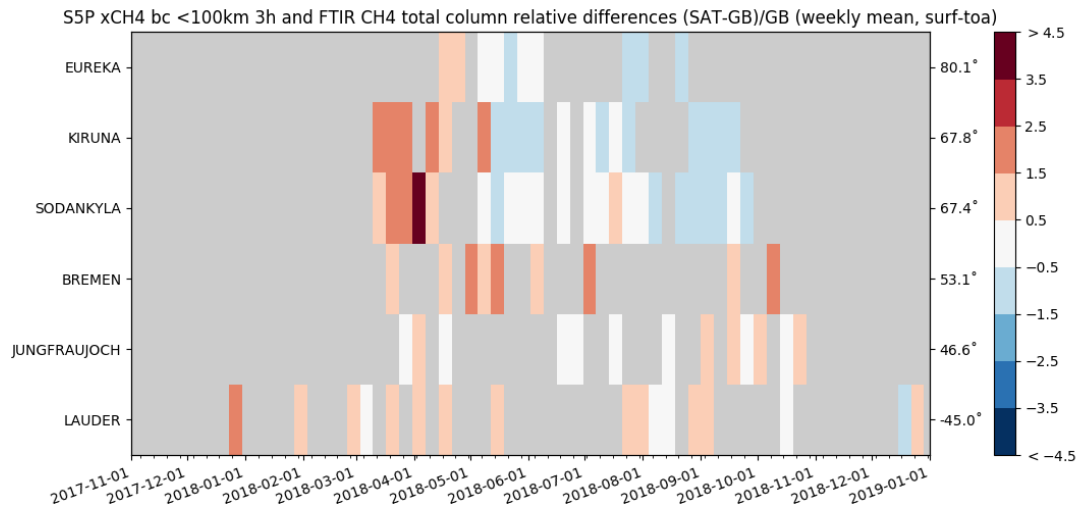
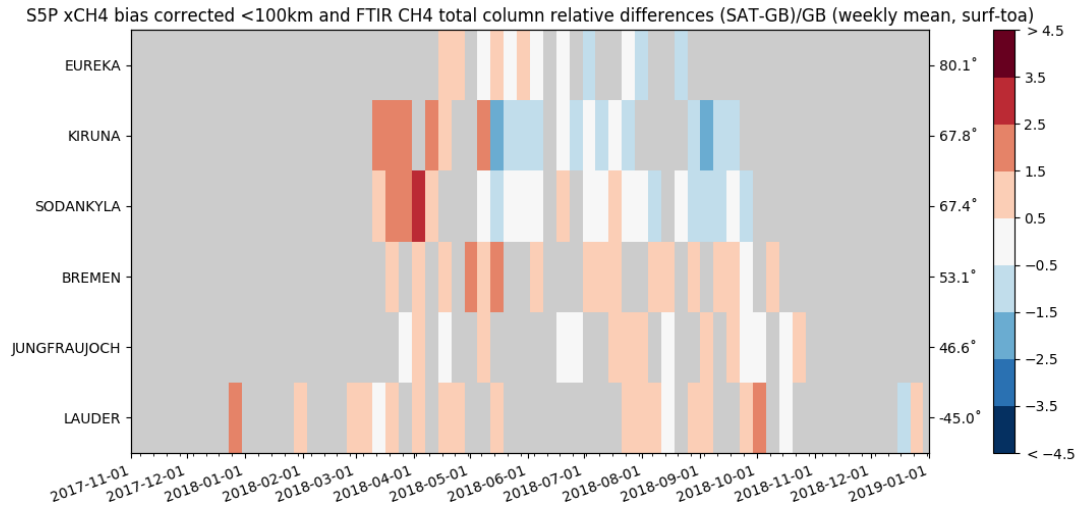
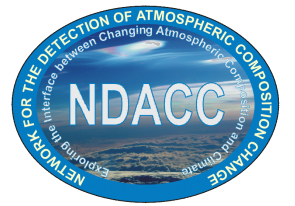
L2_CH4 (B. Langerock and M. K. Sha)



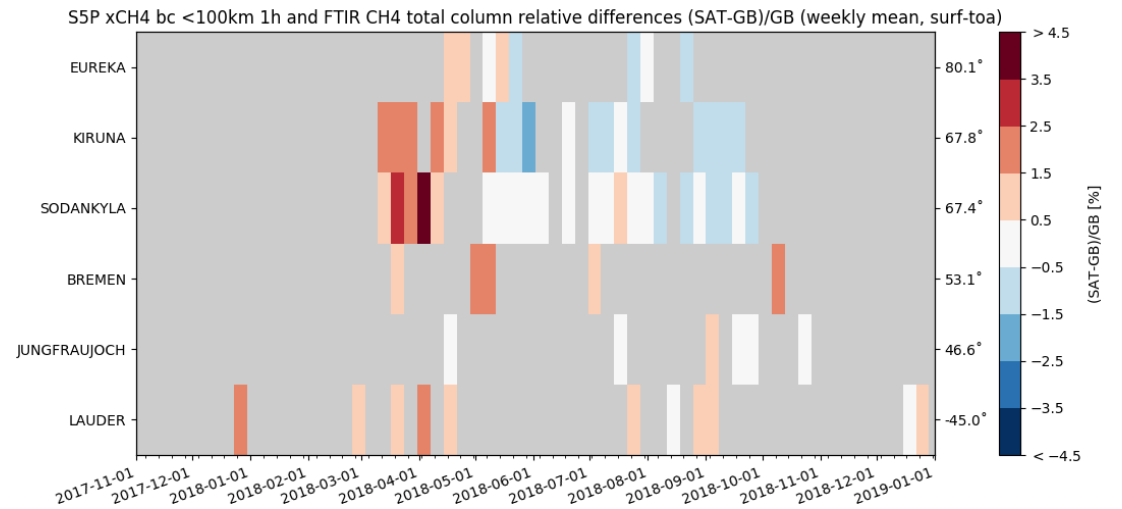
- <50km, $\Delta t < 6h$
- at least 4 pixels in co-location
- co-locations centred on summer months
- bias correction removes underestimation for high lat stations during summer



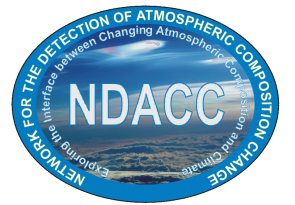
L2_CH4 (B. Langerock and M. K. Sha)



- <100km
- at least 4 pixels in co-location
- + Jungfrauoch
- much more co-locations for Lauder
- stats are not so robust: number of co-locations depends strongly on Δt

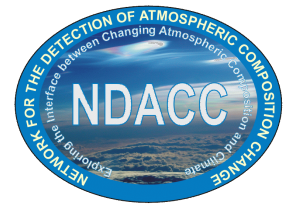


L2_CH4 (B. Langerock and M. K. Sha)



ID	S5P TROPOMI Level-2 Data Product	Vertical Resolution	Target Bias	Target Precision
L2_O3	Total O ₃	total column	3.5-5%	1.6%-2.5%
L2_O3_PR	O ₃ profile (incl. troposphere)	6 km	10-30%	10%
L2_O3_TCL	O ₃ tropospheric column	tropospheric column	25%	10%
L2_NO2	NO ₂ stratospheric column	stratospheric column	<10%	0.5 Pmolec.cm ⁻²
	NO ₂ tropospheric column	tropospheric column	25-50%	0.7 Pmolec.cm ⁻²
L2_SO2	Enhanced total SO ₂	stratospheric column	30%	0.15-0.3 DU
	Total SO ₂	total column	30-50%	1-3 DU
L2_HCHO	Total HCHO	total column	40-80%	4-12 Pmolec.cm ⁻²
L2_CO	Total CO	total column	10%	10%
L2_CH4	Total CH ₄	total column	1.5%	1%
L2_HFC	Total HFC	total column	0.05%	0.05%

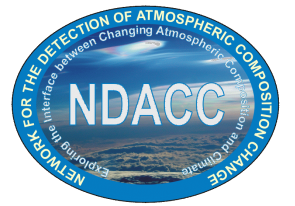
L2_CH4 (B. Langerock and M. K. Sha)



Standard S5P – XCH4 product using NDACC FTIR < 50km $\Delta t=6h$

site	# days	Std	correlation	rel diff bias(%)	rel diff std(%)	lat
EUREKA	13	1.4	0.31	-0.39	0.74	80.1
KIRUNA	35	0.9	0.13	-0.79	1.41	67.8
SODANKYLA	47	1.0	0.16	-0.47	1.16	67.4
BREMEN	19	1.2	0.68	0.59	0.63	53.1
LAUDER	12	1.3	0.65	0.10	0.75	-45.0
		1.2	0.39	-0.19	0.94	

