Inter-comparison between TCCON and NDACC XCO measurements

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+ TCCON and NDACC teams
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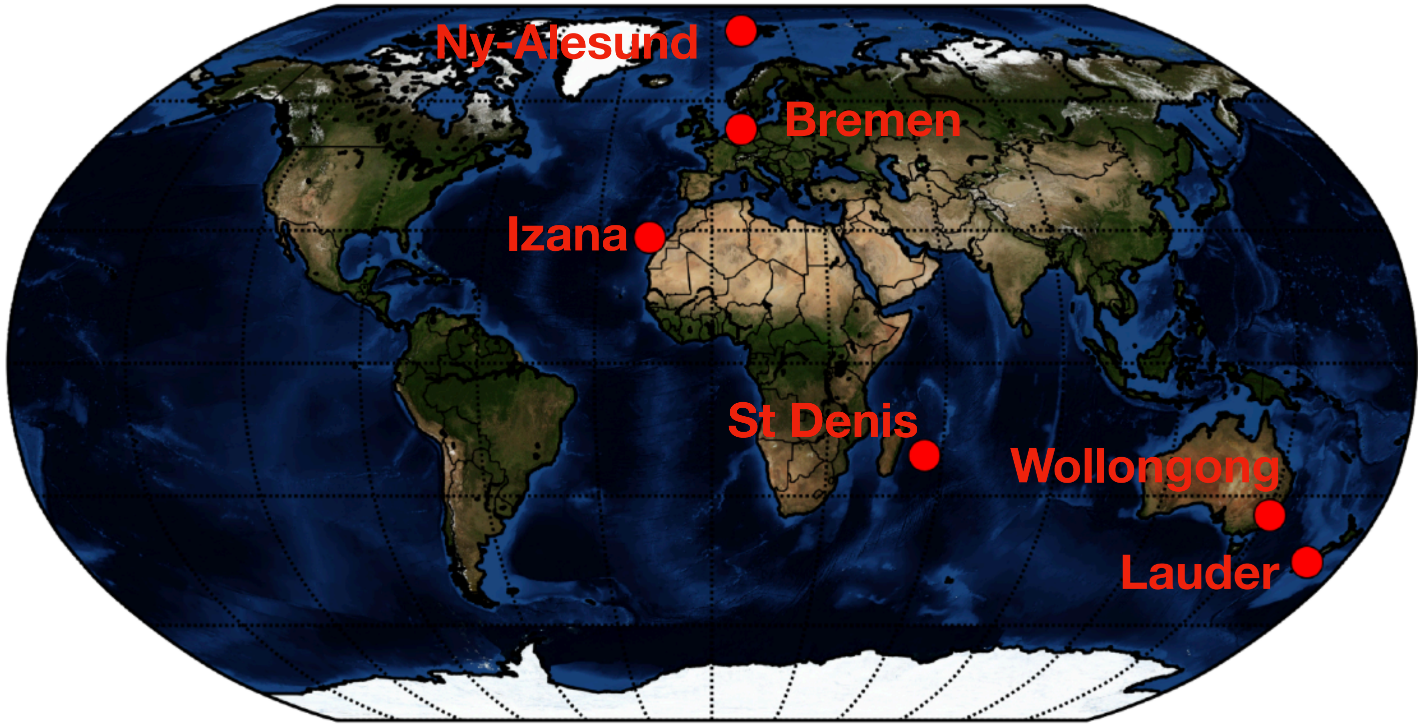
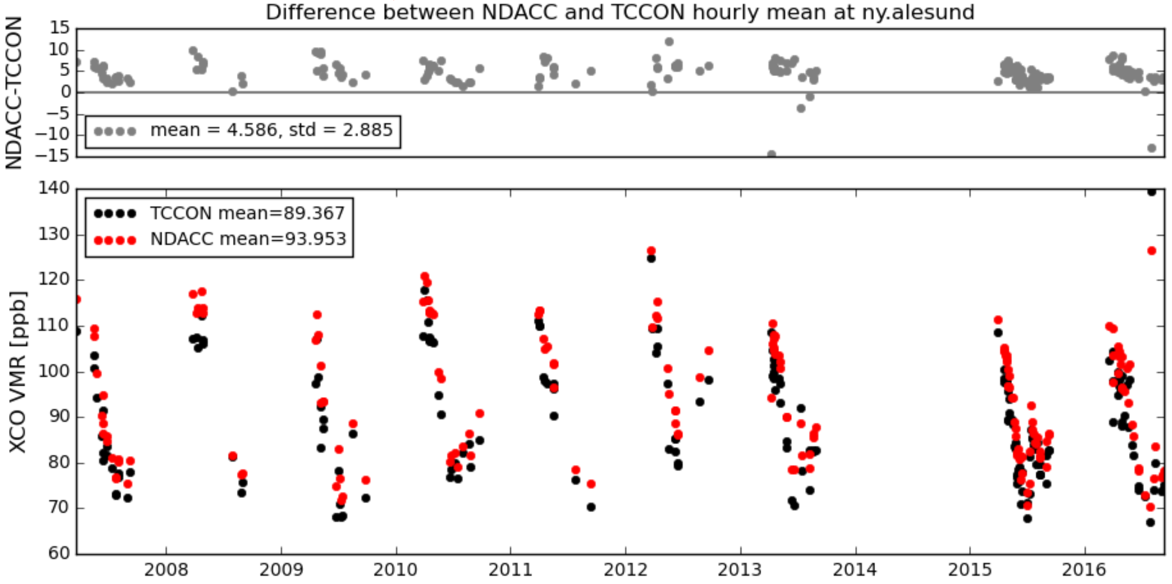
Introduction

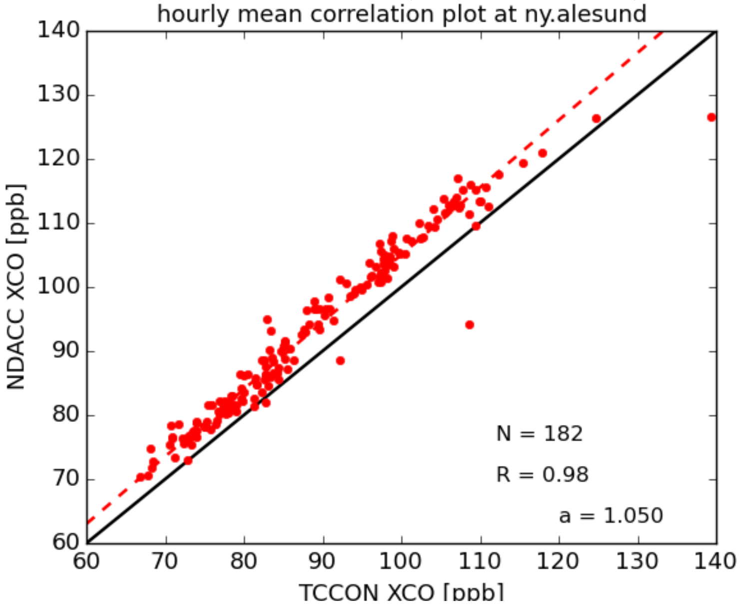
- TCCON and NDACC ground-based FTIR measurements both provide CO data.
- Borsdorff et al., (2016) used TCCON and NDACC CO data to validate the SCIAMACHY observations, and they found that NDACC XCO data is **3.8 ppb** larger than TCCON measurements.
- Kiel et al., (2016) showed that the NDACC XCO is **4.47 ± 0.17 ppb** larger than that from TCCON measurements at Karlsruhe during 2010-2014.
- In this study, we select 6 sites (Ny Alesund, Bremen, Izana, St Denis, Wollongong, Lauder) in 2007-2017 to study the difference between the TCCON and NDACC CO measurements.
- Questions: consistent bias? Why?

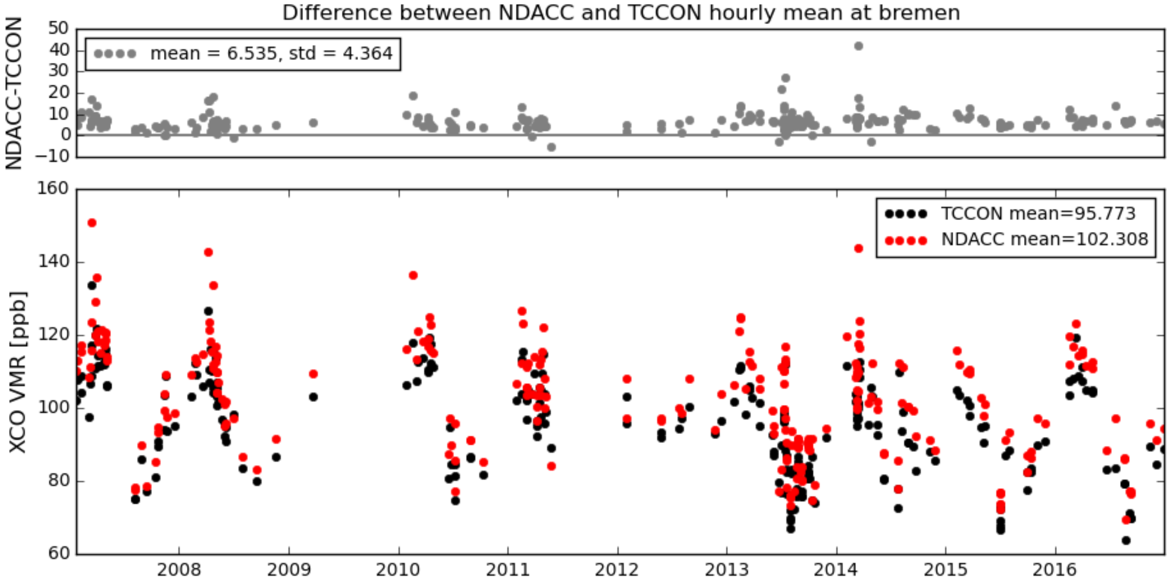
Site	Lat	Long	Alt (km)	Time coverage TCCON/NDACC
Ny-Alesund	78.9N	11.9E	0.02	2007-2016/ 2007-2016
Bremen	53.1N	8.8E	0.19	2007-2016/ 2007-2016
Izana	28.3N	16.5W	2.37	2007-2017/ 2007-2017
St Denis	21S	55.4E	0.08	2011-2017/ 2009-2015
Wollongong	34.4S	150.9E	0.03	2008-2017/ 2008-2017
Lauder	45S	169.7E	0.37	2010-2017/ 2010-2017

