Refine the Calibration of PROFFAST 2

TCCON-NDACC-COCCON Meeting in Spa

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Why redo the calibration?

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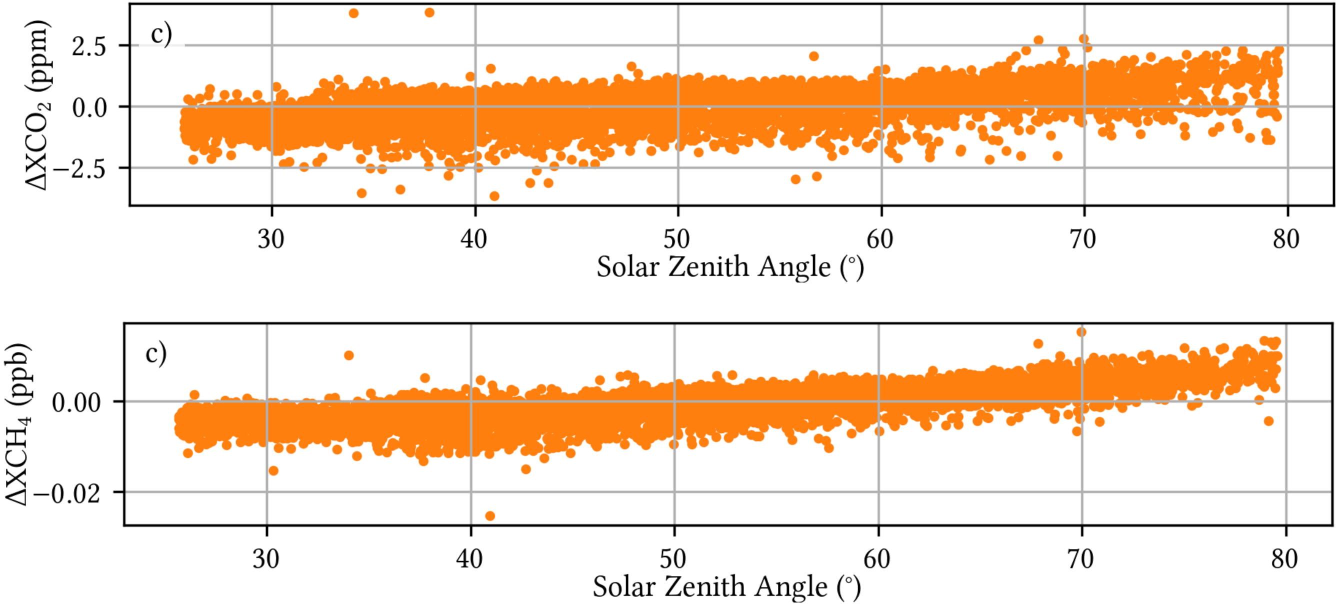
- Last calibration was released in January 2022 with (PROFFAST 2.2, or PROFFASTpylot 1.1)
  - Shows a residual offset for larger solar zenith angles (SZA)
  - Considered only COCCON reference and KA-TCCON data

- The new calibration is based on 3 EM27/SUNs and 2 TCCON sites:
  - SN37 (reference EM27/SUN) compared with TCCON-KA
  - SN39 compared with TCCON-SO (2017 – 2018)
  - SN122 compared with TCCON-SO (2020 – mid 2021)

Status of the old calibration

Δ Xgas: SN37(COCCON reference) vs. TCCON-KA



How to Calibrate?

Determine

Air mass Dependent Correction Factors (ADCFs)

&

Air mass Independent Correction Factors (AICFs)

How to Calibrate?