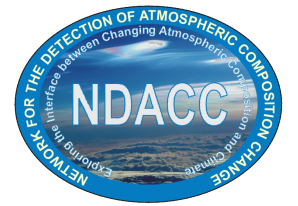
L2_CH4 (B. Langerock and M. K. Sha)



Bias corrected S5P – XCH4 product using NDACC FTIR < 50km $\Delta t=6h$

site	# days	Std	correlation	rel diff bias(%)	rel diff std(%)	lat
EUREKA	13	1.1	0.69	0.47	0.53	80.1
KIRUNA	35	0.9	0.14	0.17	1.45	67.8
SODANKYLA	47	1.0	0.20	0.57	1.14	67.4
BREMEN	19	1.2	0.68	1.12	0.61	53.1
LAUDER	12	1.3	0.70	0.61	0.71	-45.0
		1.1	0.48	0.59	0.89	

L2_CH4 (B. Langerock and M. K. Sha)



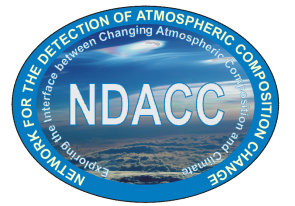
Bias corrected S5P – XCH4 product using NDACC FTIR < 100km $\Delta t=3h$

site	# days	Std	correlation	rel diff bias(%)	rel diff std(%)	lat
EUREKA	25	2.3	0.41	-0.03	1.49	80.1
KIRUNA	45	1.0	0.10	0.03	1.37	67.8
SODANKYLA	57	1.0	0.06	0.36	1.16	67.4
BREMEN	13	0.9	0.74	1.46	0.49	53.1
JUNGFRAUJOCH	19	0.8	0.82	0.24	0.48	46.6
LAUDER	20	1.3	0.80	0.76	0.58	-45.0
		1.2	0.49	0.47	0.93	

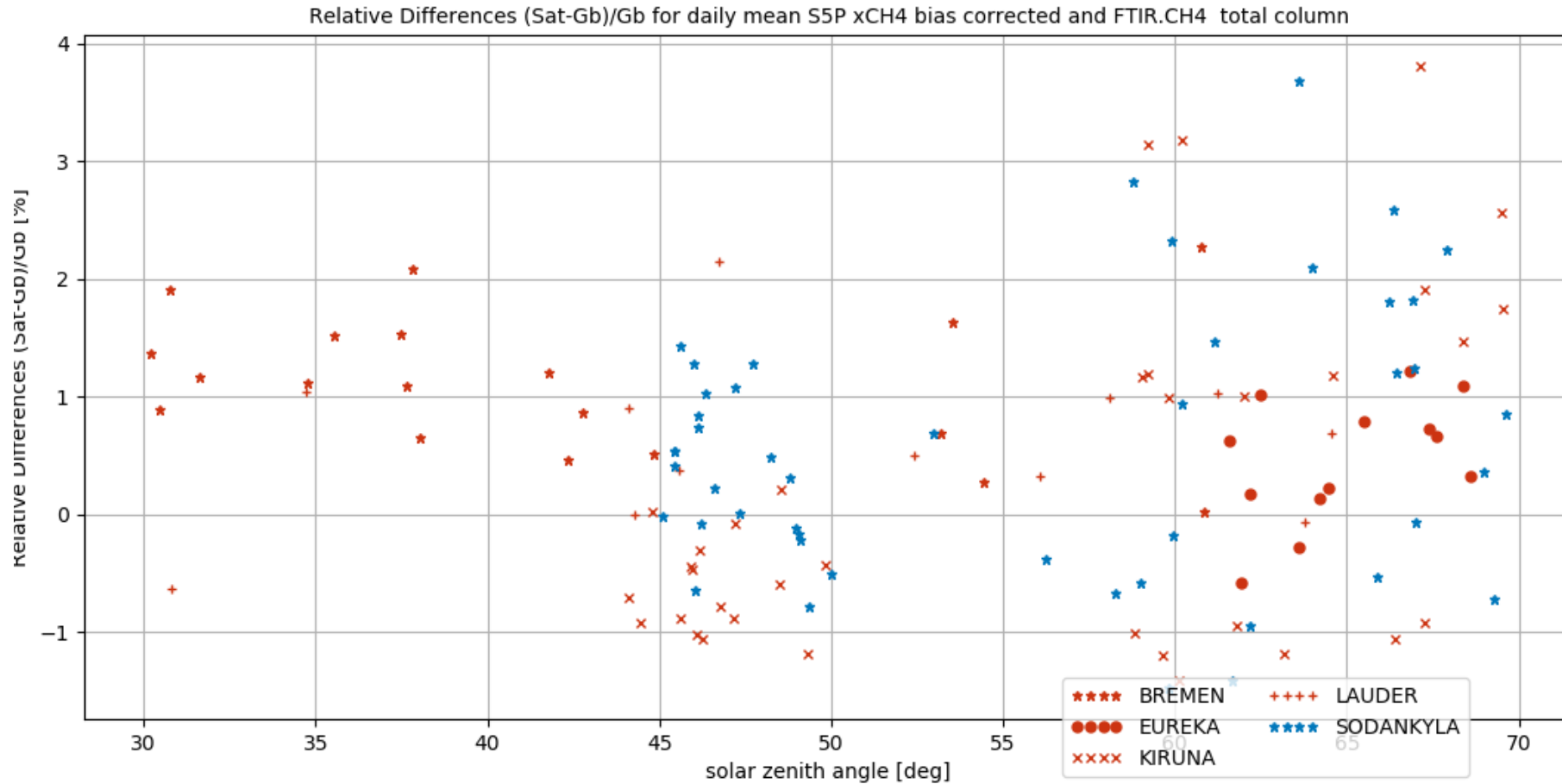
Conclusions

- all scenario's: mission requirements are met across available NDACC sites
- statistics is not robust to make statements on correlation (-> TCCON)

L2_CH4 (B. Langerock and M. K. Sha)



SZA / Rel diff (bias corrected, <50km) ———> higher spread at SZA>60°



L2_CH4 (B. Langerock and M. K. Sha)



TCCON FTIR characteristics

- Highly homogenized network; global coverage (80° N – 45° S) with about 26 stations
- High accuracy / precision: 0.2% / 0.3% for CH₄
- S5P Prior CH₄ is substituted with the TCCON CH₄ prior
- Altitude correction is done for each pixel to the ground station height

S5P setup

- FTIR smoothed with SAT AVK
- $\Delta t=1h$
- 50km radius and 100km radius
- QA filtering: qa_value>50
- Normal xCH₄ product and bias-corrected xCH₄ product
- Data processor version: 01.02.02 (RPRO & OFFL)

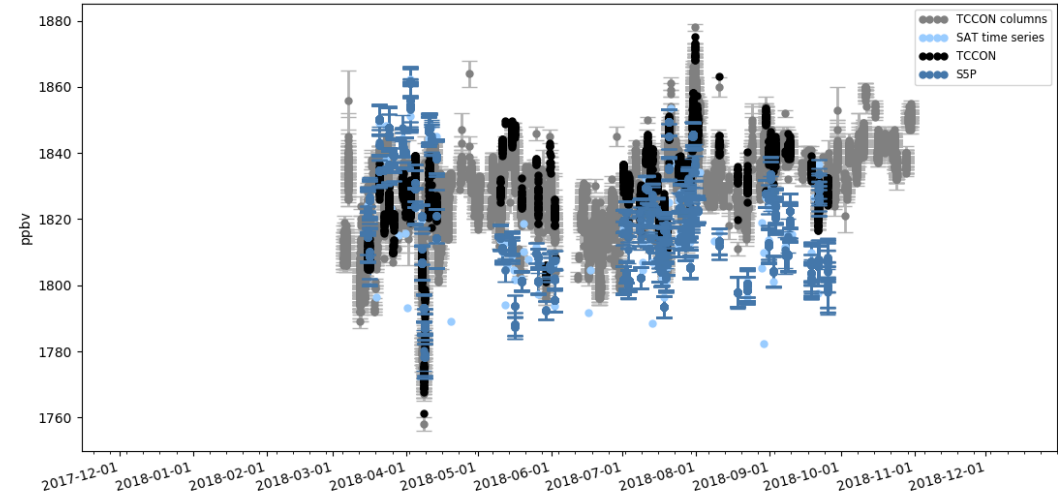
L2_CH4 (B. Langerock and M. K. Sha)