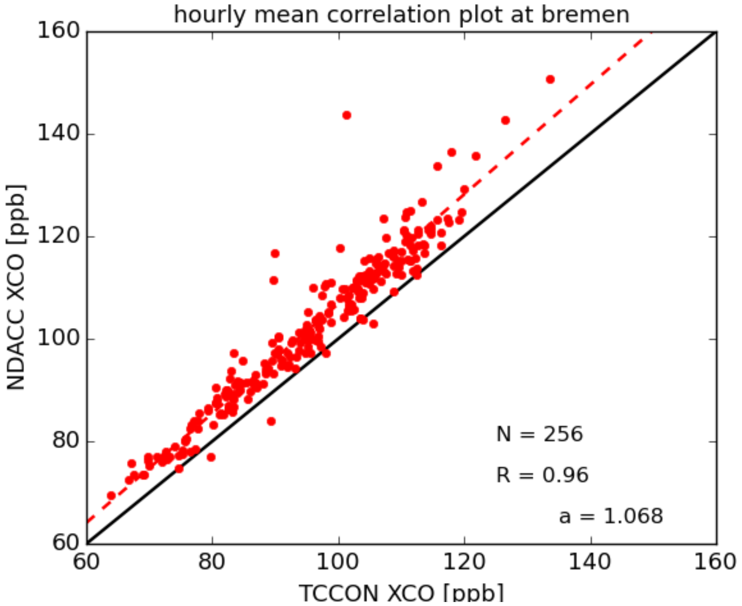


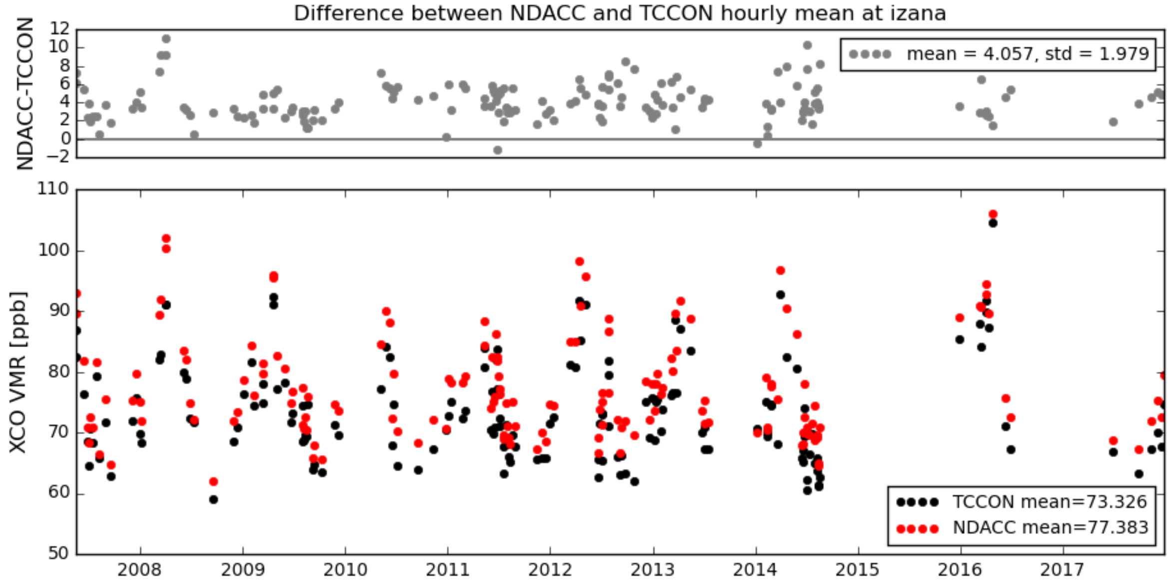
Direct comparison - NH

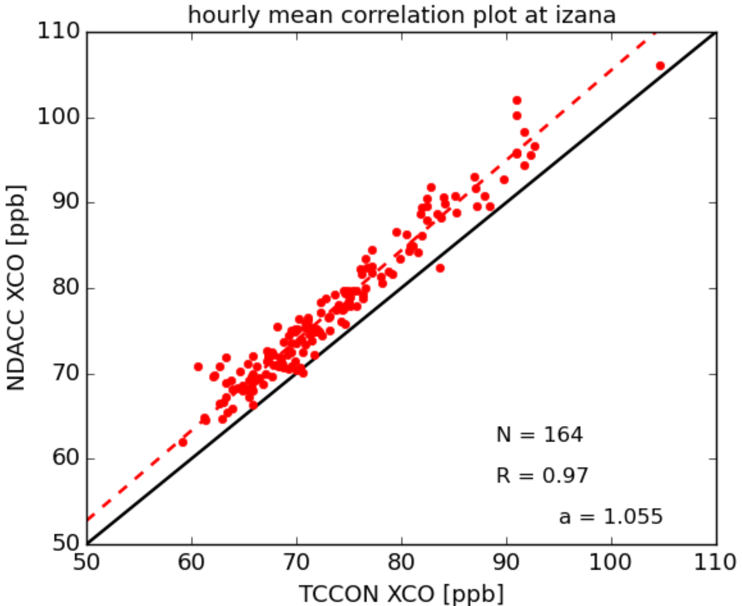






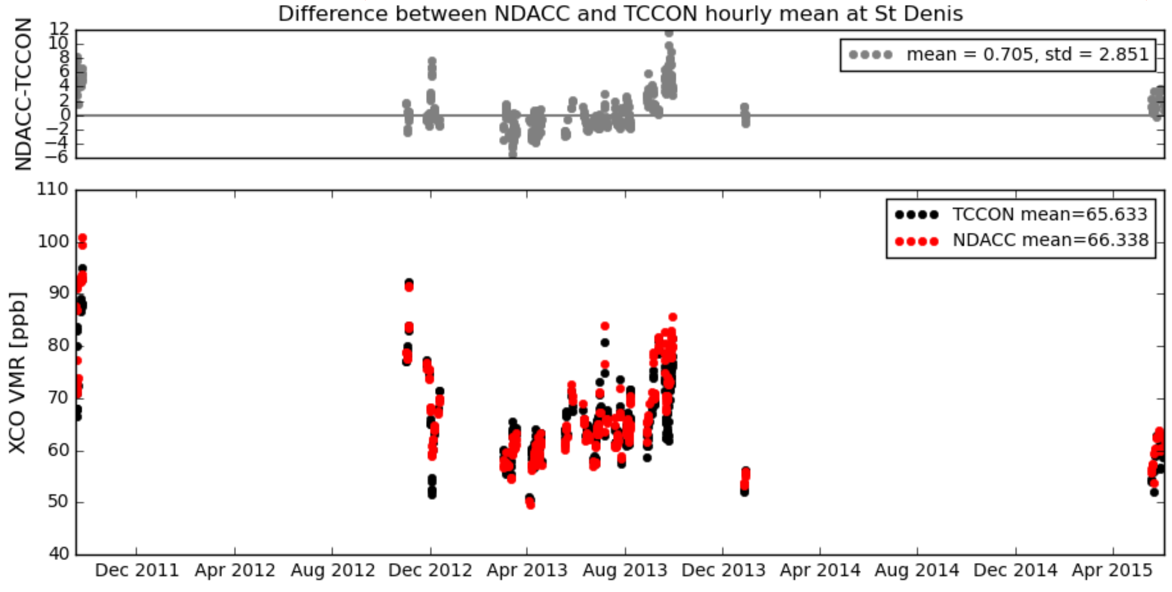


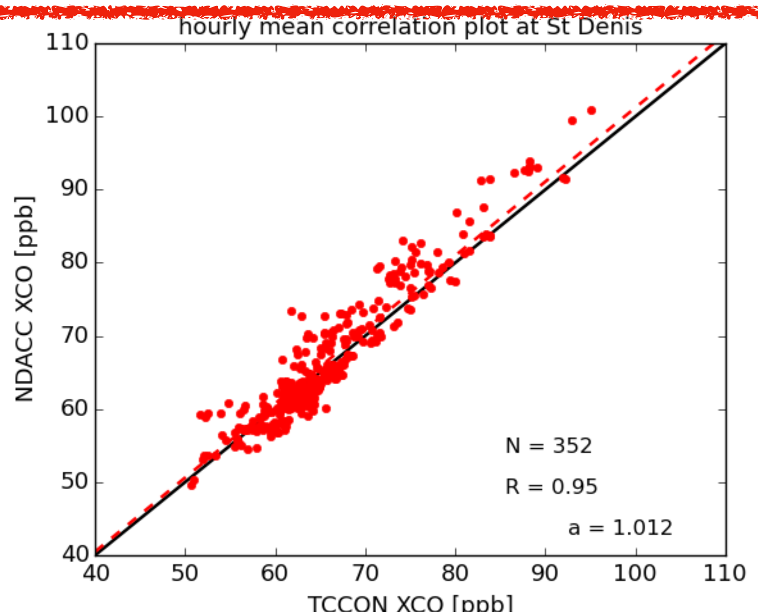


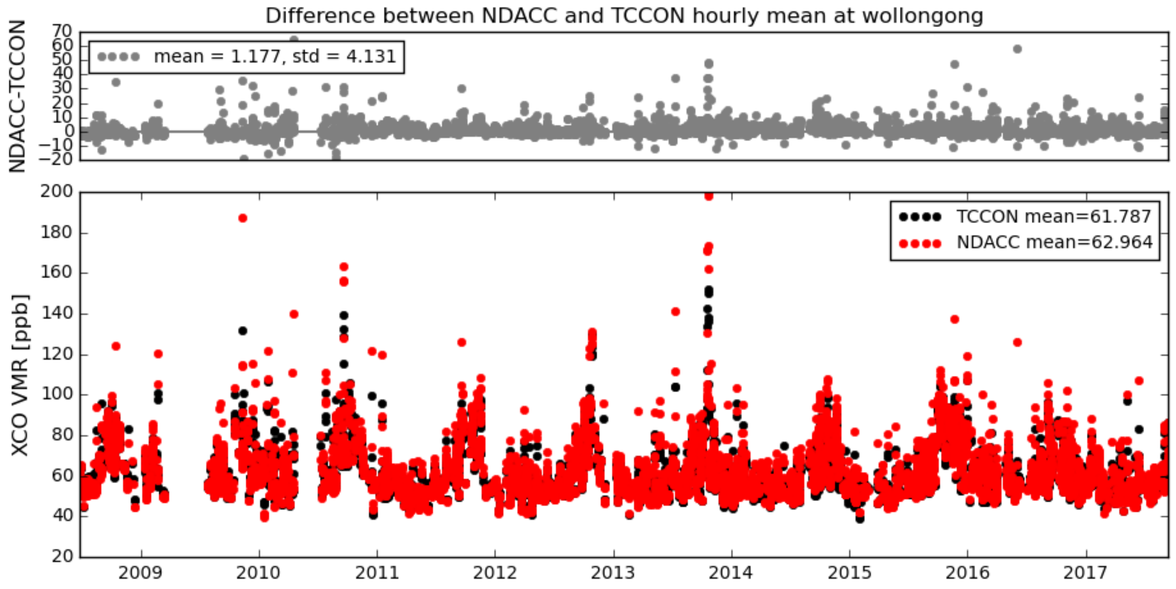


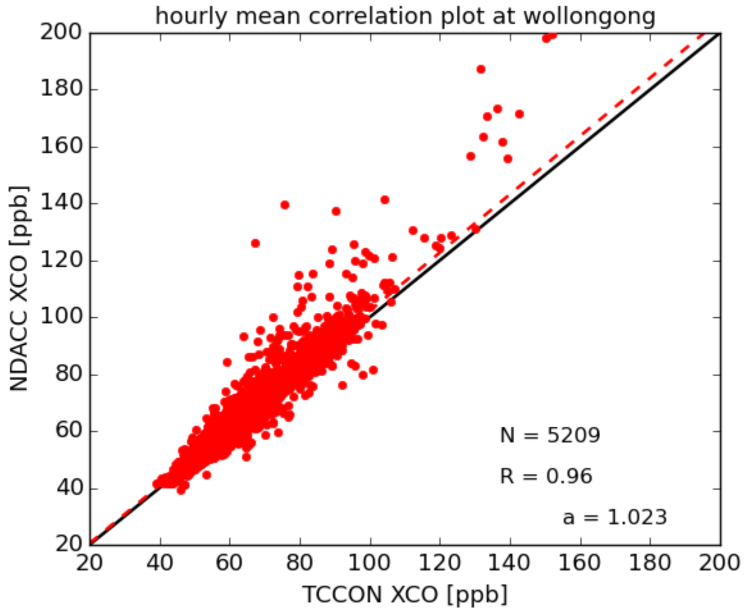
Capture the seasonal variations very well R~0.97

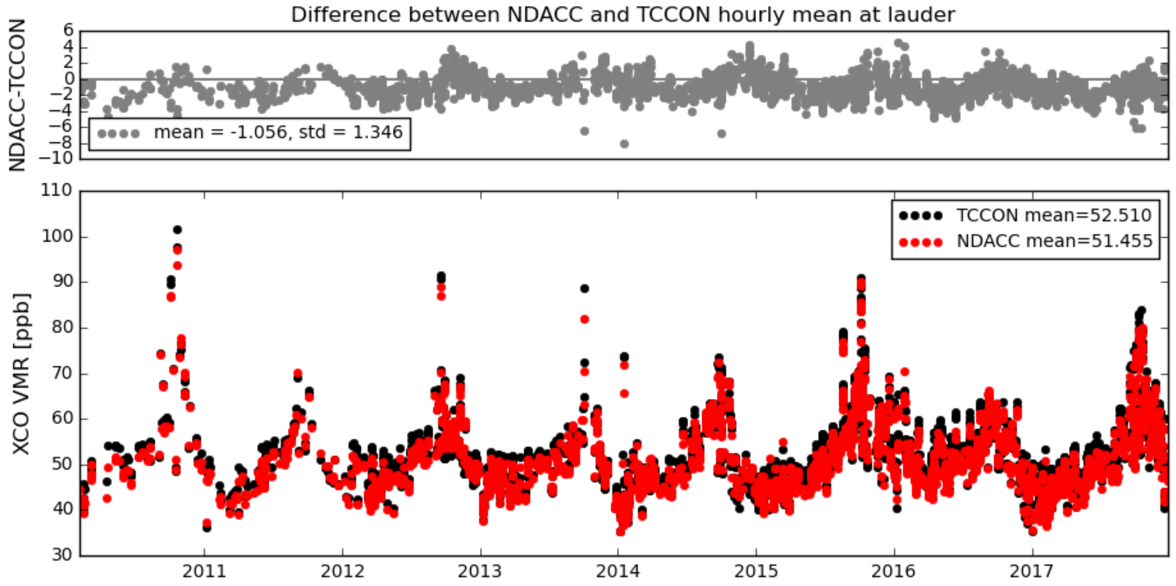
Direct comparison - SH

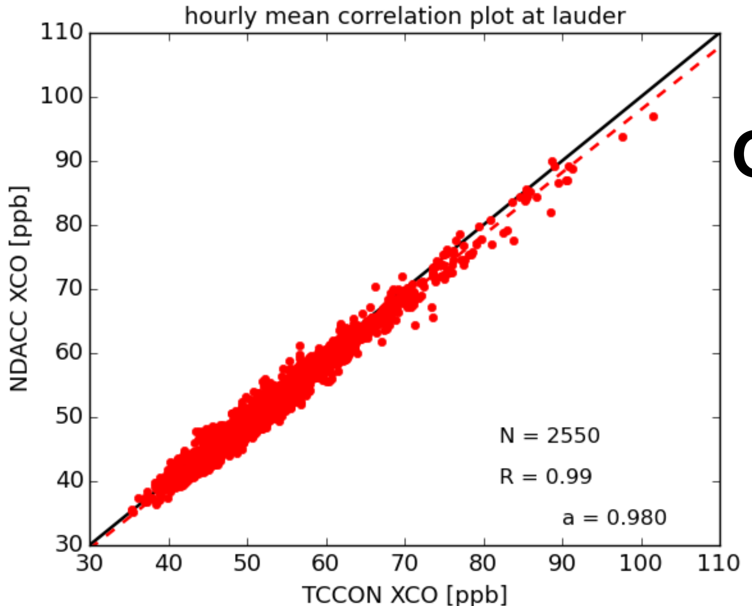

Difference between NDACC and TCCON hourly mean at St Denis


hourly mean correlation plot at St Denis


Difference between NDACC and TCCON hourly mean at wollongong


hourly mean correlation plot at wollongong


Difference between NDACC and TCCON hourly mean at lauder


hourly mean correlation plot at lauder

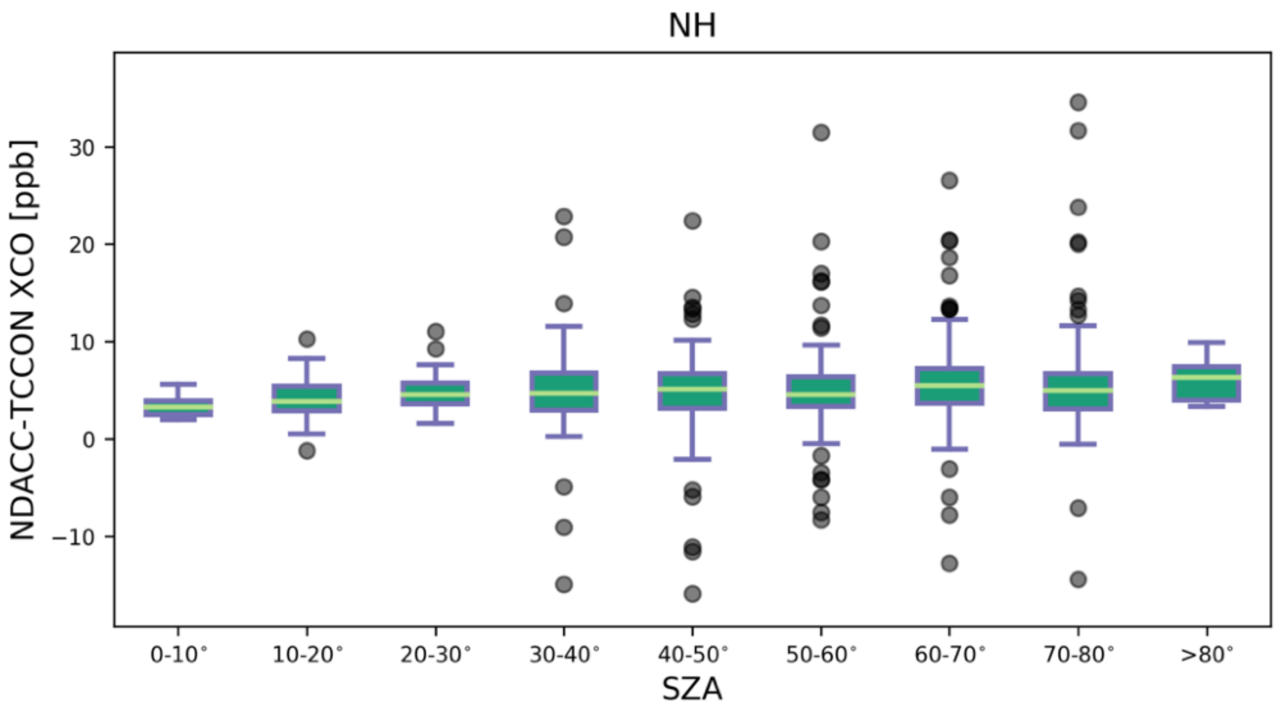
Capture the seasonal variations very well R~0.97