1) Improve ADCFs (Independent of TCCON)

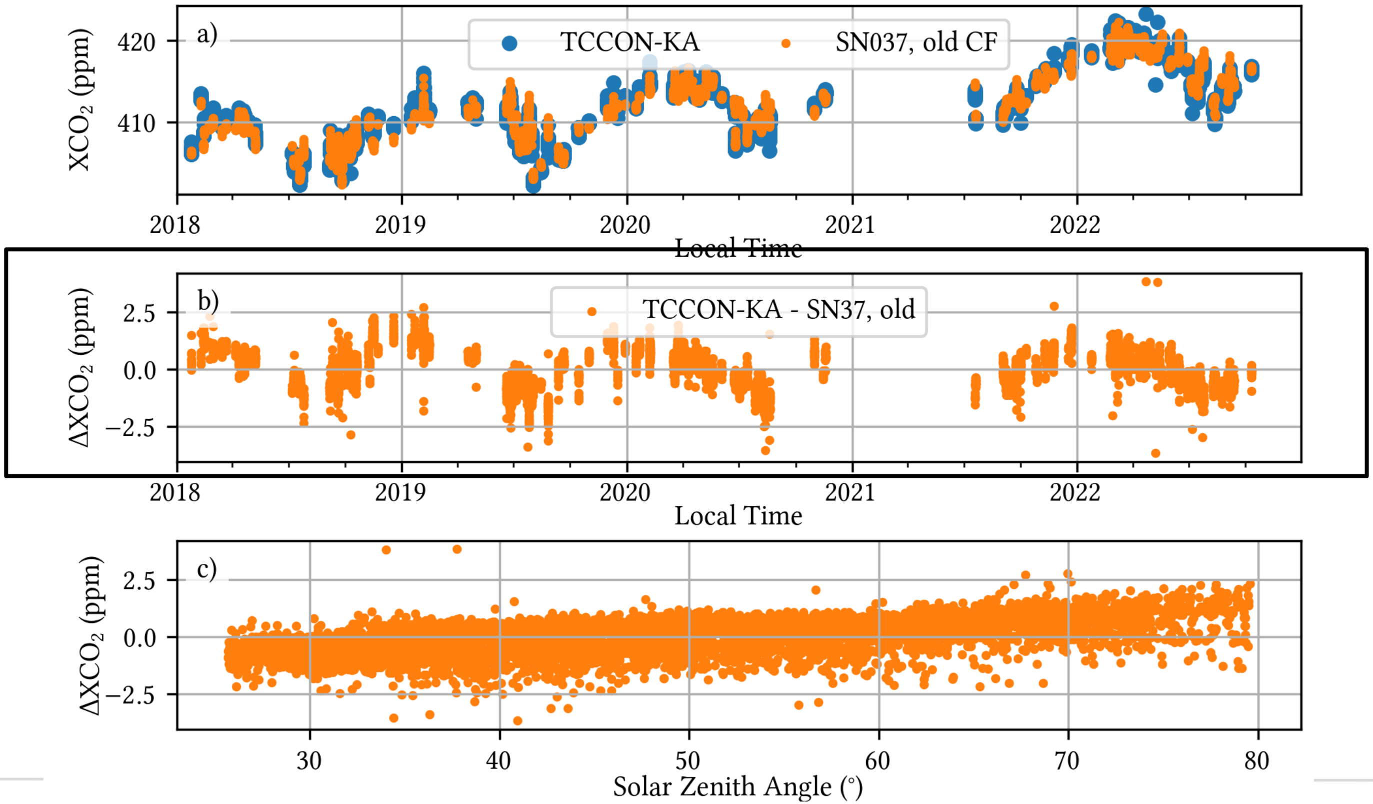
1. For **each day**: Calculate the **mean of** all **measurements** with $20 \leq \text{SZA} \leq 50$
2. **Divide** the measurements of each day **by** this **average**
3. **Fit** $f(\text{SZA}) = 1 + a \cdot \text{sza}^2$ to the data
4. Estimate ADCFs in order to **minimize "a"**
5. **Reprocess** with **new ADCFs** and repeat with step 1

3) Improve AICFs (Calibration to match with TCCON):

1. **Bin** the **measurements** of TCCON and COCCON **in 10 minute bins**
2. **Divide** the **bins** by each other and average the resulting quotients:
   $c = \frac{1}{N} \sum_i q_i$
3. $\text{AICF}_{\text{new}} = c \cdot \text{AICF}_{\text{old}}$
4. **Reprocess** with new ADCFs and repeat with step 1.