Bias corrected S5P-XCH4

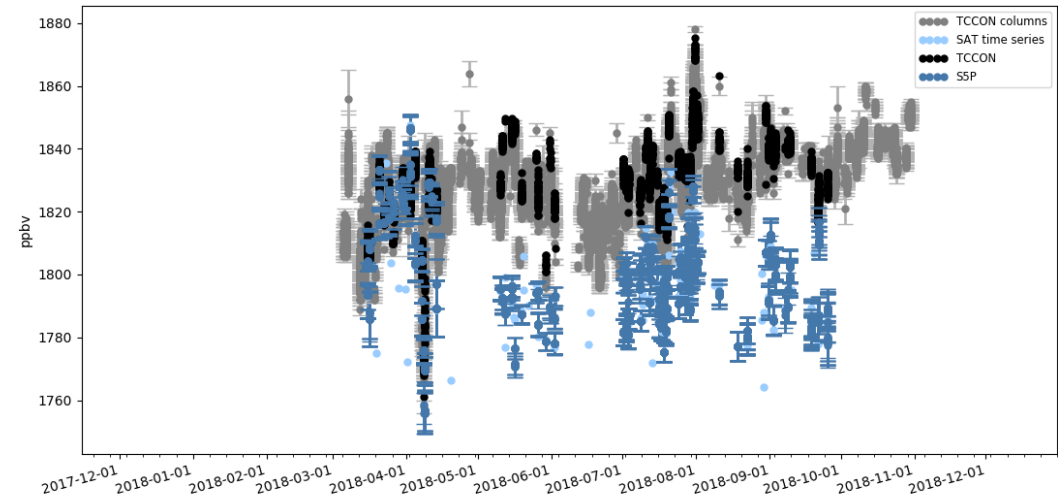
High bias during winter / spring and low bias during summer / autumn

S5P-TCCON xCH4 smooth 100km bc 1hr and FTIR.CH4 dry air mol fraction (xCH4) values (surf - toa, SODANKYLA (lat.=67.4°), 2018-03-15 till 2018-09-25, 3070 meas.)



Standard S5P-XCH4

S5P-TCCON xCH4 smooth 100km 1hr and FTIR.CH4 dry air mol fraction (xCH4) values (surf - toa, SODANKYLA (lat.=67.4°), 2018-03-15 till 2018-09-25, 3070 meas.)

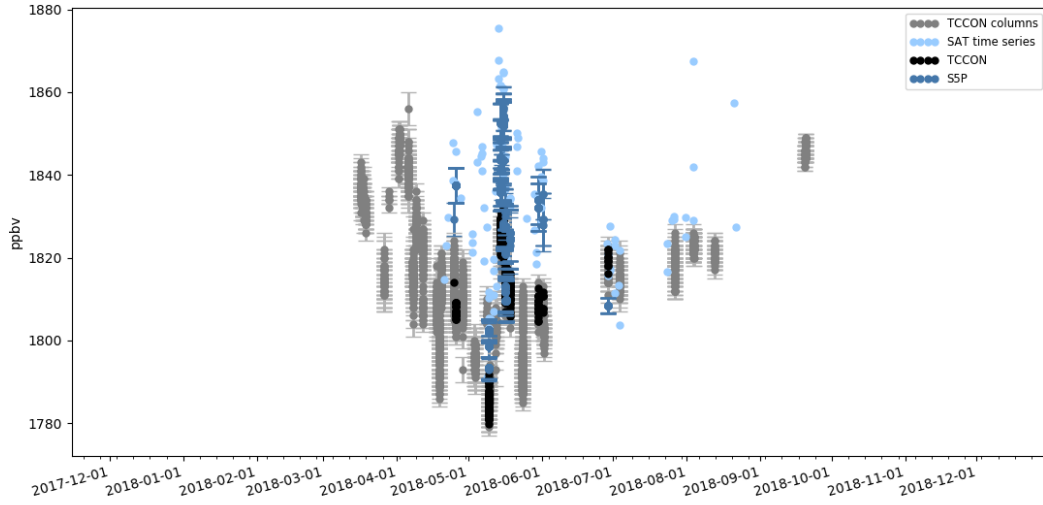


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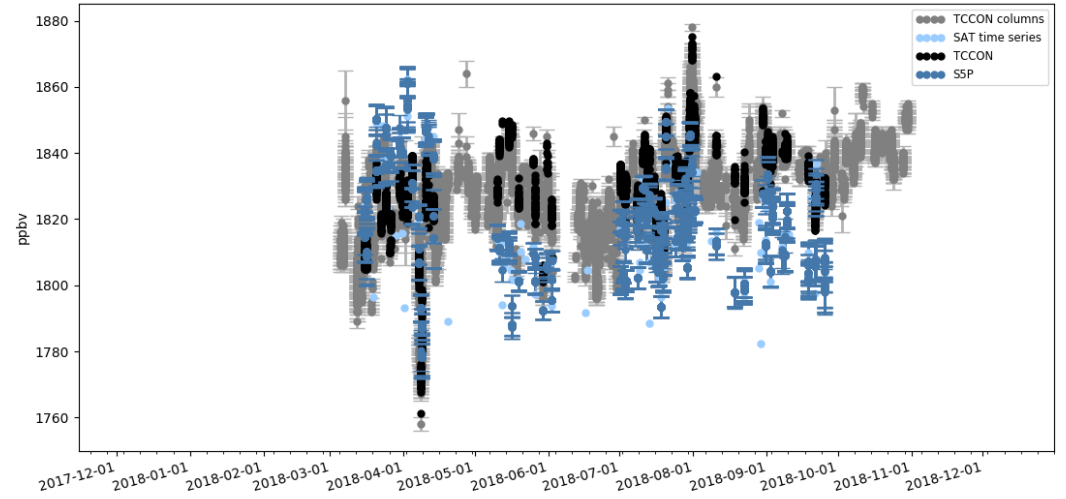


Bias corrected S5P-XCH4

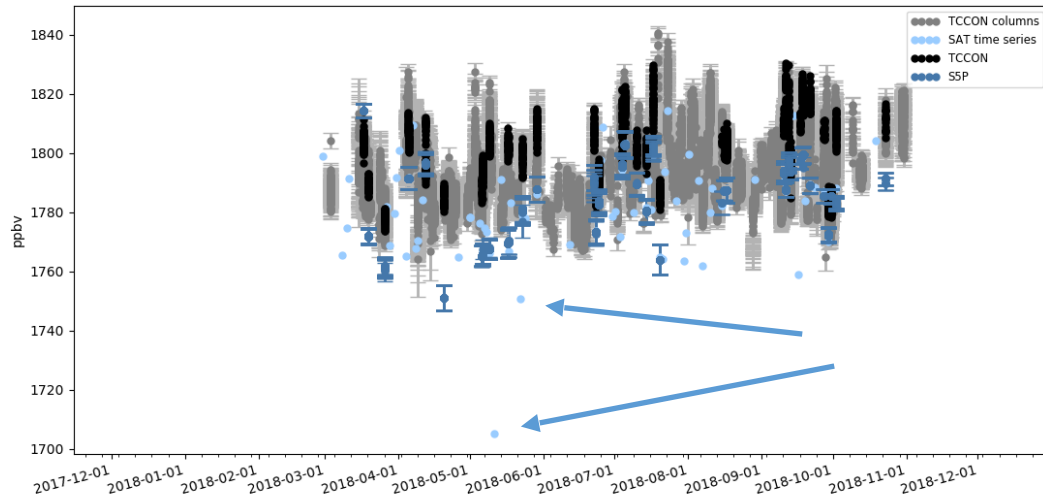
S5P-TCCON xCH4 smooth 100km bc 1hr and FTIR.CH4 dry air mol fraction (xCH4) values (surf - toa, EUREKA (lat.=80.0°), 2018-04-24 till 2018-06-28, 524 meas.)



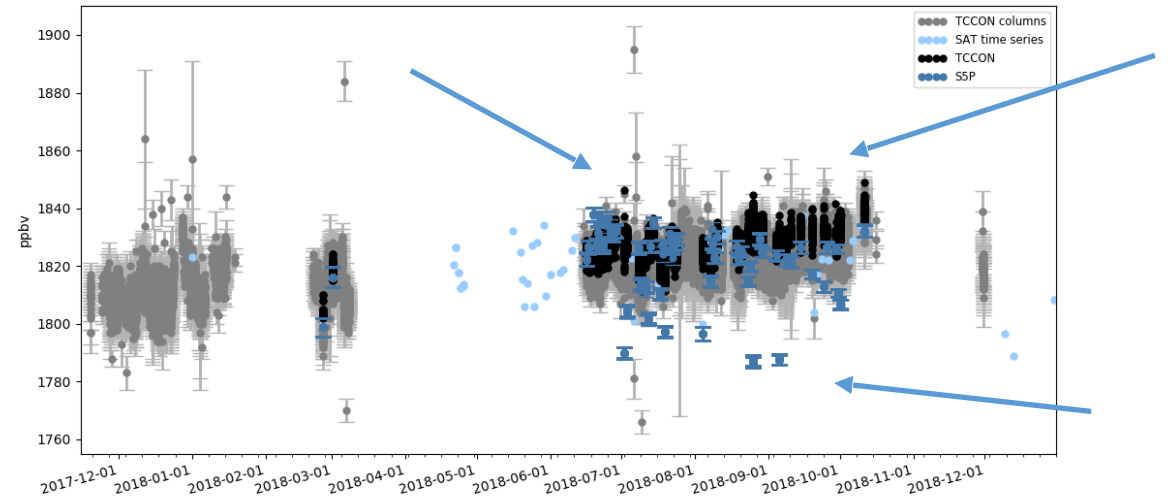
S5P-TCCON xCH4 smooth 100km bc 1hr and FTIR.CH4 dry air mol fraction (xCH4) values (surf - toa, SODANKYLA (lat.=67.4°), 2018-03-15 till 2018-09-25, 3070 meas.)