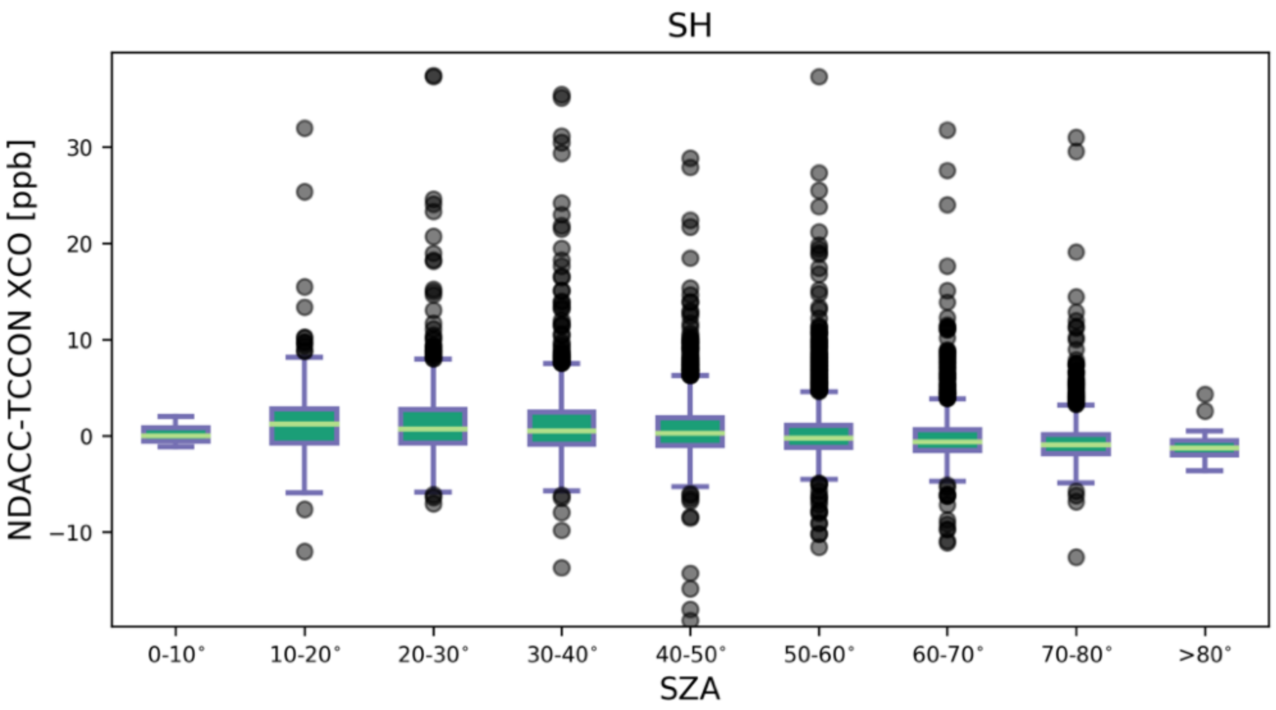
Relative difference

(NDACC-TCCON) /NDACC	NyAlesund	Bremen	Izana	St Denis	Wollongong	Lauder
Mean±SD [%]	4.9±3.1	6.4±4.3	5.2±2.6	1.1±4.3	1.9±6.6	-2.0±2.6

=> The mean bias are about 5.5 % and 0.3 % at NH and SH, respectively

Does the bias has a airmass dependence?

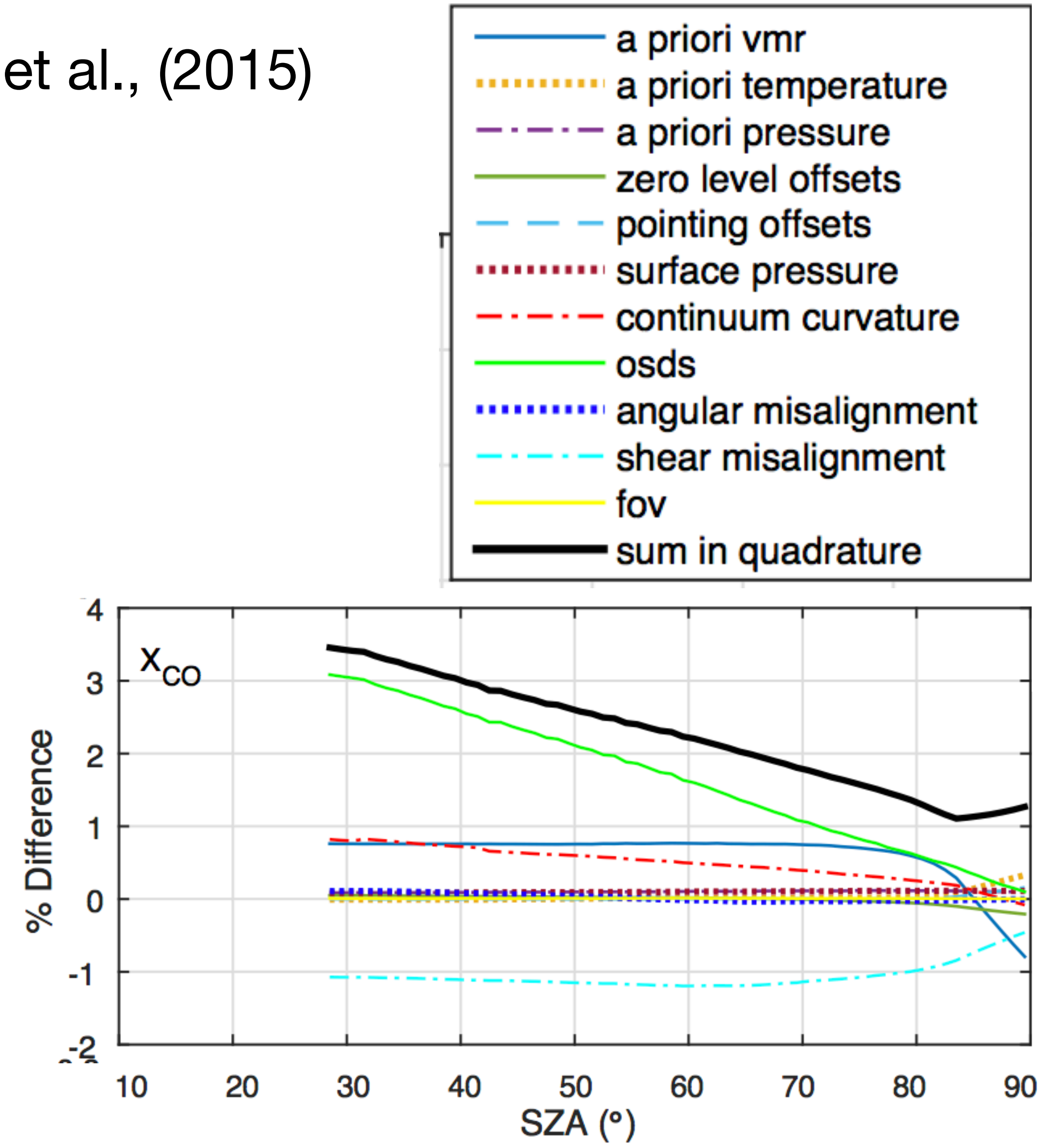


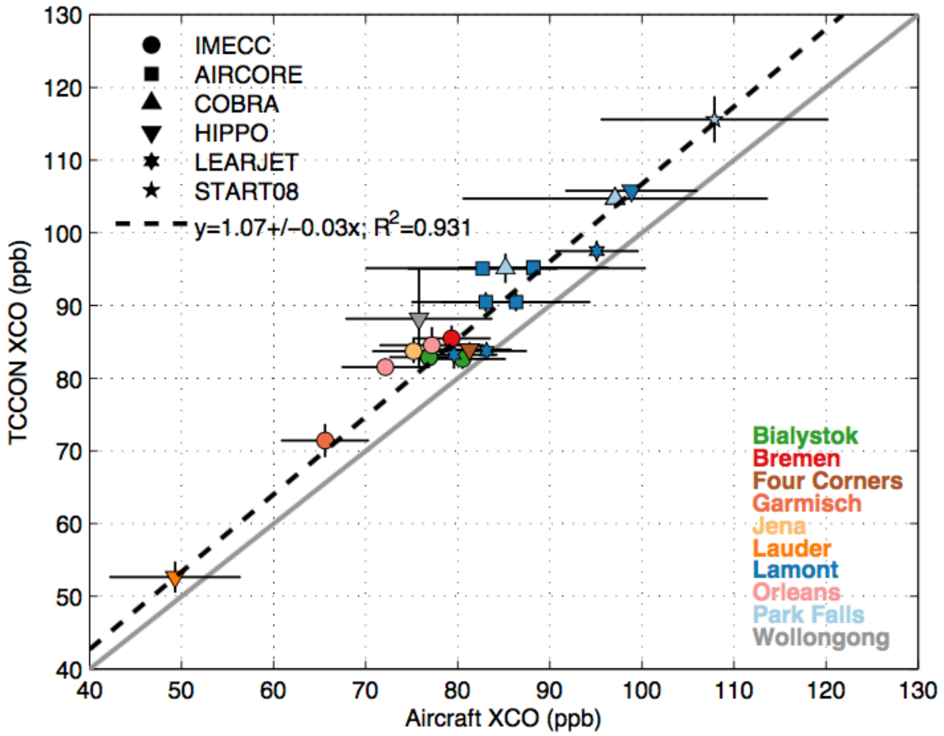


=> Compare to the scatter, the difference from SZA is very small

TCCON uncertainty

Wunch et al., (2015)





TCCON data are calibrated to WMO standards, by applying a scaling factor of 1.067 (with uncertainty of 0.02)

Random error : < 3.5% , decreasing with SZA.
Largest contribution: Observer-Sun Doppler Stretch (osds), a priori vmr, continuum curvature …

**Note that: the smoothing error is not included in the systematic uncertainty of TCCON*

NDACC uncertainty

NDACC reports systematic and random uncertainties with retrieved total column data

Site	NyAlesund	Bremen	Izana	St Denis	Wollongong	Lauder
sys/ran[%]	5.0/6.5	3.4/4.0	2.1/0.5	2.5/1.0	2.1/2.2	2.1/1.8

The NDACC uncertainty is variable at difference sites

- *NDACC **systematic uncertainty** is mainly from spectroscopy and temperature;*
- *NDACC **random uncertainty** is mainly from SZA and temperature;*
- ***Smoothing error** is very small*

	Systematic [%]	Random [%]
Smoothing	0.3	0.1
Measurement	-	0.1
Spectroscopy	2.0	-
SZA	0.1	0.7
Temperature	1.5	0.7
Total	2.5	1.0

NDACC CO retrieval settings been harmonised:
-> same retrieval windows; the same spectroscopy (HITRAN 2008); the a priori profile from WACCM model

Why is there an apparent different bias between TCCON and NDACC XCO in NH and SH ?

XCO calculating method of TCCON and NDACC

TCCON

$$X_{CO} = 0.2095 \times \frac{TC_{CO,r}}{TC_{O_2,r}} \times \frac{1}{\alpha \cdot [1 + \beta \times SPF(\theta)]}$$

Scaling factor

Airmass dependent factor

NDACC

$$X_{CO} = \frac{TC_{CO,r}}{TC_{dry,air}} = \frac{TC_{CO,r}}{P_s/(gm_{air}^{dry}) - TC_{H_2O}(m_{H_2O}/m_{air}^{dry})}$$

In both case, based on OEM (Rodgers 2000)

$$TC_{CO,r} = TC_{CO,a} + \vec{A} \cdot (\overrightarrow{PC_t} - \overrightarrow{PC_a}) + \varepsilon$$

A: Averaging kernel

a,r,t: a priori, retrieved, true

PC: partial column

TC: total column

Site	Nyalesund	Bremen	Izana	Stdenis	Wollongong	Lauder	Mean
$\frac{TC_{O_2}/0.2095}{TC_{dry,air}}$	1.015+0.002	1.015+0.002	1.018+0.002	1.015+0.002	1.016+0.002	1.019+0.002	1.016
$\beta \times SPF(\theta)$	-0.020+0.006	-0.008+0.009	-0.002+0.007	-0.004+0.008	-0.005+0.008	-0.008+0.008	-0,008

$$\alpha' = \overline{TC_{O_2}/(0.2095TC_{dry,air})} \cdot \alpha \cdot [1 + \overline{\beta \times SPF(\theta)}] = 1.008\alpha = 1.0757$$

The the difference between TCCON and NDACC XCO data is:

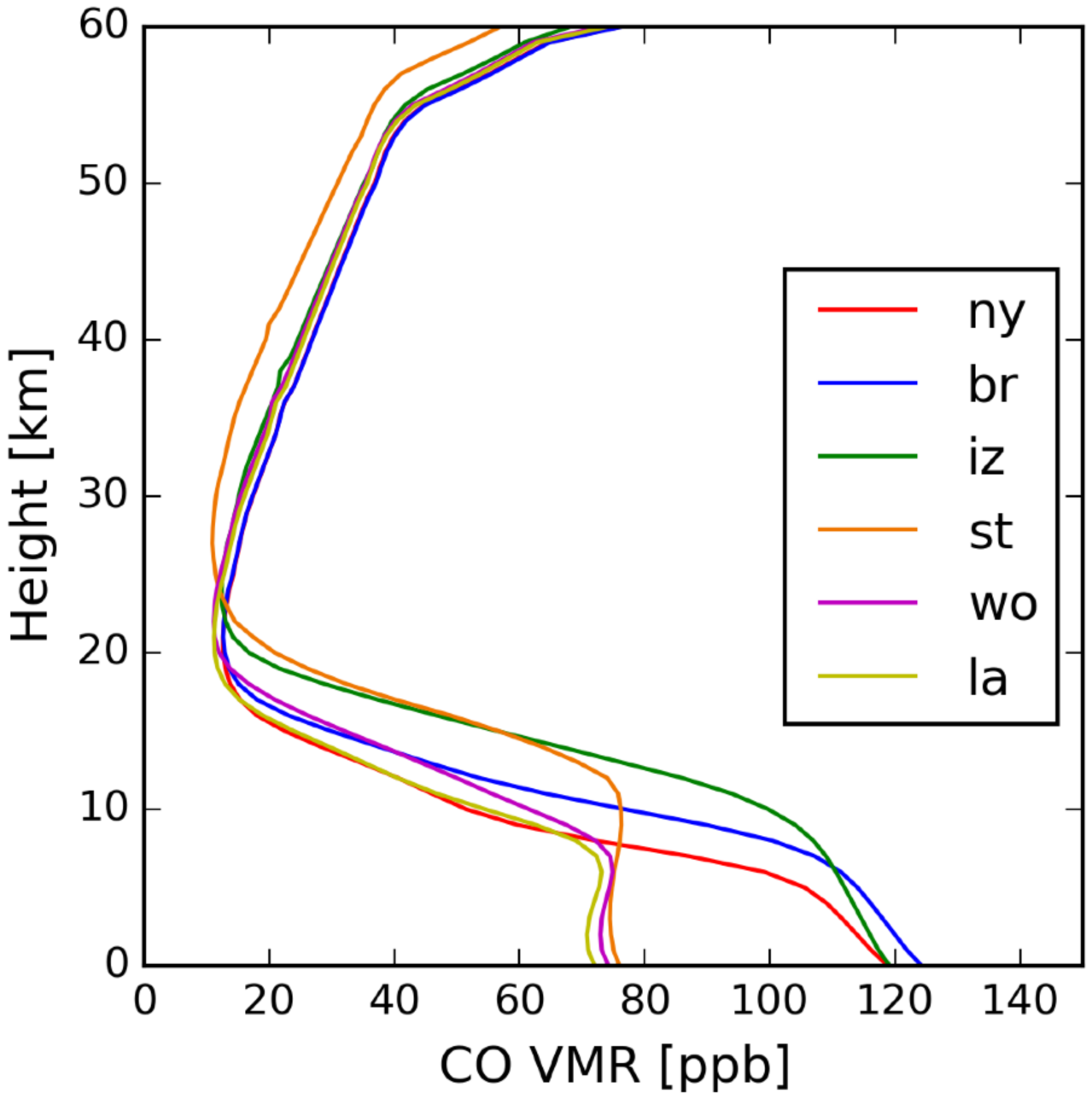
$$X_{CO,TCCON} - X_{CO,NDACC} = \frac{1}{TC_{air,dry}}(TC_{CO,r,TCCON}/\alpha' - TC_{CO,r,NDACC})$$

$$= \frac{1}{TC_{air,dry}}[[TC_{CO,a,TCCON} + \overrightarrow{A_{TCCON}} \cdot (\overrightarrow{PC_t} - \overrightarrow{PC_{a,TCCON}}) + \varepsilon_{TCCON}]/\alpha' - [TC_{CO,a,NDACC} + \overrightarrow{A_{NDACC}} \cdot (\overrightarrow{PC_t} - \overrightarrow{PC_{a,NDACC}}) + \varepsilon_{NDACC}]]$$

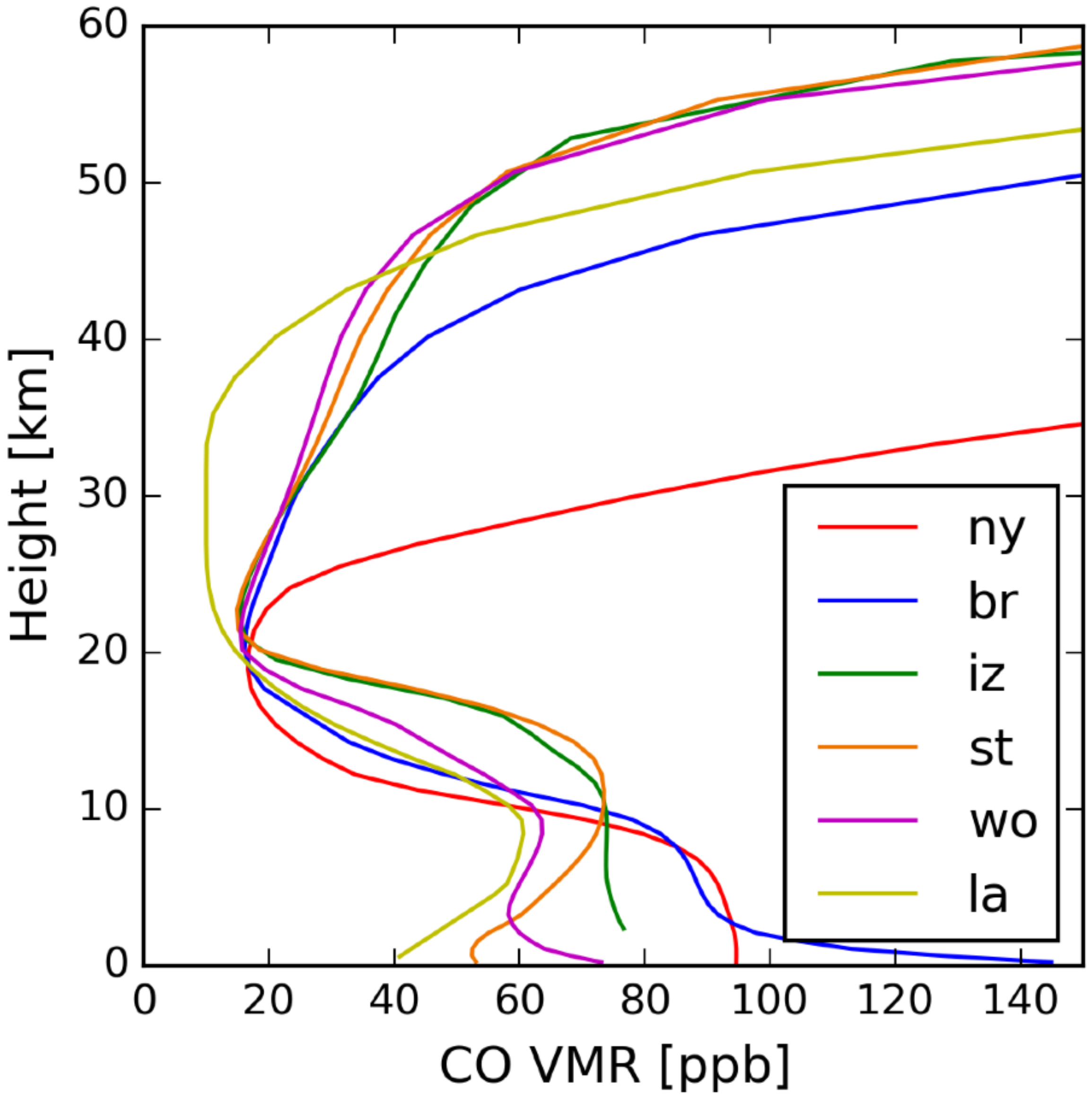
The difference comes from the difference in **a priori profiles**, **averaging kernels** and **retrieval uncertainties**

TCCON and NDACC CO a priori profiles

TCCON apriori - GGG code
Mean in 2013
(on daily basis)



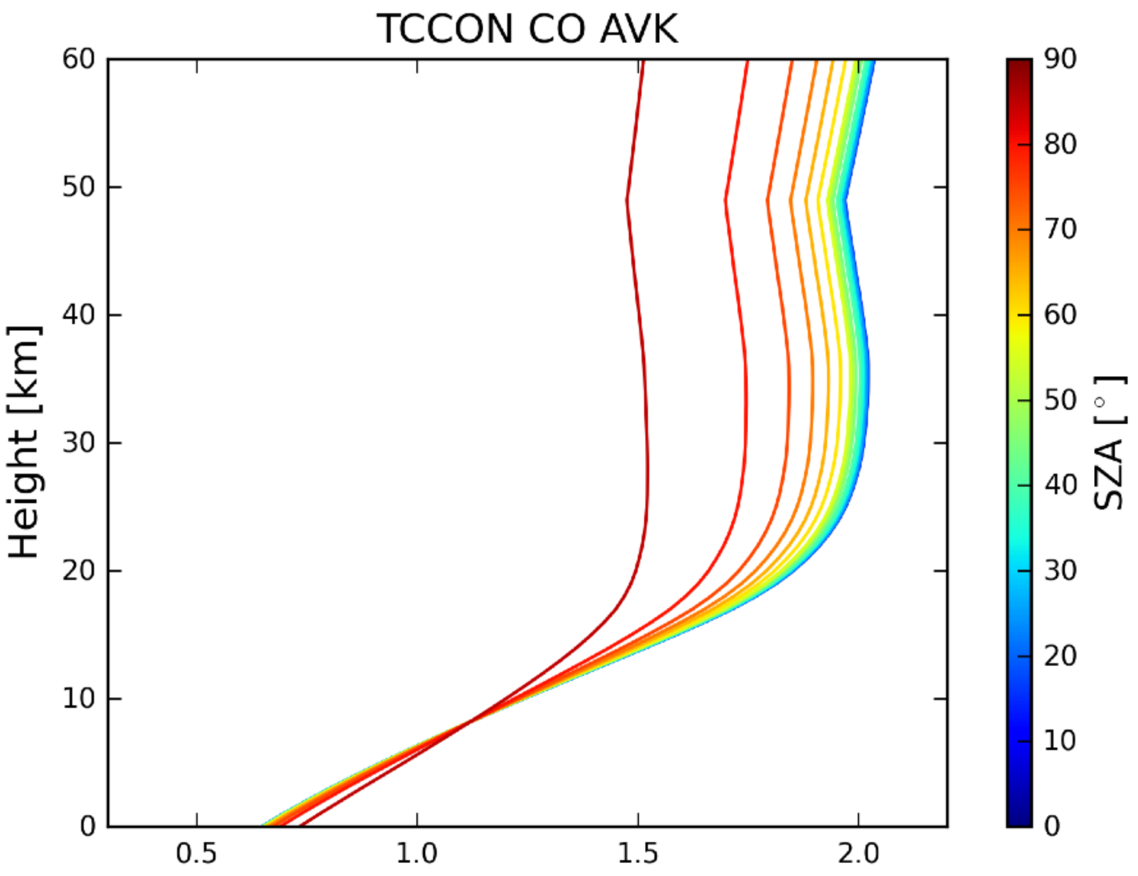
NDACC a priori - WACCM model
Mean 1980-2020
(fixed)



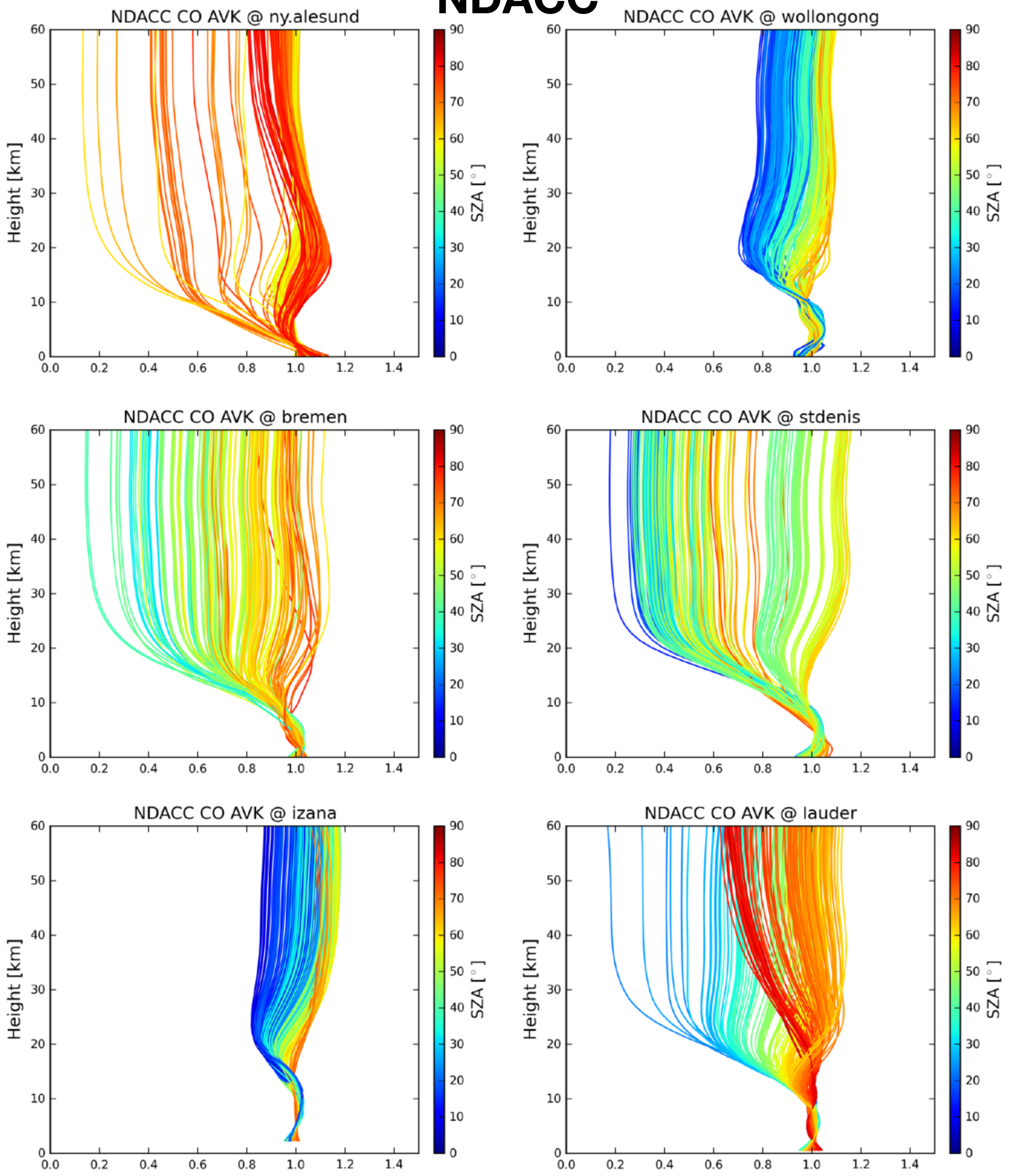
Very different TCCON a priori profiles at SH and SH

Averaging kernels of TCCON and NDACC

TCCON



NDACC



Sensitivities are very different between TCCON and NDACC

Update a priori profile for TCCON and NDACC

According to Rodgers and Conner (2003)

$$TC_{CO,r} = TC_{CO,a} + \vec{A} \cdot (\overrightarrow{PC_t} - \overrightarrow{PC_a}) + \varepsilon$$

$$TC'_{CO,r} = TC_{CO,op} + \vec{A} \cdot (\overrightarrow{PC_t} - \overrightarrow{PC_{op}}) + \varepsilon$$

$$\downarrow$$

$$TC'_{CO,r} = TC_{CO,r} + (\vec{I} - \vec{A}) \cdot (\overrightarrow{PC_{op}} - \overrightarrow{PC_a}) + \varepsilon$$