S5P-TCCON xCH4 smooth 100km bc 1hr and FTIR.CH4 dry air mol fraction (xCH4) values (surf - toa, WOLLONGONG (lat.=34.4°), 2018-03-17 till 2018-10-23, 1506 meas.)



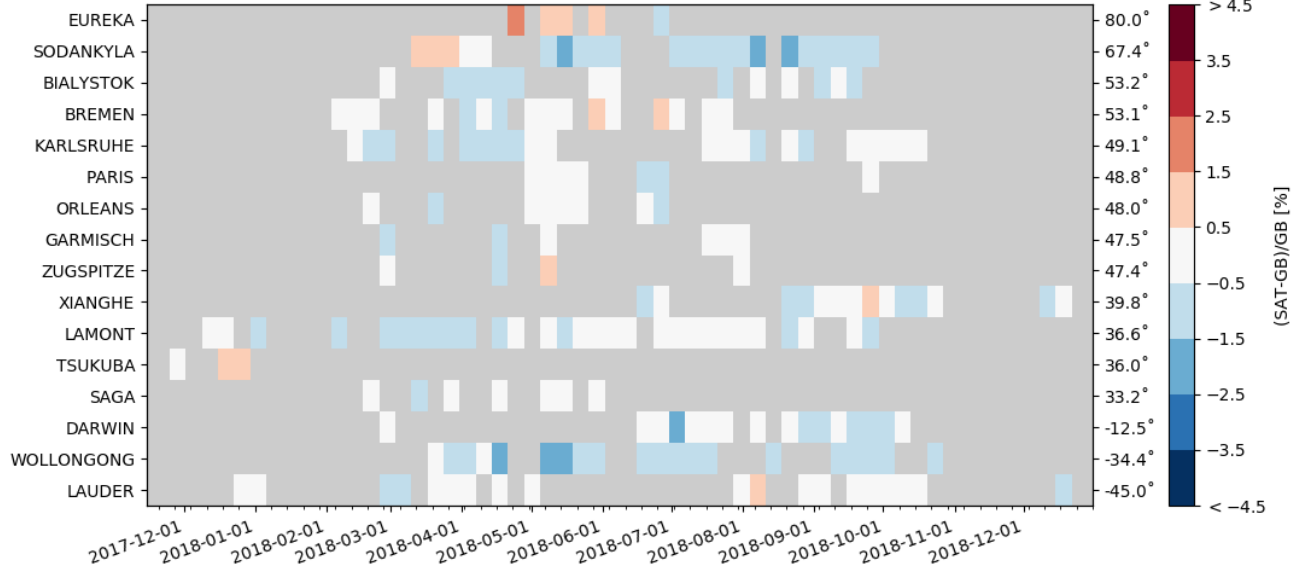
S5P-TCCON xCH4 smooth 100km bc 1hr and FTIR.CH4 dry air mol fraction (xCH4) values (surf - toa, DARWIN (lat.=12.5°), 2018-02-25 till 2018-10-11, 2866 meas.)



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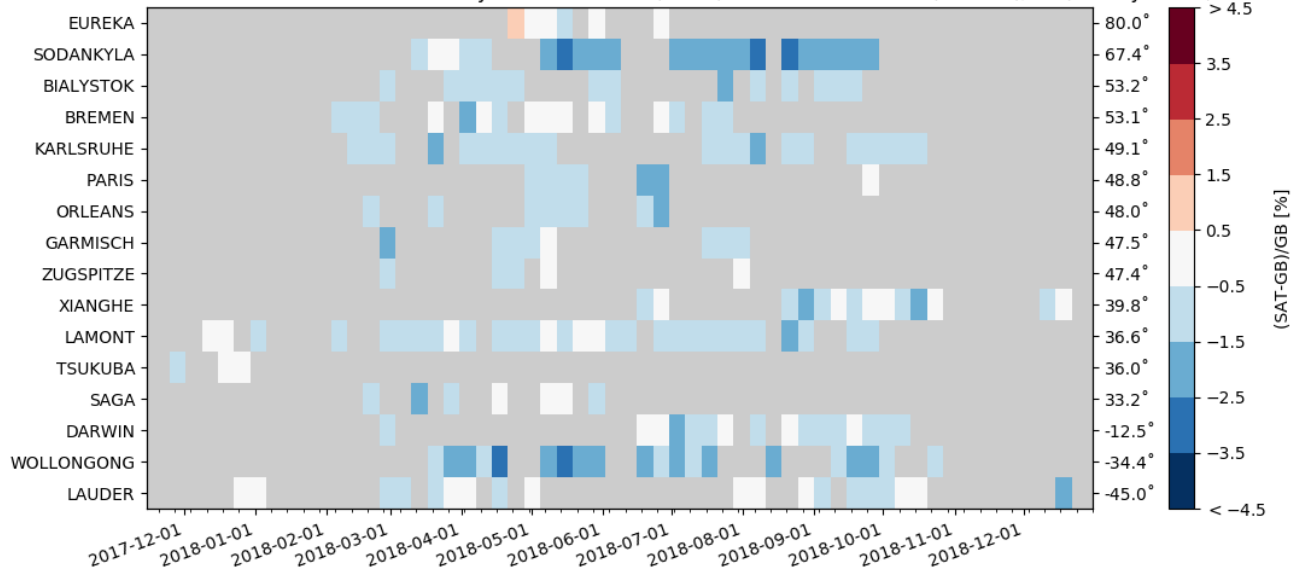
S5P-TCCON xCH4 smooth 100km bc 1hr and FTIR CH4 dry air mol fraction (xCH4) relative differences (SAT-GB)/GB (weekly mean, surf-toa)



Bias corrected S5P-XCH4

Bias corrected S5P XCH4 data show better match improved overall bias relative to TCCON

S5P-TCCON xCH4 smooth 100km 1hr and FTIR CH4 dry air mol fraction (xCH4) relative differences (SAT-GB)/GB (weekly mean, surf-toa)



Standard S5P-XCH4

Validation of standard S5P – XCH4 product using TCCON FTIR

Site	#	Std	Correlation	Rel diff bias (%)	Rel diff std (%)	Lat
EUREKA	643	0.9	0.63	-0.26	0.62	80.0
SODANKYLA	3070	0.8	0.32	-1.62	0.93	67.4
BIALYSTOK	1821	0.8	0.37	-0.99	0.57	53.2
BREMEN	636	1.0	0.55	-0.58	0.57	53.1
KARLSRUHE	1185	0.6	0.60	-1.17	0.50	49.1
PARIS	1014	0.5	0.37	-0.93	0.71	48.8
ORLEANS	709	0.7	0.72	-1.14	0.37	48.0
GARMISCH	319	0.7	0.81	-0.87	0.46	47.5
ZUGSPITZE	26	1.3	0.60	-1.12	0.76	47.4
XIANGHE	584	1.5	0.65	-0.64	0.65	39.8
LAMONT	2744	1.1	0.71	-0.72	0.44	36.6
TSUKUBA	194	0.7	0.30	-0.12	0.35	36.0
SAGA	629	0.9	0.48	-0.62	0.49	33.2
DARWIN	2866	0.4	0.13	-0.56	0.75	-12.5
WOLLONGONG	1506	0.8	0.63	-1.56	0.66	-34.4
LAUDER	1689	0.9	0.81	-0.68	0.42	-45.0
Mean		0.9	0.54	-0.85	0.58	

Validation of bias corrected S5P – XCH4 product using TCCON FTIR

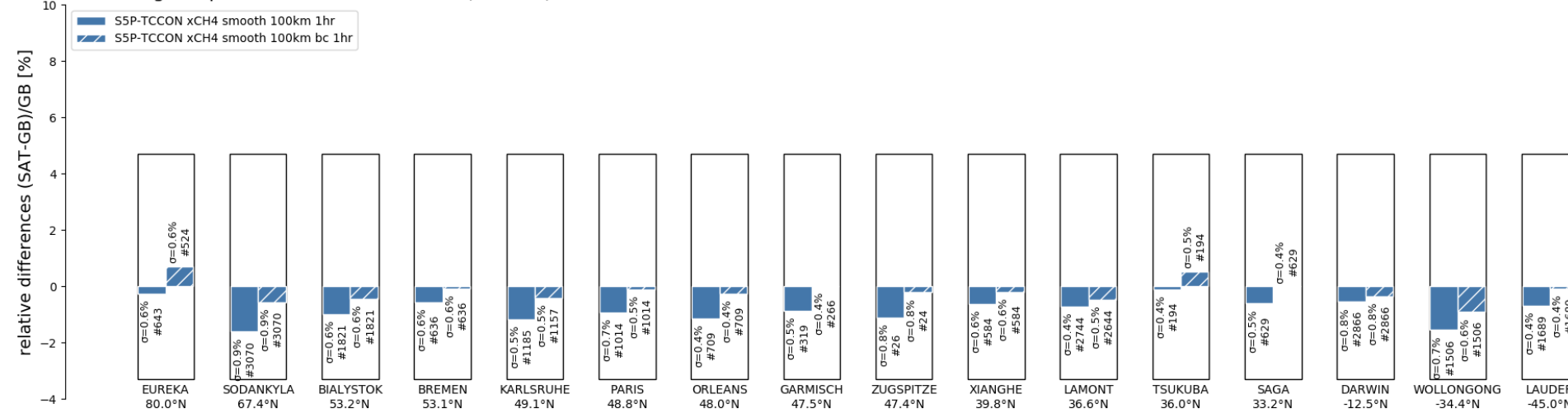
Site	#	Std	Correlation	Rel diff bias (%)	Rel diff std (%)	Lat
EUREKA	524	0.8	0.78	0.71	0.59	80.0
SODANKYLA	3070	0.8	0.32	-0.58	0.92	67.4
BIALYSTOK	1821	0.7	0.46	-0.46	0.56	53.2
BREMEN	636	0.9	0.53	-0.10	0.61	53.1
KARLSRUHE	1157	0.6	0.59	-0.41	0.49	49.1
PARIS	1014	0.7	0.36	-0.12	0.50	48.8
ORLEANS	709	0.7	0.67	-0.27	0.36	48.0
GARMISCH	266	0.7	0.86	-0.00	0.42	47.5
ZUGSPITZE	24	1.5	0.59	-0.23	0.76	47.4
XIANGHE	584	1.3	0.69	-0.21	0.63	39.8
LAMONT	2644	1.0	0.61	-0.49	0.55	36.6
TSUKUBA	194	0.5	0.37	0.53	0.47	36.0
SAGA	629	1.1	0.52	0.00	0.43	33.2
DARWIN	2866	0.4	0.01	-0.35	0.77	-12.5
WOLLONGONG	1506	0.9	0.63	-0.92	0.62	-34.4
LAUDER	1689	0.9	0.81	-0.09	0.42	-45.0
Mean		0.9	0.55	-0.19	0.57	

L2_CH4 (B. Langerock and M. K. Sha)

Bias corrected S5P-XCH4

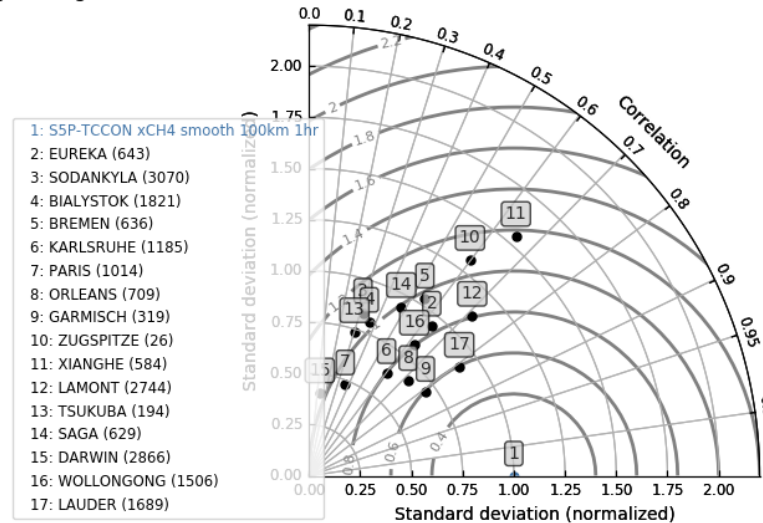


Histogram plot of relative differences (SAT-GB)/GB for S5P-TCCON xCH4 smooth 100km 1hr, S5P-TCCON xCH4 smooth 100km bc 1hr and FTIR CH4 timeseries

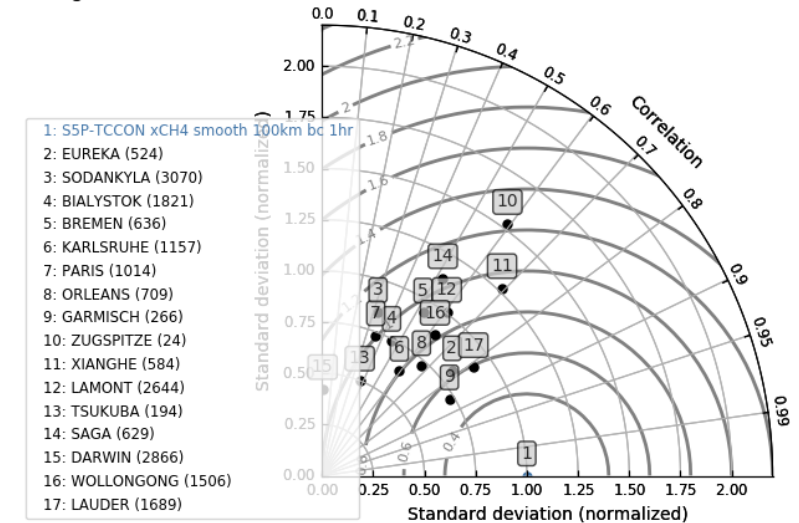


Correlation not so good due to low SAT values and SZA (seasonal) dependent bias

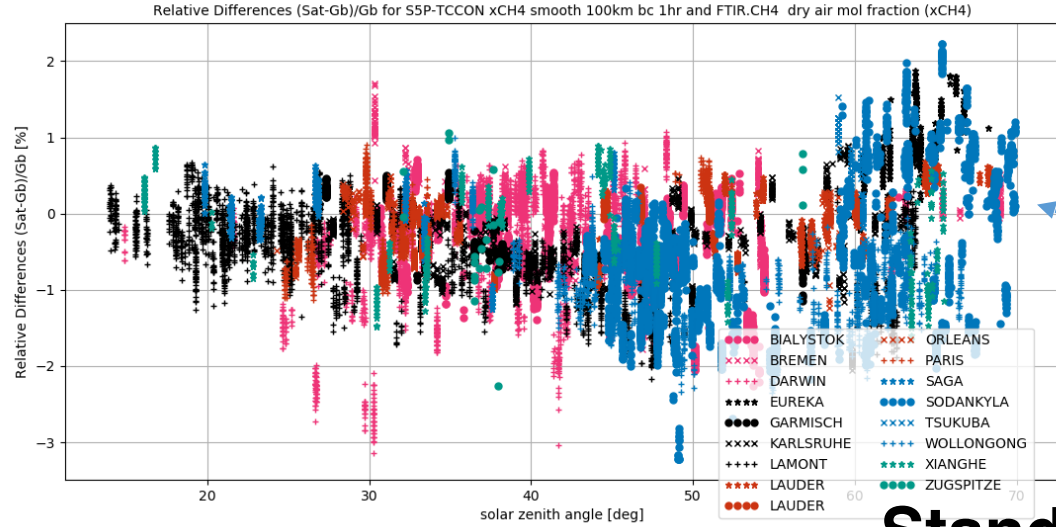
ylor diagram for S5P-TCCON xCH4 smooth 100km 1hr and FTIR.CH4 timeser