Then, the same a priori profile $\overrightarrow{PC_{op}}$ is applied for both TCCON and NDACC; for the difference between the adjusted TCCN and NDACC XCO data:

$$X'_{CO,r,TCCON} - X'_{CO,r,NDACC} = \frac{1}{\alpha' TC_{air,dry}}[TC_{CO,op} + \overrightarrow{A_{TCCON}} \cdot (\overrightarrow{PC_t} - \overrightarrow{PC_{op}}) + \varepsilon_T] - \frac{1}{TC_{air,dry}}[TC_{CO,op} + \overrightarrow{A_{NDACC}} \cdot (\overrightarrow{PC_t} - \overrightarrow{PC_{op}}) + \varepsilon_N]$$

$$= \frac{1}{TC_{air,dry}}[(1/\alpha' - 1)TC_{CO,op} + (\overrightarrow{A_{TCCON}}/\alpha' - \overrightarrow{A_{NDACC}}) \cdot (\overrightarrow{PC_t} - \overrightarrow{PC_{op}}) + \varepsilon_T + \varepsilon_N]$$

If the a priori profile is very close to the true status, then

$$X_{CO,r,TCCON} - X_{CO,r,NDACC} = (1/\alpha' - 1)X_{CO,op} + \varepsilon_T + \varepsilon_N = -0.07X_{CO,op} + \varepsilon_T + \varepsilon_N$$

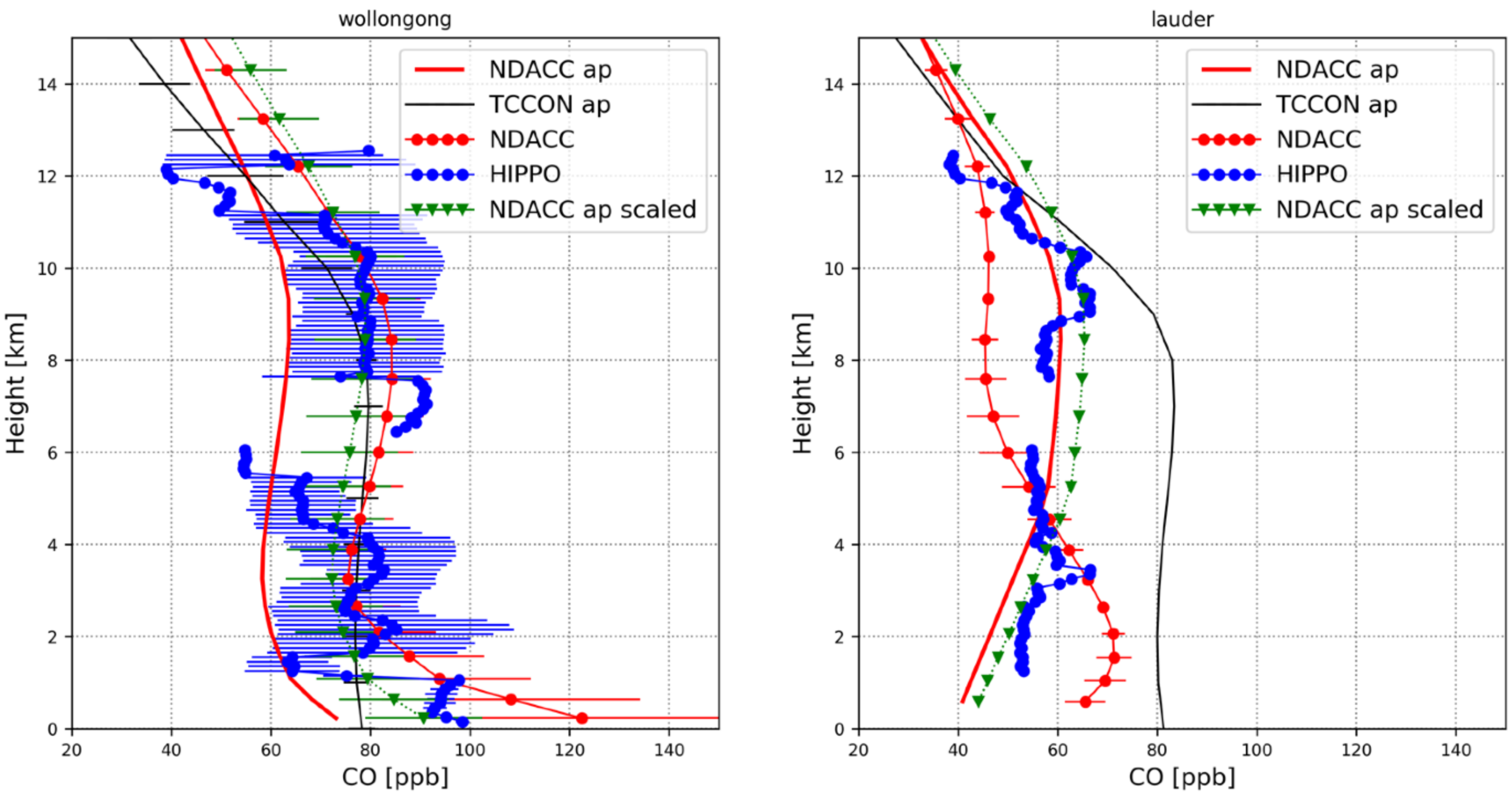
Test: the same a priori profile is applied for TCCON and NDACC

Method 1 - scaled WACCM profile

Method 2 - CAMS model (surface-12km)+scaled WACCM profile (above 12 km)

CAMS expID : oper0001
Resolution: T511 L60 (~40x40 km)
Mainly focus on the troposphere

Method 1- Using scaled WACCM profile as the a priori profile



As an example, the scaled WACCM profiles are shown at Wollongong and Lauder, when the HIPPO (aircraft) measurements are available.

$$\overrightarrow{x_{N,scaled}} = \overrightarrow{x_{N,ap}} * TC_{N,r}/TC_{N,ap}$$

(NDACC'-TCCON') /NDACC'	NyAlesund	Bremen	Izana	St Denis	Wollongong	Lauder	Mean
mean±SD [%]	8.5±4.2	6.2±4.6	7.7±3.2	6.3±5.1	6.2±7.6	5.6±3.5	6.8

=> after updating the TCCON priori, the bias between SH and NH is almost gone

$$X_{CO,r,NDACC} - X_{CO,r,TCCON} = (1 - 1/\alpha')X_{CO,op} + \varepsilon_T + \varepsilon_N = 0.070X_{CO,r,NDACC} + \varepsilon_T + \varepsilon_N$$

The mean bias of 6.8% is close to 7.0%, and the difference is within the systematic uncertainty of NDACC data (~2.5%)

Method 2- Using CAMS model as the a priori profile for surface -12 km and scaled NDACC a priori profile for above 12 km

-> We generate the coarse vertical profile from CAMS model < test only for one year (2013)>

TCCON & NDACC in 2013

(NDACC-TCCON) /NDACC	NyAlesund	Bremen	Izana	St Denis	Wollongong	Lauder	Mean
mean±SD [%]	4.3±4.9	7.3±4.8	5.5±1.7	0.5±4.3	1.5±7.0	-1.6±2.5	2.9

Update TCCON & NDACC

(NDACC'-TCCON') /NDACC'	NyAlesund	Bremen	Izana	St Denis	Wollongong	Lauder	Mean
mean+SD [%]	8.7±5.0	7.3±4.3	7.8±1.9	4.3±3.9	5.0±7.4	4.4±2.5	6.3

=> the mean is 6.3%
the bias between NH and SH still exists, but it is reduced.

Smoothing error estimation

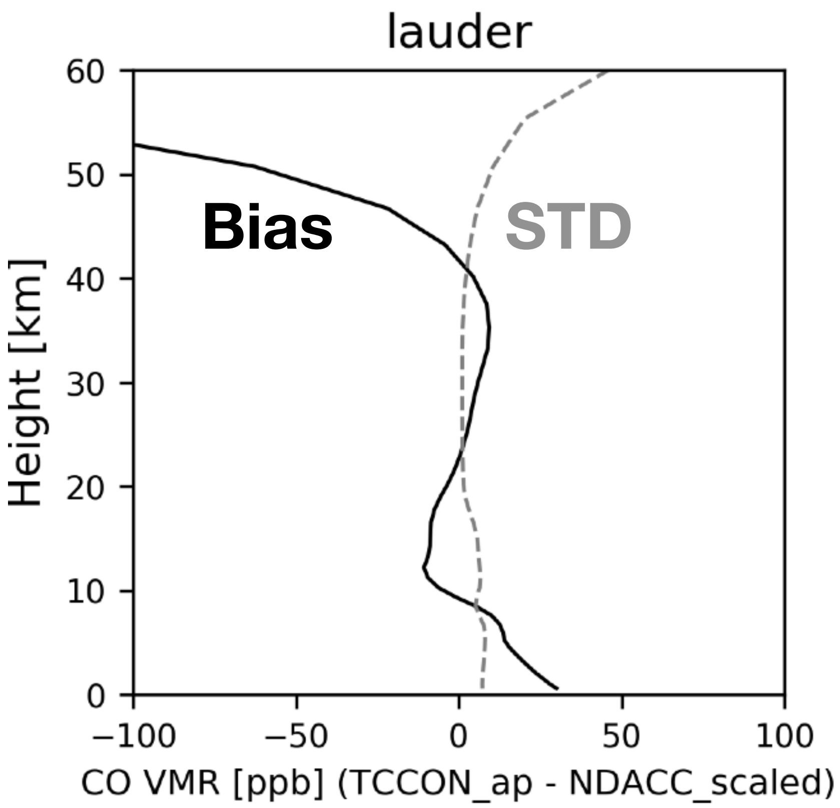
According to Rodgers (2000)

$$\sigma_s^2 = (\vec{I} - \vec{A})^T S_a (\vec{I} - \vec{A})$$

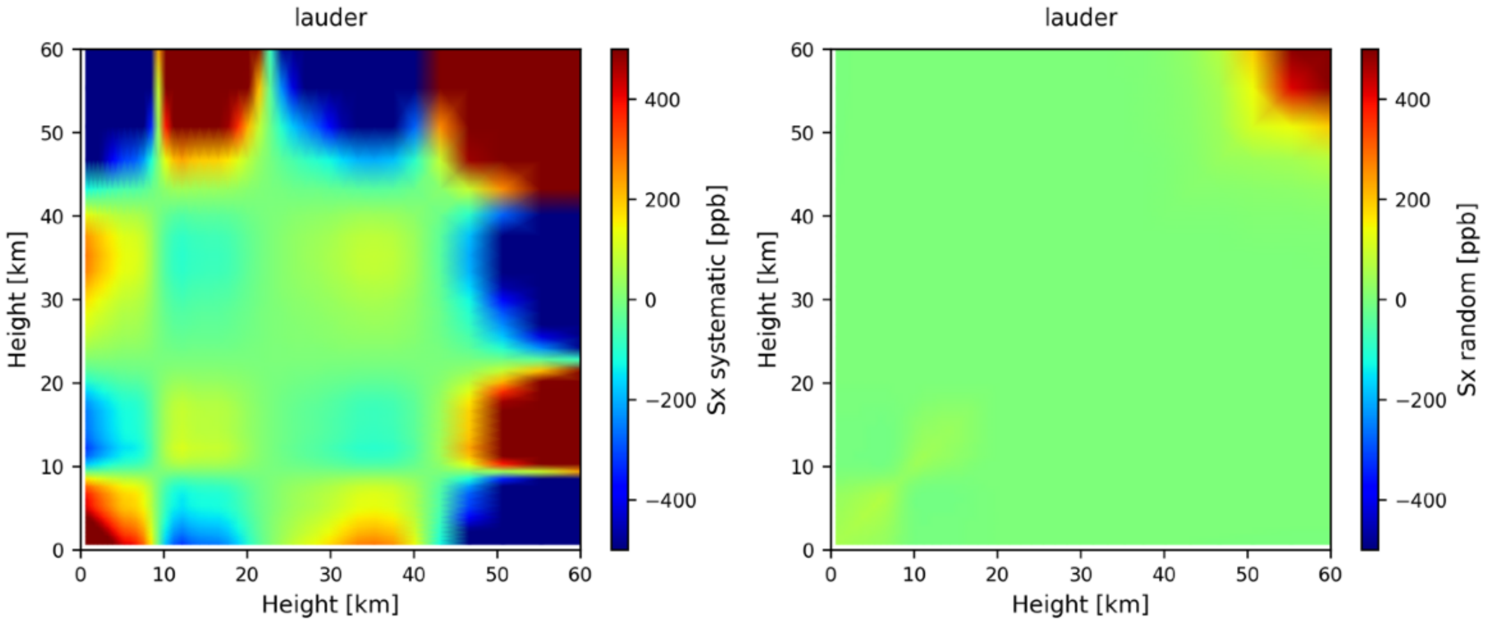
Systematic ↙ Random ↘

Bias **Covariance**

Using the scaled WACCM a priori profile as the true status



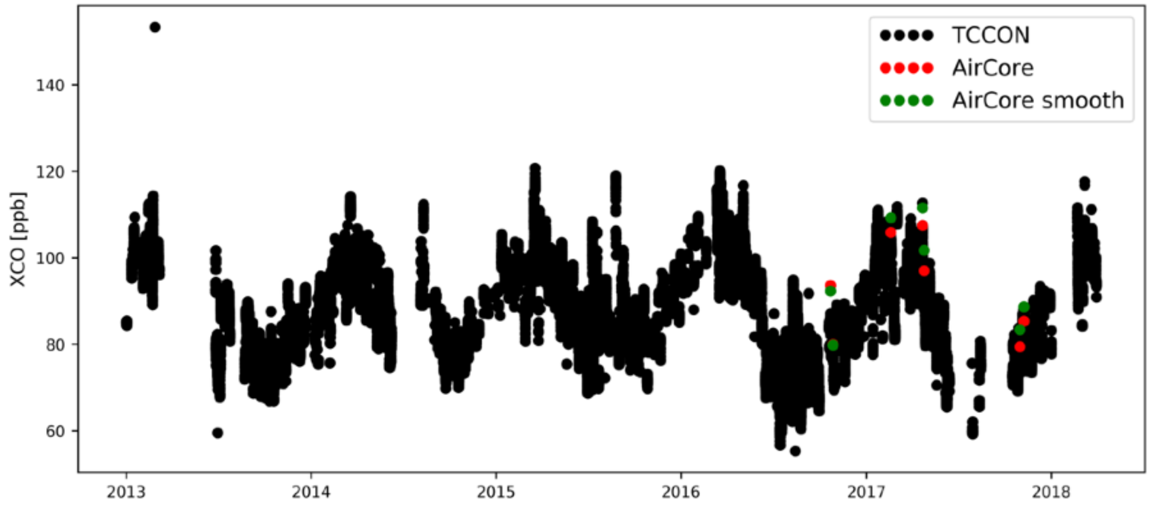
Sys±ran [%]	TCCON	NDACC
Ny-Alesund	3.7±2.0	0.8±0.3
Bremen	0.2±2.3	0.3±0.4
Izana	3.0±1.9	0.4±0.1
St Denis	5.0±2.1	0.2±0.4
Wollongong	3.9±3.6	0.1±0.5
Lauder	7.9±2.0	0.1±0.2