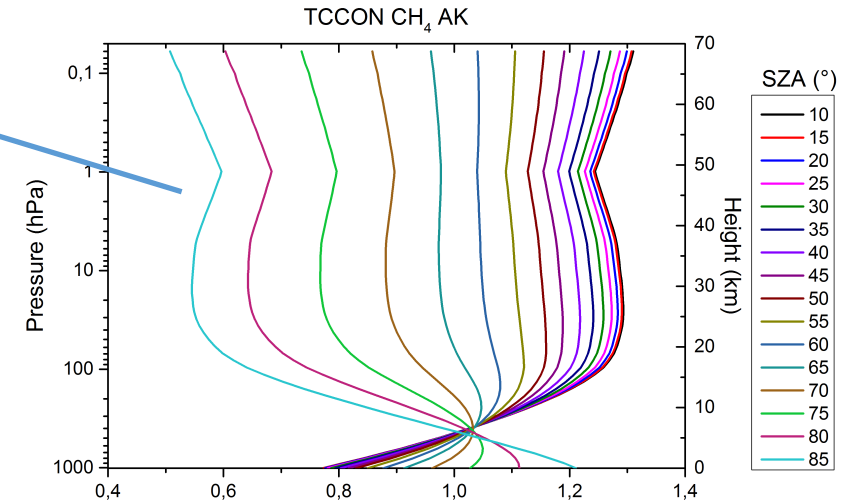
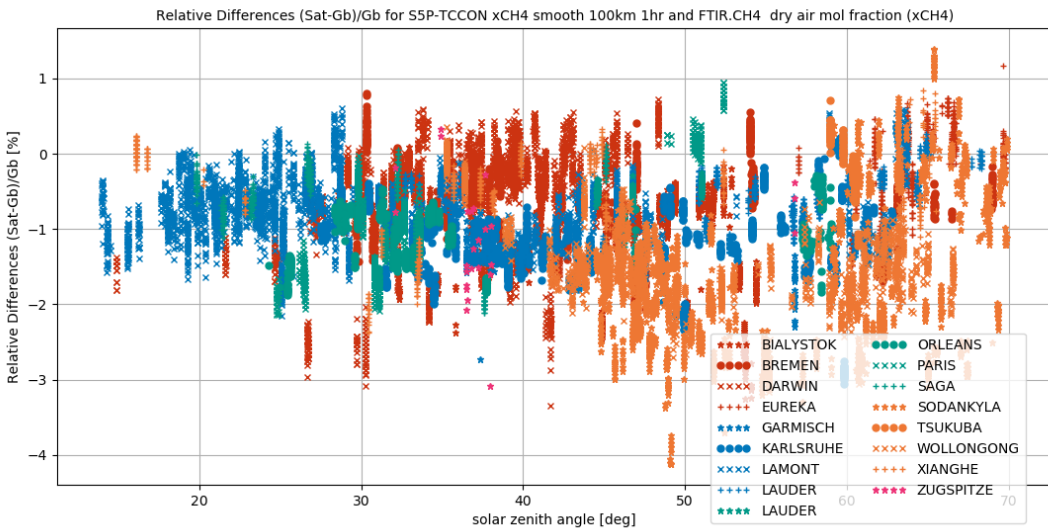
or diagram for S5P-TCCON xCH4 smooth 100km bc 1hr and FTIR.CH4 timeser



Bias corrected S5P-XCH4



Standard S5P-XCH4



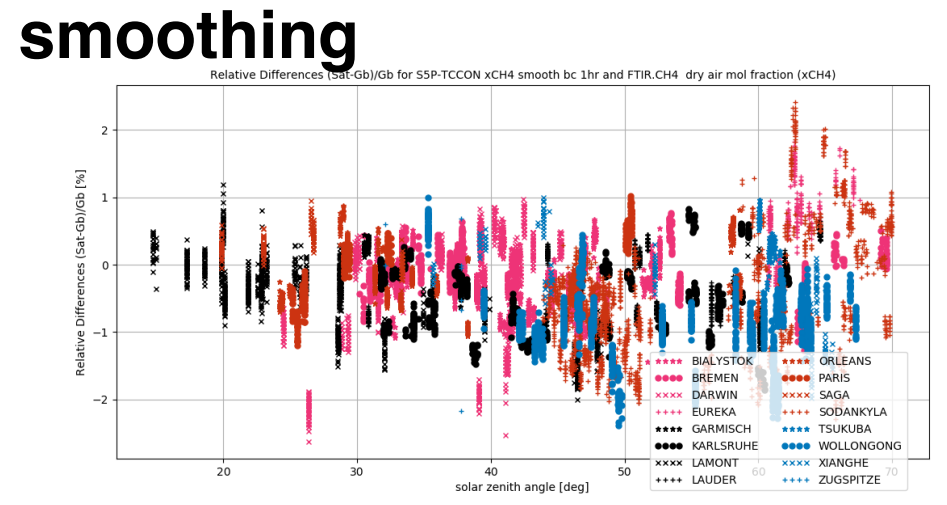
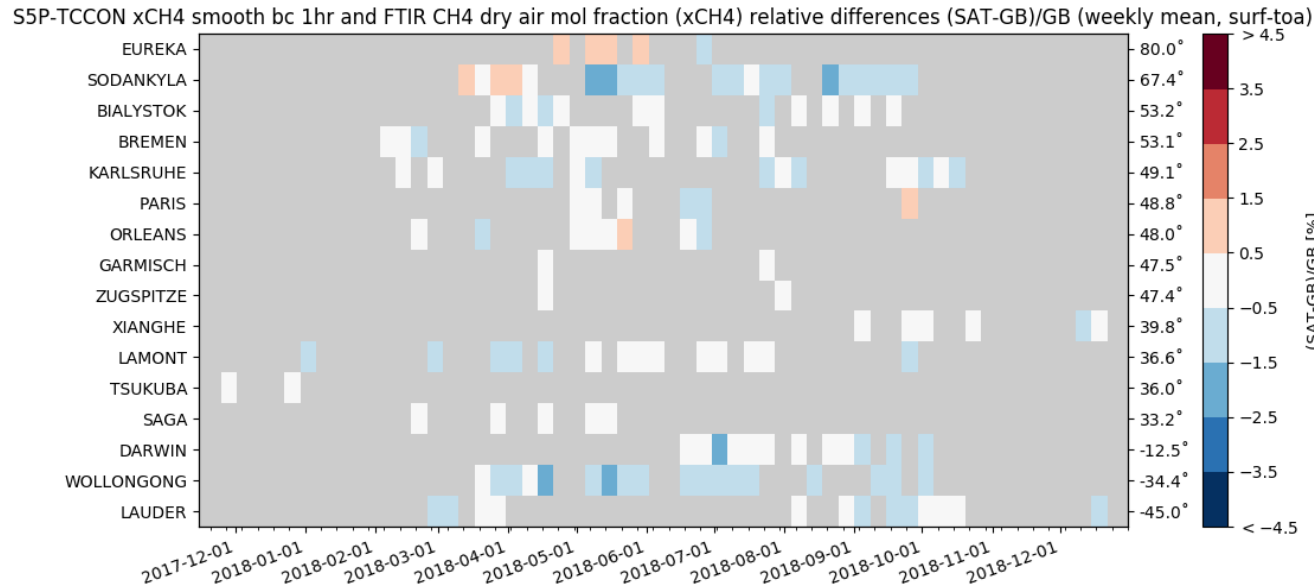
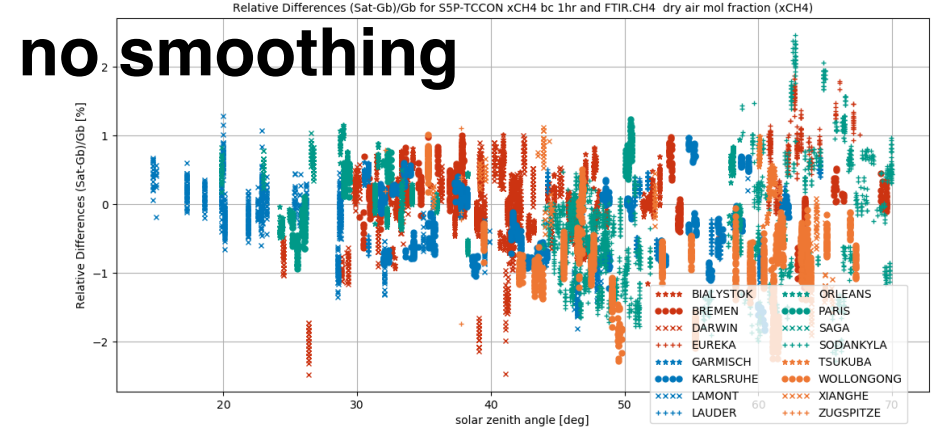
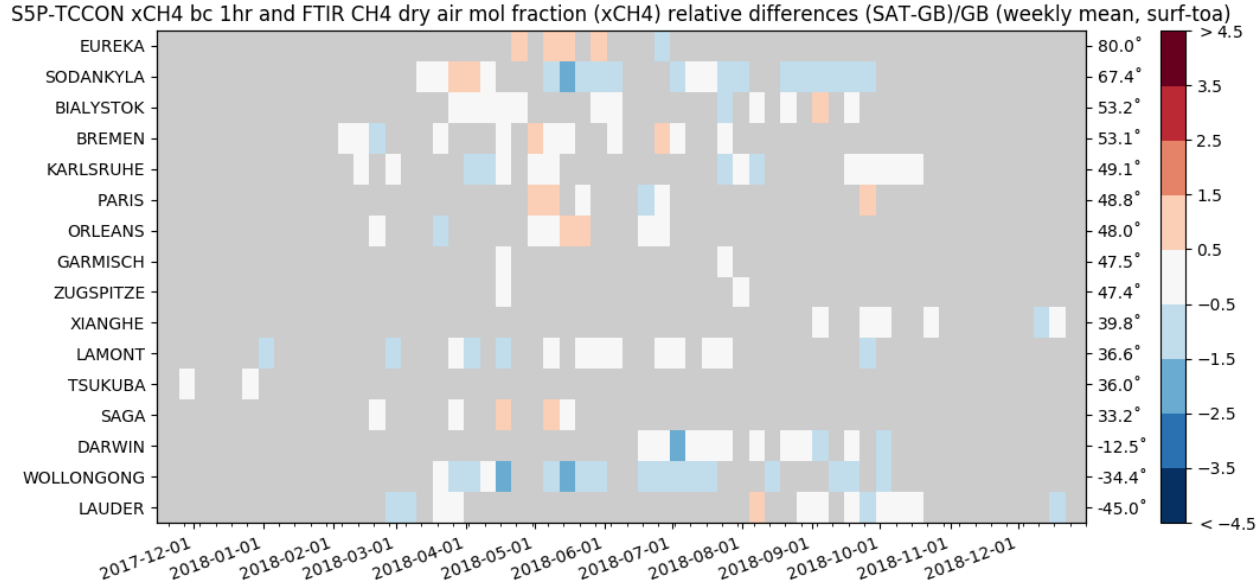
TCCON column averaging kernel – dependent on measurement SZA

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Smoothing - TCCON

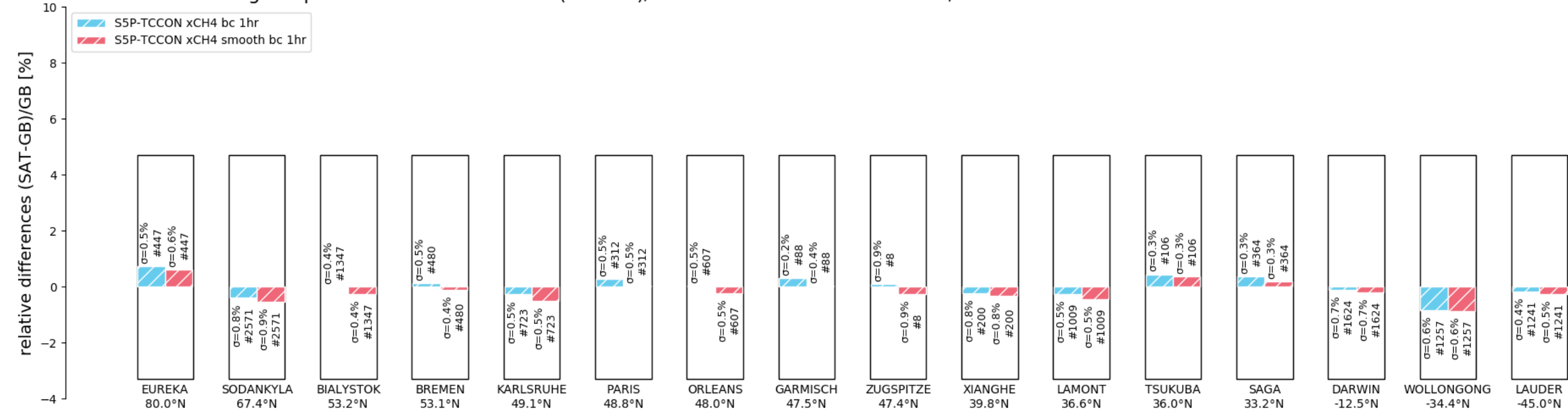


Co-location: $r = 50$ km



Co-location: r = 50 km

Histogram plot of relative differences (SAT-GB)/GB for S5P-TCCON xCH4 bc 1hr, S5P-TCCON xCH4 smooth bc 1hr and FTIR CH4 timeseries



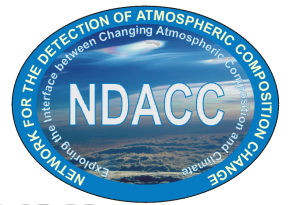
↑
to be investigated

no smoothing: mean rel bias = 0%, rel bias std = 0.53%
 smoothing: mean rel bias = -0.18%, rel bias std = 0.54%

Sensitivity tests – validation of S5P–XCH4 using TCCON FTIR

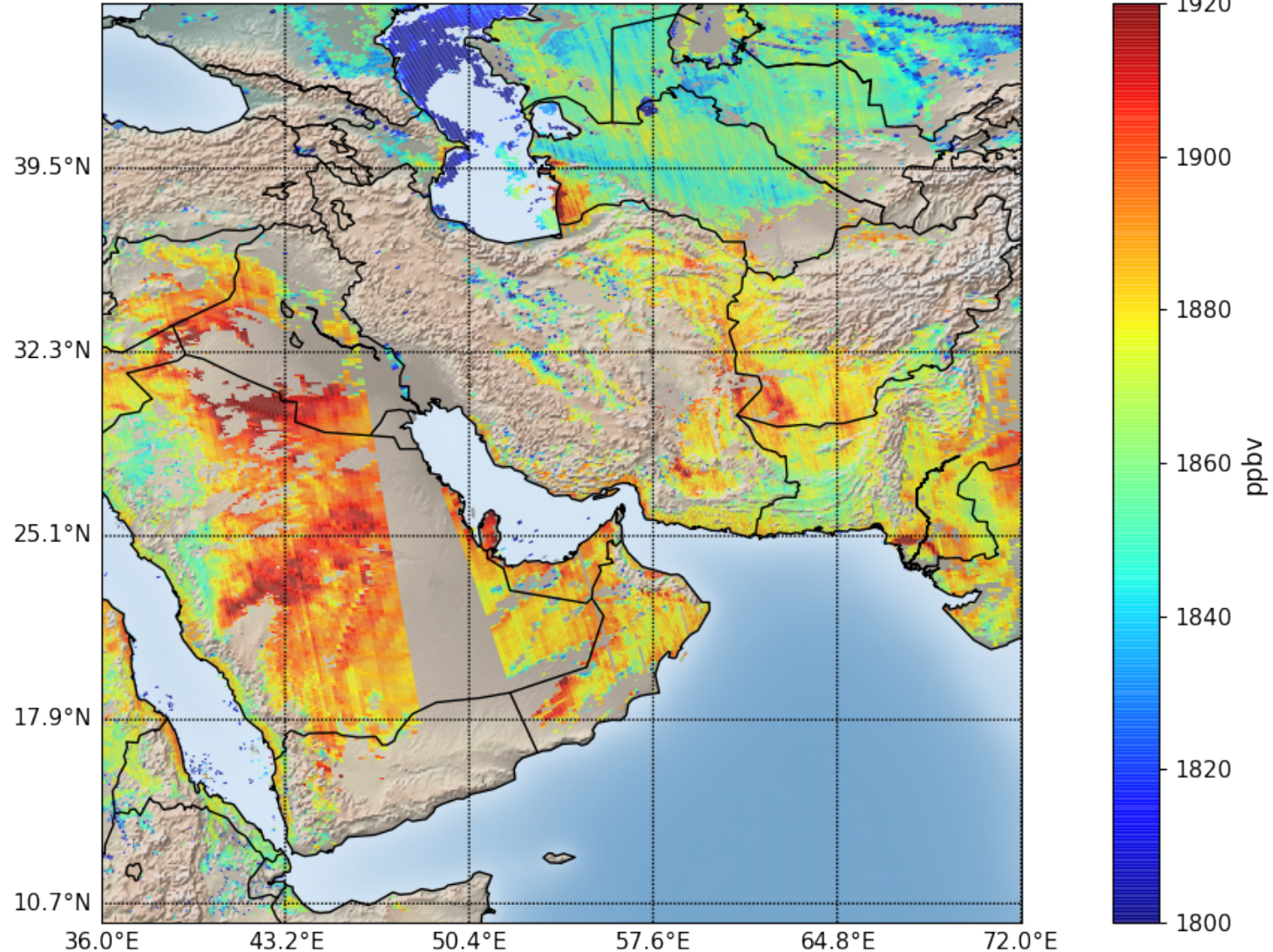
Test cases	Std	Correlation	Rel diff bias (%)	Rel diff std (%)
Biasc 1hr => 50 km	0.9	0.52	0.00	0.53
Biasc 1hr => 100 km	0.9	0.56	0.00	0.56
Biasc smoothing 1 hr => 50 km	0.8	0.50	-0.18	0.54
Biasc smoothing 1 hr => 100 km	0.9	0.55	-0.19	0.57
Biasc 100 km 1 hr => smoothing	0.9	0.55	-0.19	0.57
Biasc 100 km 1 hr => no smoothing	0.9	0.56	0.00	0.56
Smoothing 100 km 1 hr => no biasc	0.9	0.54	-0.85	0.58
Smoothing 100 km 1 hr => biasc	0.9	0.55	-0.19	0.57
Biasc smoothing 100 km => 1 hr	0.9	0.55	-0.19	0.57
Biasc smoothing 100 km => 30 min	0.9	0.55	-0.20	0.57
Biasc smoothing 100 km 1 hr => circ	0.9	0.55	-0.19	0.57
Biasc smoothing 100 km 1 hr => cone	0.9	0.50	-0.20	0.53