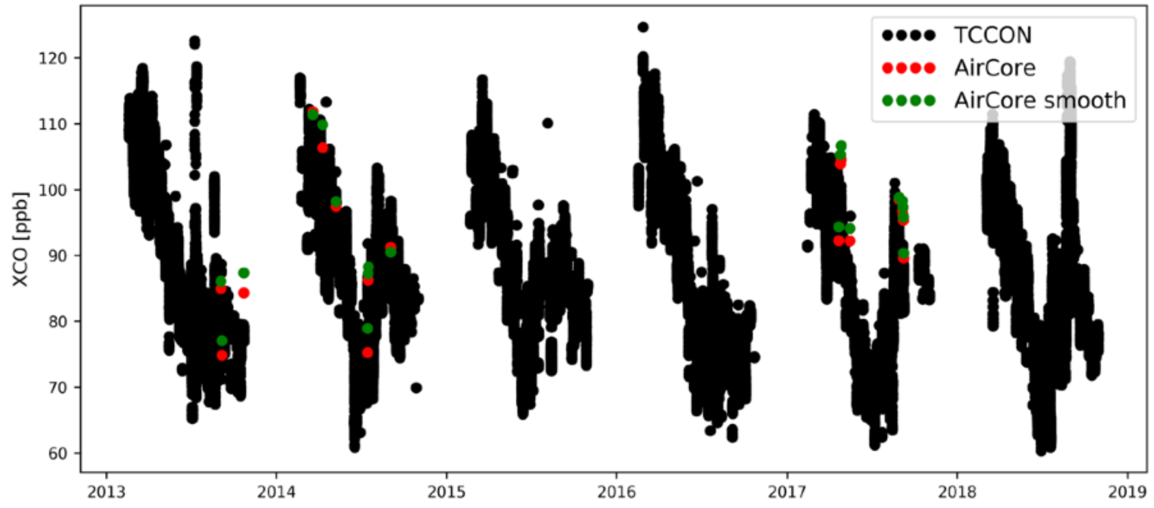


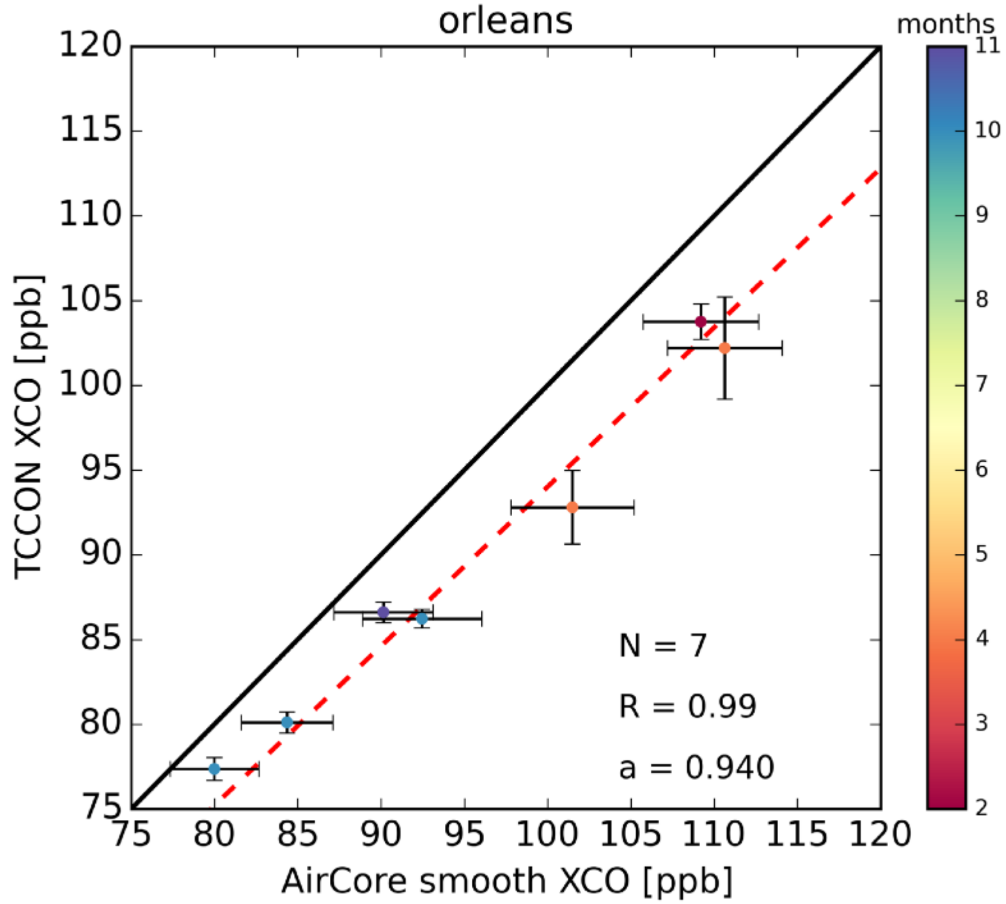
An example: the Sa systematic and random matrixes for TCCON retrievals at Lauder

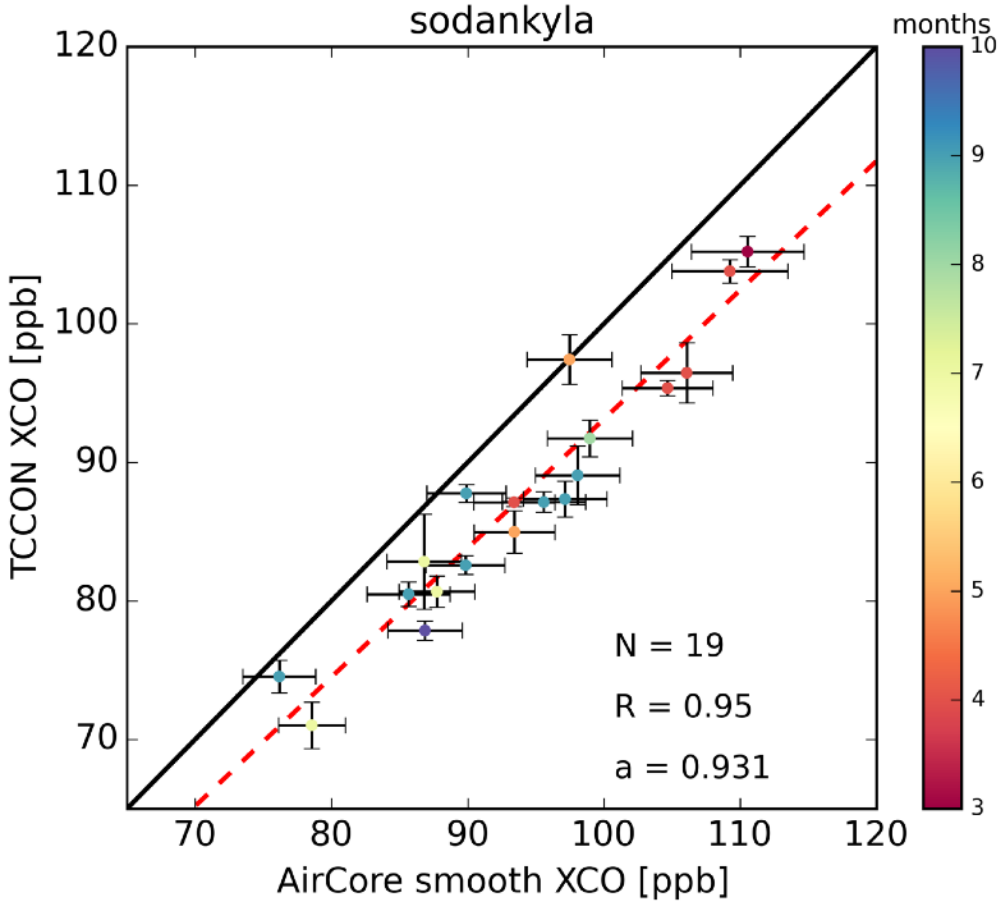
=>The hemispheric dependence in the bias is mainly due to the smoothing error of TCCON XCO data

AirCore vs TCCON XCO measurements





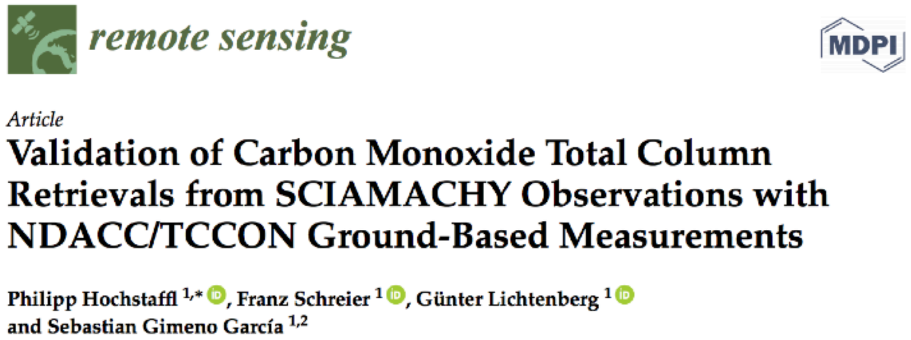




TCCON XCO measurements are 6.0±1.9%(orleans) and 6.9±2.5%(sodankyla) lower than smoothed AirCore measurements

Conclusions

- The standard TCCON XCO is about 5.5%/0.3% less than the NDACC XCO in the NH/SH.
- After applying the optimal a priori profile, the bias between the TCCON and NDACC XCO becomes about 6.0-7.0%, and the hemispheric dependence is significantly reduced.
- The TCCON XCO systematic smoothing error is estimated up to 7.9% (lauder). The user should take the smoothing error into account when comparing to satellite observations or model simulations.
- AirCore measurements at Orleans and Sodankyla confirm that the scaling factor of TCCON XCO data should not be 1.067.



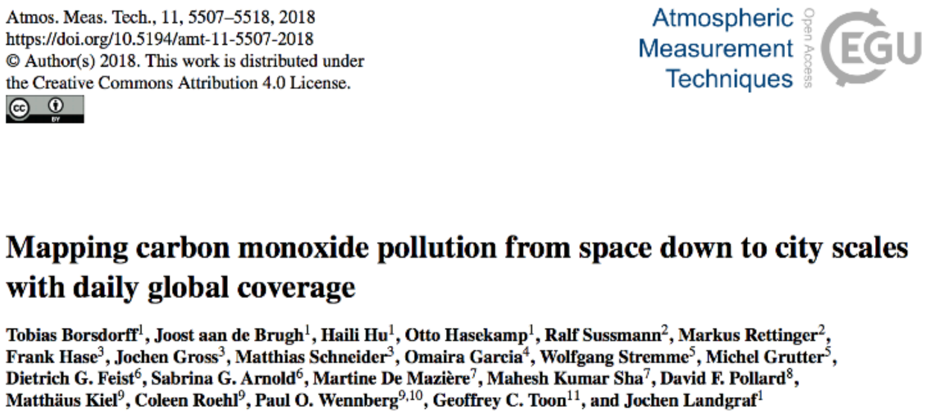
remote sensing

MDPI

Article

Validation of Carbon Monoxide Total Column Retrievals from SCIAMACHY Observations with NDACC/TCCON Ground-Based Measurements

Philipp Hochstaffl [1,*], Franz Schreier [1], Günter Lichtenberg [1] and Sebastian Gimeno García [1,2]



Atmos. Meas. Tech., 11, 5507–5518, 2018
https://doi.org/10.5194/amt-11-5507-2018
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Atmospheric Measurement Techniques

Mapping carbon monoxide pollution from space down to city scales with daily global coverage

Tobias Borsdorff[1], Joost aan de Brugh[1], Haili Hu[1], Otto Hasekamp[1], Ralf Sussmann[2], Markus Rettinger[2], Frank Hase[3], Jochen Gross[3], Matthias Schneider[3], Omaira Garcia[4], Wolfgang Stremme[5], Michel Grutter[5], Dietrich G. Feist[6], Sabrina G. Arnold[6], Martine De Mazière[7], Mahesh Kumar Sha[7], David F. Pollard[8], Matthäus Kiel[9], Coleen Roehl[9], Paul O. Wennberg[9,10], Geoffrey C. Toon[11], and Jochen Landgraf[1]

* *A manuscript based on this is almost ready for submission*

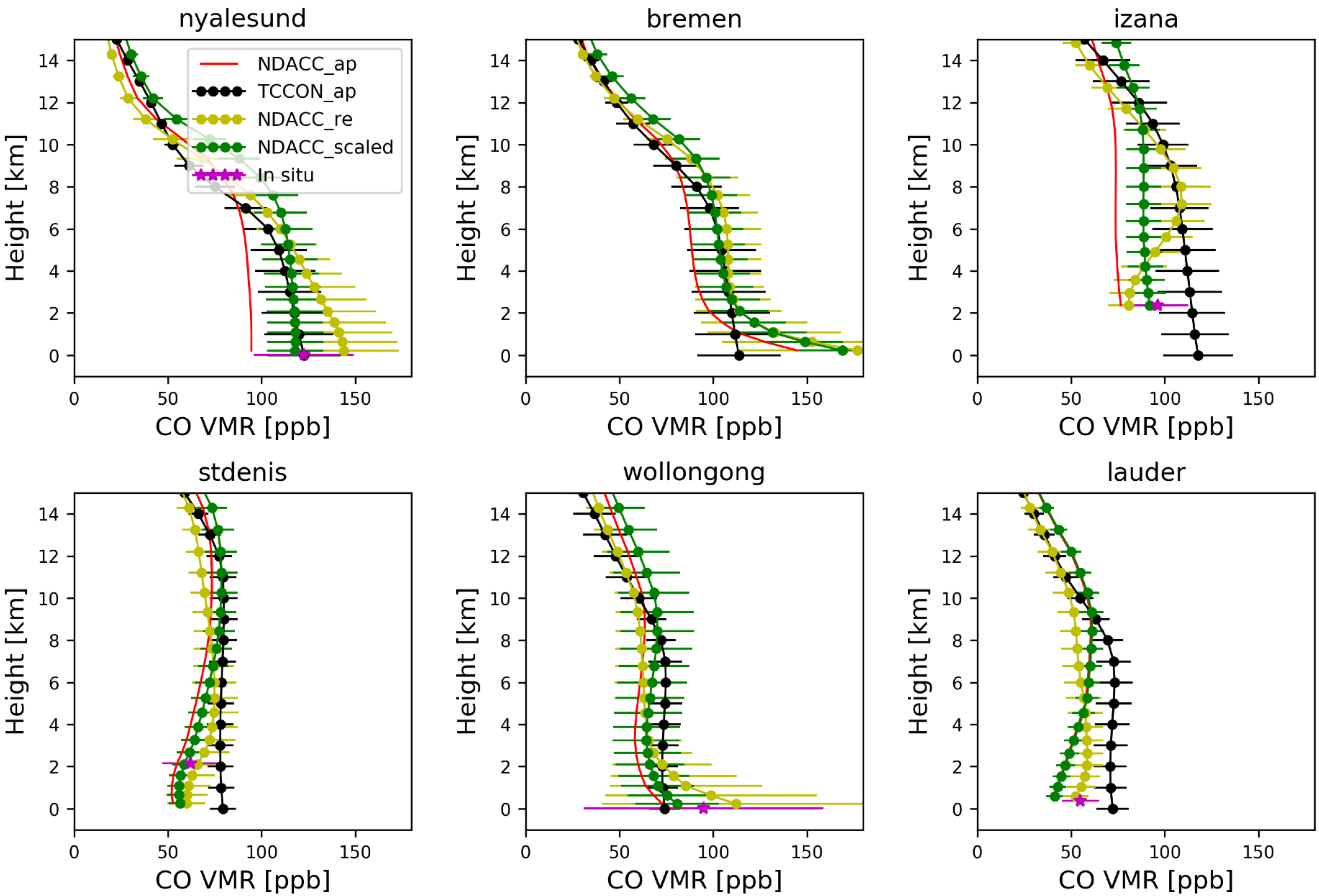
Thanks a lot for your attention!