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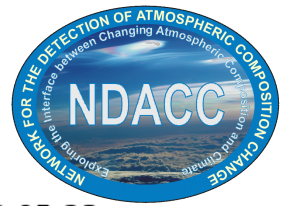


- Animation shows May 22/23 all pixels and 23 with $qa > 0.5$
- stripes
- low values above Caspian sea after filtering on $qa > 0.5$

SAT data CH₄ column volume mixing ratio dry air in 14 S5P files for 2018-05-23

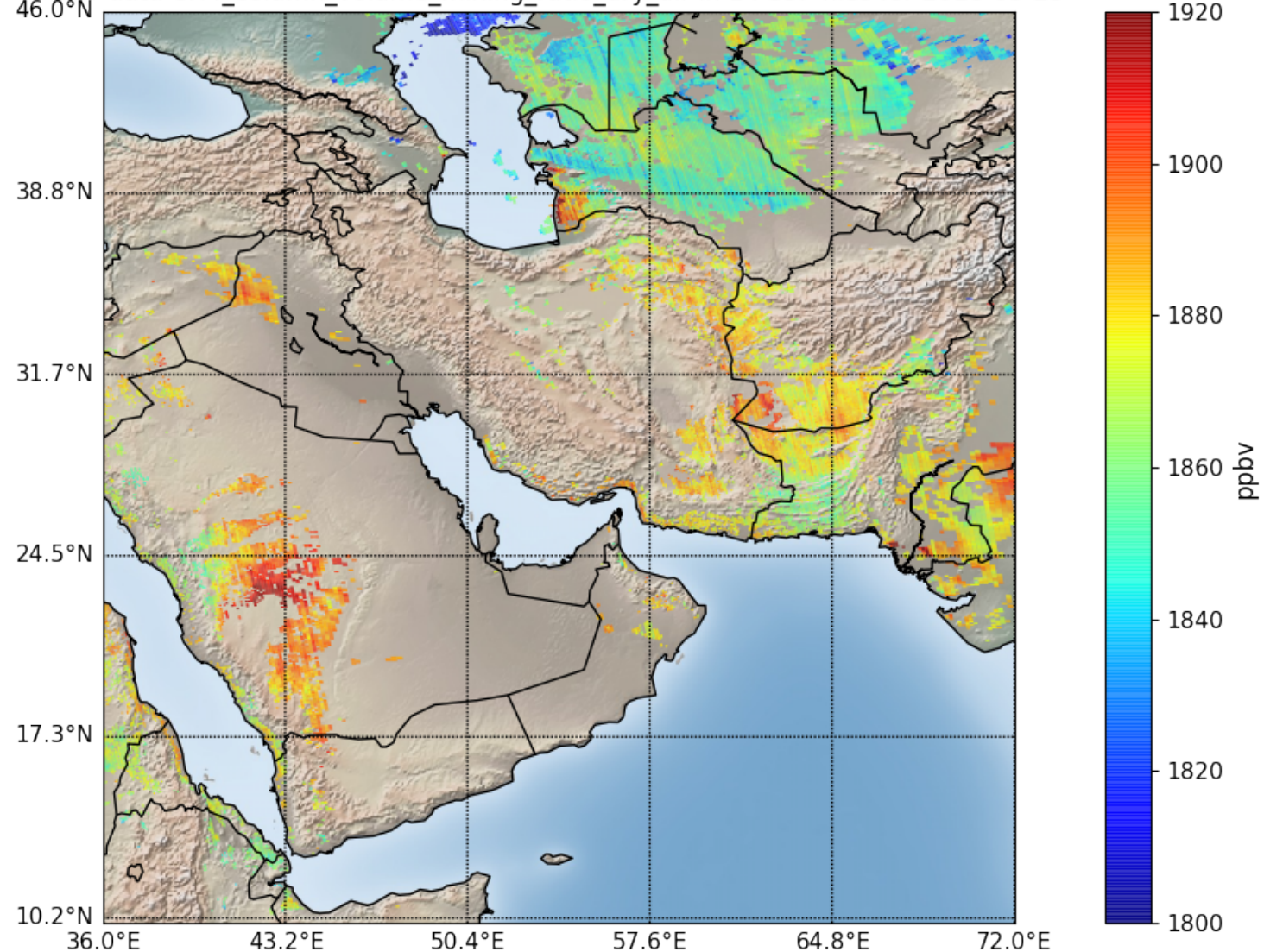


L2_CH4 (B. Langerock and M. K. Sha)

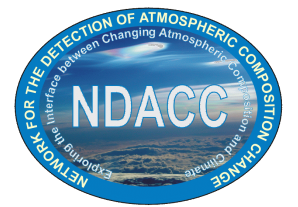
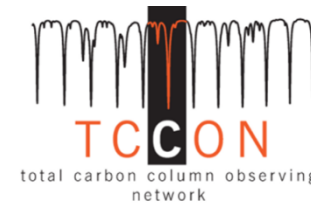


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SAT data CH₄ column volume mixing ratio dry air in 14 S5P files for 2018-05-23



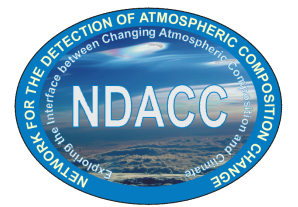
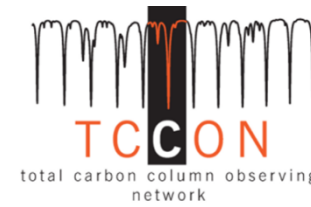
L2_CH4 (B. Langerock and M. K. Sha)



Conclusions

- **Validation of TROPOMI XCH₄ with NDACC XCH₄:**
 - Mean bias of $0.47\% \pm 0.93\%$ (6 stations; < 100 km, $\Delta t=3h$)
 - ➔ **S5P xCH₄ accuracy and precision compliant with mission requirement;**
- **Validation of TROPOMI XCH₄ with TCCON XCH₄:**
 - Mean bias of $-0.19\% \pm 0.57\%$ (16 stations; < 100 km, $\Delta t=1h$)
 - ➔ **S5P xCH₄ accuracy and precision compliant with mission requirement;**
 - Correlation coefficient is 0.55
- NDACC: few stations and few co-located pixels makes statistics not robust, but bias and std is within mission requirement
- Low SAT values need to be investigated -> QA values?
- Stripes and remaining pixels above ocean...
- Mission requirements: target bias **OK** precision **OK**
- Overall recommendation: Yes, the CH₄ product is ready for release to the public along with the product readme file

L2_CH4 (B. Langerock and M. K. Sha)



Notes

Disclaimer: The presented work has been performed in the frame of the Sentinel-5 Precursor Validation Team (S5PVT) or Level 1/Level 2 Product Working Group activities. Results are based on preliminary (not fully calibrated/validated) Sentinel-5 Precursor data that will still change.

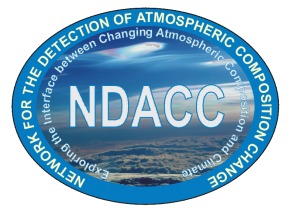
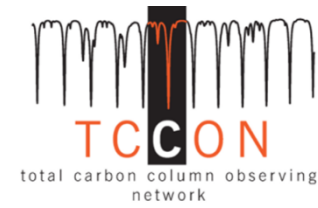
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The NDACC-IRWG data have been funded by the individual national agencies of each partner.

The VDAF validation work has been funded by ESA and BELSPO / BIRA-IASB.

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Thank you for your attention!