Extra slides

Method 1- Using scaled WACCM profile as the a priori profile

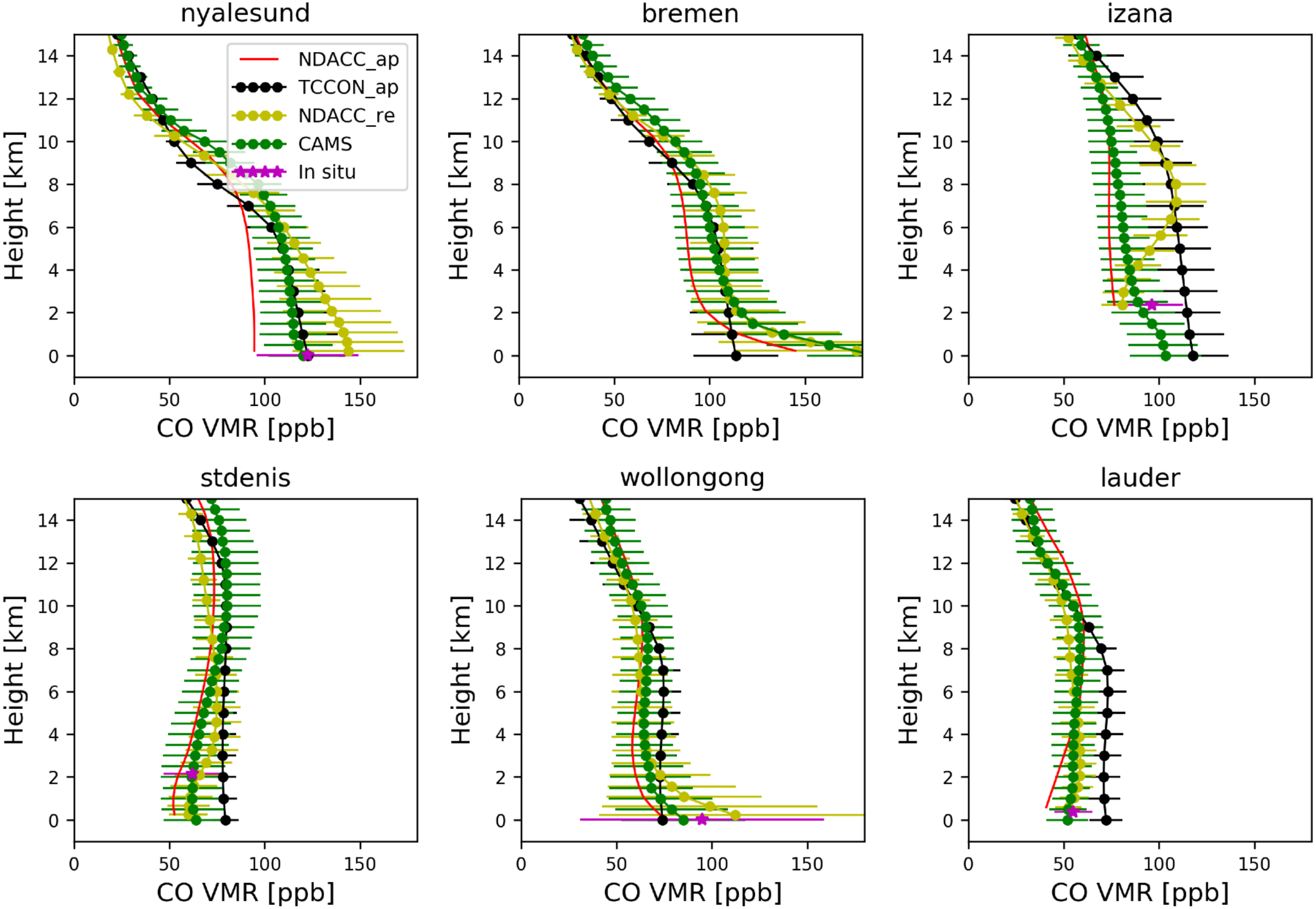
CO profiles from TCCON ap, NDACC ap, scaled NDACC ap and surface CO VMR from in situ measurements in 2013

$$\overrightarrow{x_{N,scaled}} = \overrightarrow{x_{N,ap}} * TC_{N,r}/TC_{N,ap}$$



Method 2- Using CAMS model as the a priori profile for surface -12 km and scaled NDACC a priori profile for above 12 km

CO profiles from TCCON, NDACC, CAMS model,
and surface CO VMR from in situ measurements in 2013

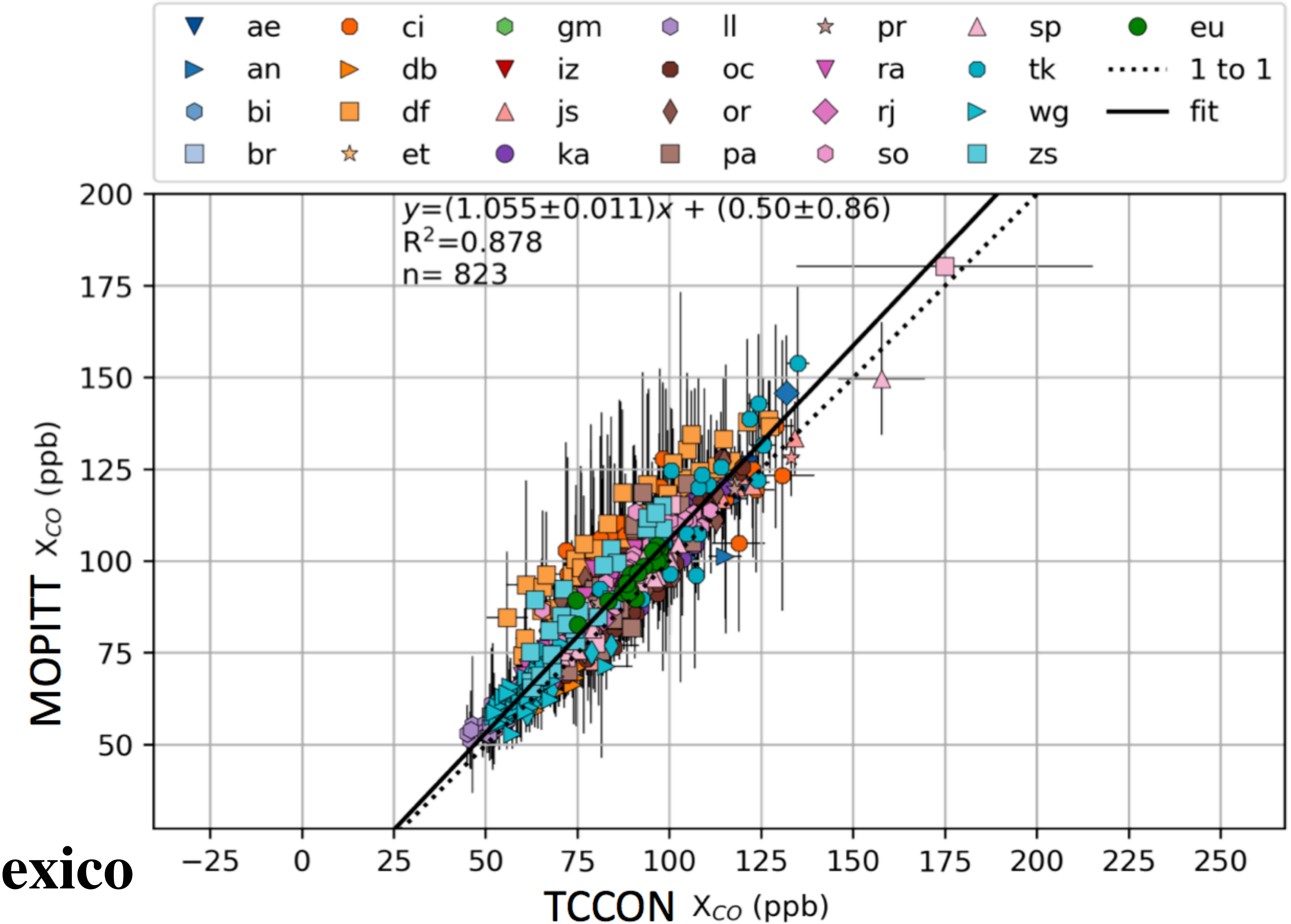


TCCON Comparison

- Nominal coincidence criterion 2°×4°
- Following methods of Wunch et al. (2011) doi: 10.5194/acp-11-12317-2011
  - Using TCCON prior as comparison ensemble ($\mathbf{x}_c = \mathbf{x}_{Ta}$)
  - Applying MOPITT averaging kernels to TCCON $\hat{\mathbf{x}} = \gamma \mathbf{x}_{Ta}$

TCCON Comparison (2016 only)

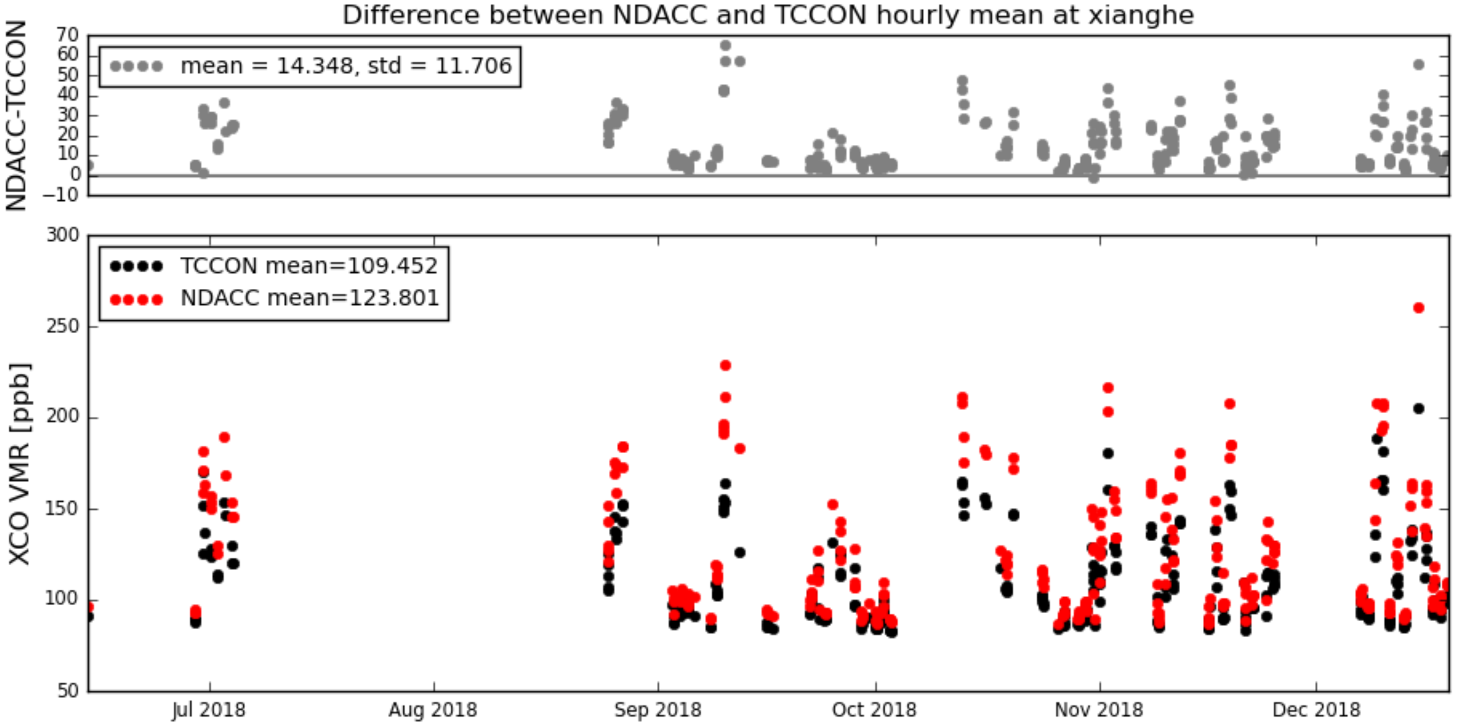
- 2016 bias on order of 5-6%

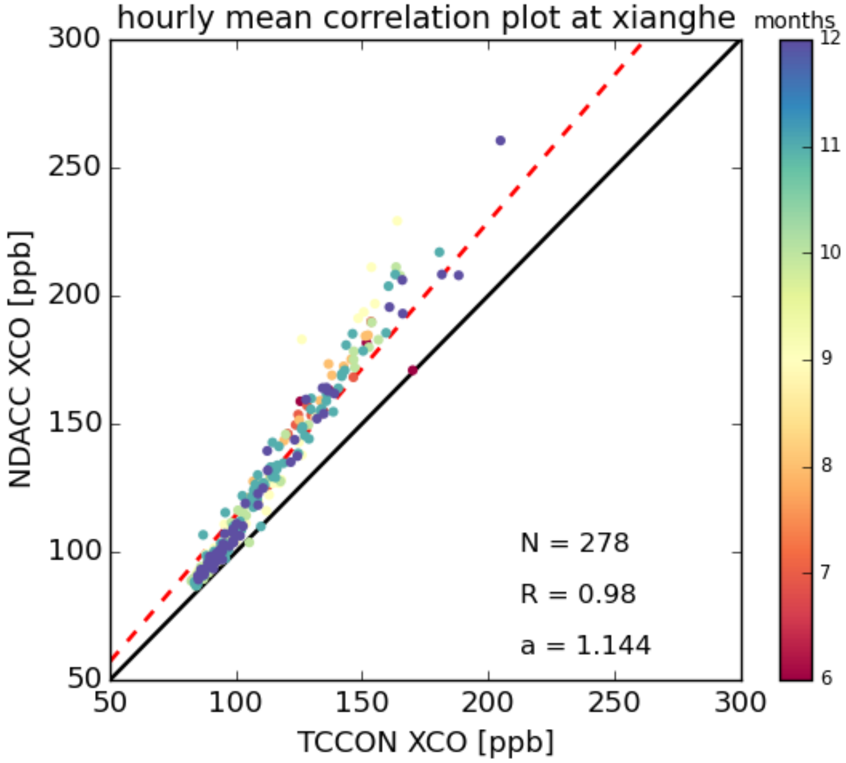


Jacob Hedelius et al., 2018 Mexico

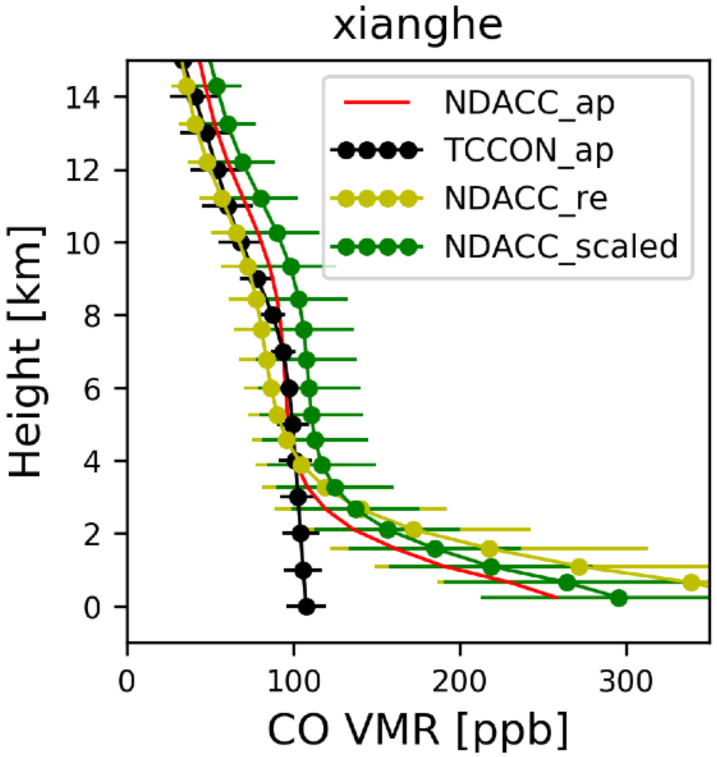
	TCCON	NDACC
Retrieval windows (cm-1)	4208.7-4257.3 4262.0-4318.8	2057.70-2058.00 2069.56-2069.76 2157.50-2159.15
Interfering species	CH4, H2O, HDO CH4, H2O, HDO	O3,CO2,OCS O3,CO2,OCS O3,CO2,N2O,H2O
Spectroscopy	ATM	HITRAN2008
Retrieval code	GGG2014 Profile scaling	SFIT4 or PROFFIT9 Profile retrieval
A priori profile	GGG2014 code (daily basis)	WACCM (fixed)
Dry air calculation	O2	Ps and H2O
Post-processing	Airmass dependent and independent correction	None

Test @ Xianghe, China (close to Beijing)





=> NDACC is 11.6+9.5(SD)% larger than TCCON XCO



As Xianghe is located in a polluted area, the CO VMR at the surface is relatively high (which is confirmed by the WACCM model and NDACC retrieved profiles). However, the TCCON a priori profile is too low, which will lead into a underestimation from the smoothing error.

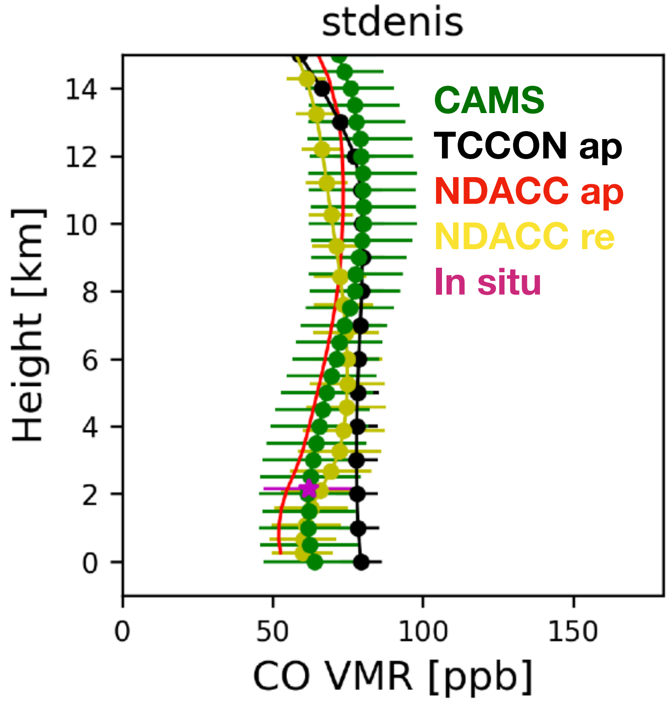
If using the scaled WACCM as the a priori profile (method 1), NDACC XCO is 5.0 + 6.9% larger than TCCON XCO

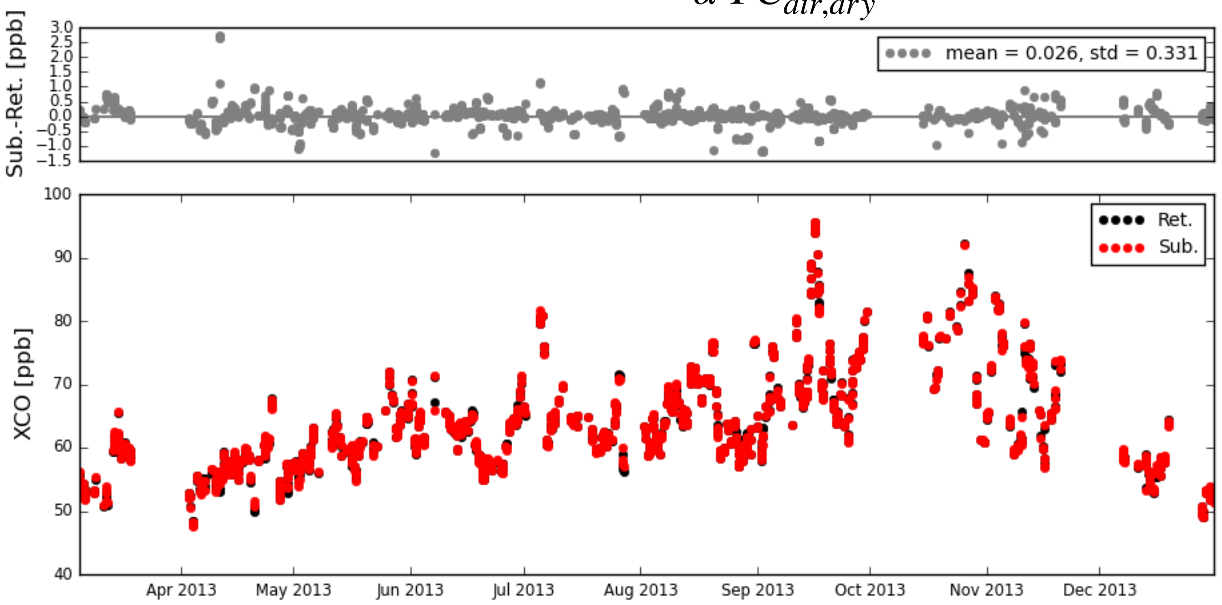
Test: the substitution method for TCCON data

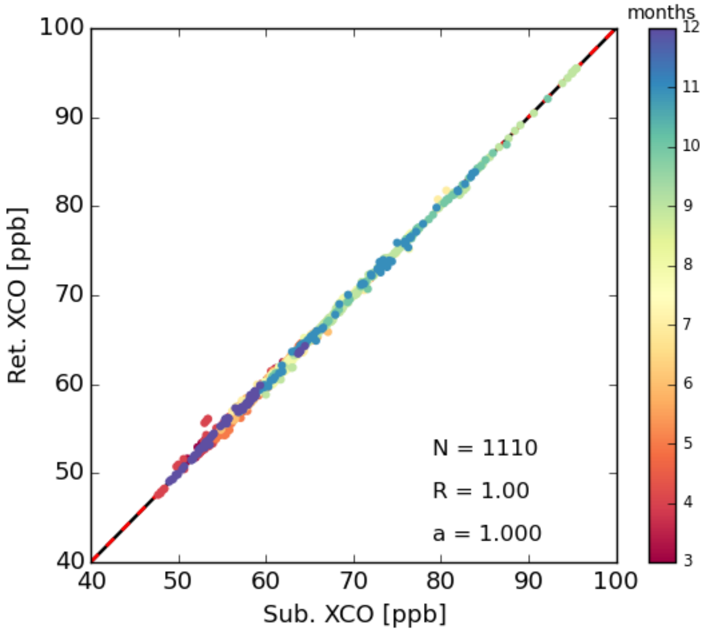
Test one year data @ St Denis

Ret. Re-run the GGG2014 code by using the CAMS as the a priori profile

Sub. $X'_{r,TCCON} = X_{r,TCCON} + \frac{1}{\alpha' TC_{air,dry}}[(\vec{I} - \overrightarrow{A_{TCCON}}) \cdot (\overrightarrow{PC_{CAMS}} - \overrightarrow{PC_a})]$

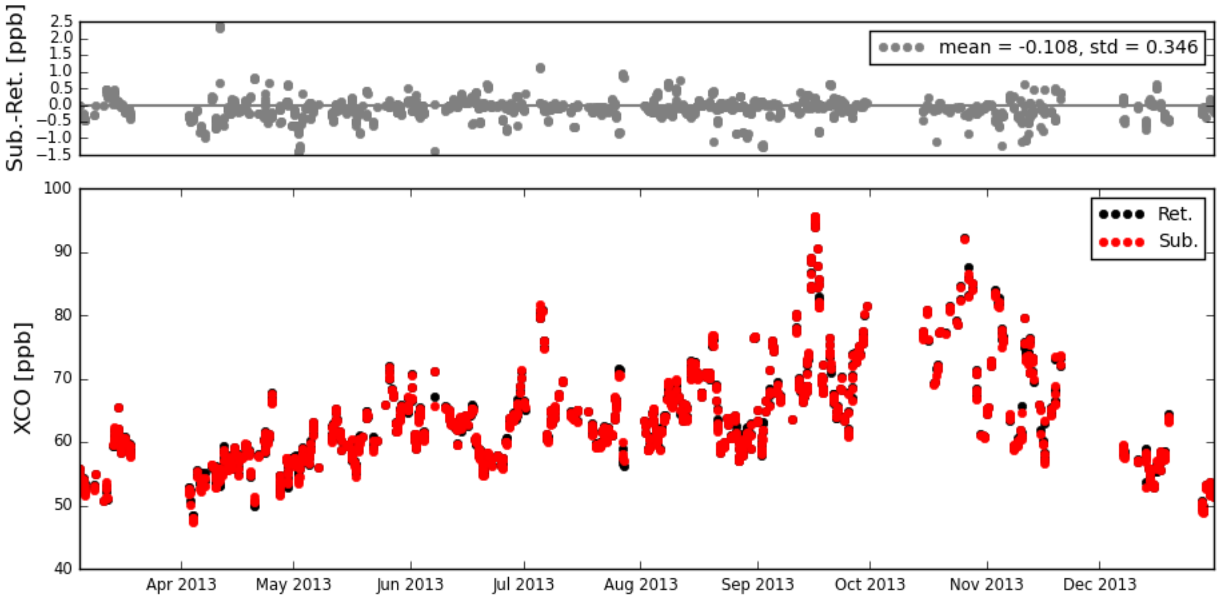


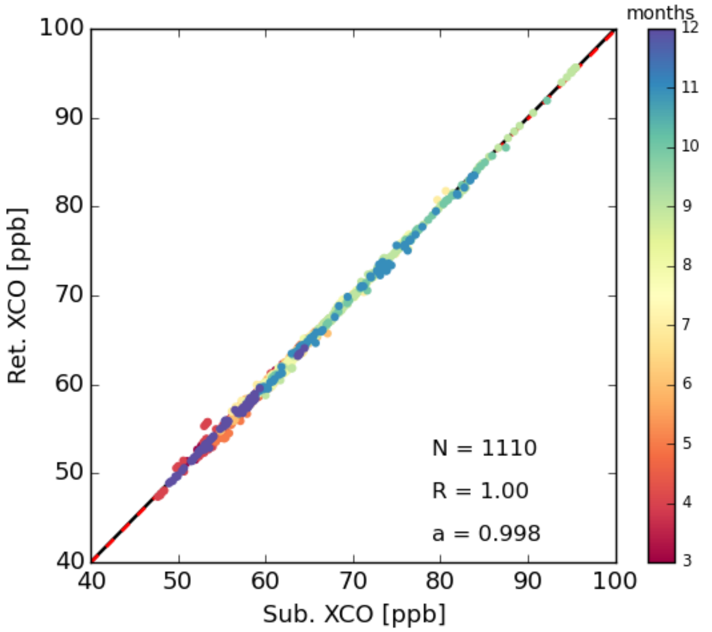




If α' is not taken into account

Sub. $X'_{r,TCCON} = X_{r,TCCON} + \frac{1}{TC_{air,dry}}[(\vec{I} - \overrightarrow{A_{TCCON}}) \cdot (\overrightarrow{PC_{CAMS}} - \overrightarrow{PC_a})]$





Taking α' in to account improves the agreement with GGG of 0.2%