Status of the old calibration

Δ Xgas: SN37(COCCON reference) vs. TCCON-KA



How to Calibrate?

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1) Improve ADCFs (Independent of TCCON)

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4. Estimate ADCFs in order to **minimize “a”**
5. **Reprocess** with **new ADCFs** and repeat with step 1

2) Introduce a third, empirical correction factor:
Correct all species with a linear correction in dependence of XH2O

3) Improve AICFs (Calibration to match with TCCON):

1. **Bin** the **measurements** of TCCON and COCCON **in 10 minute bins**
2. **Divide** the **bins** by each other and average the resulting quotients: $c = \frac{1}{N} \sum_i q_i$
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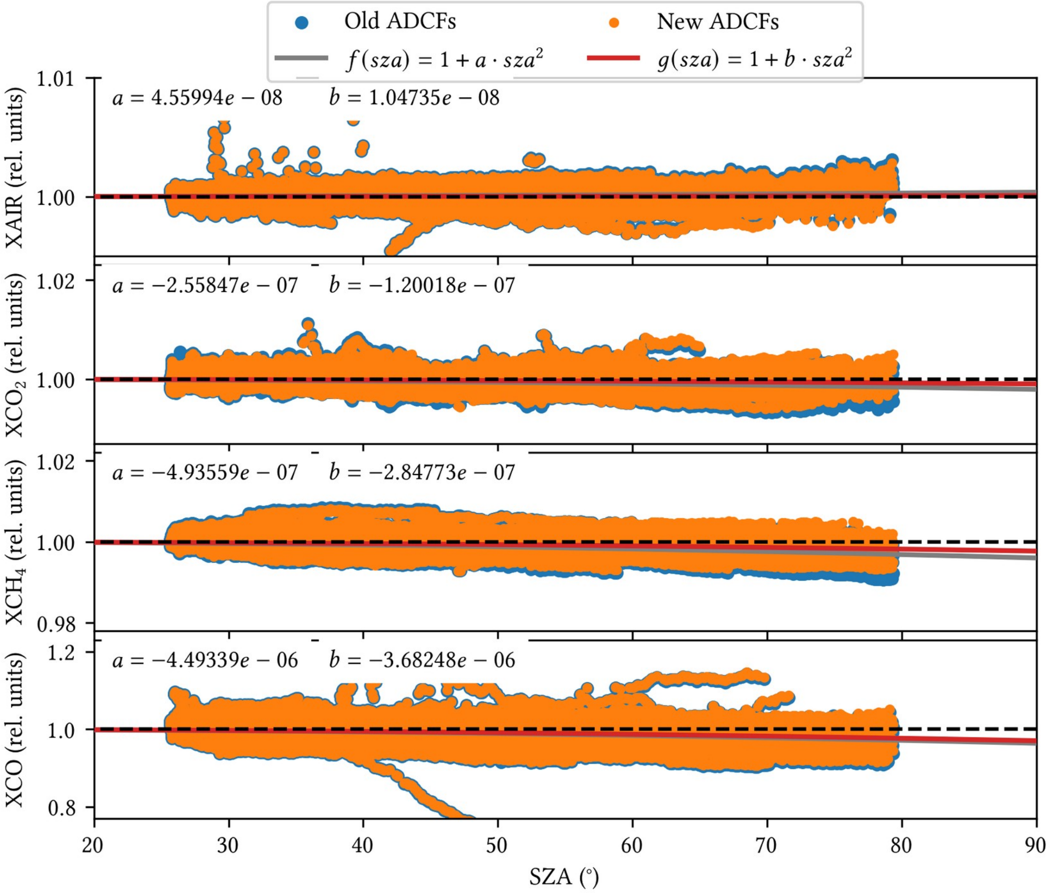
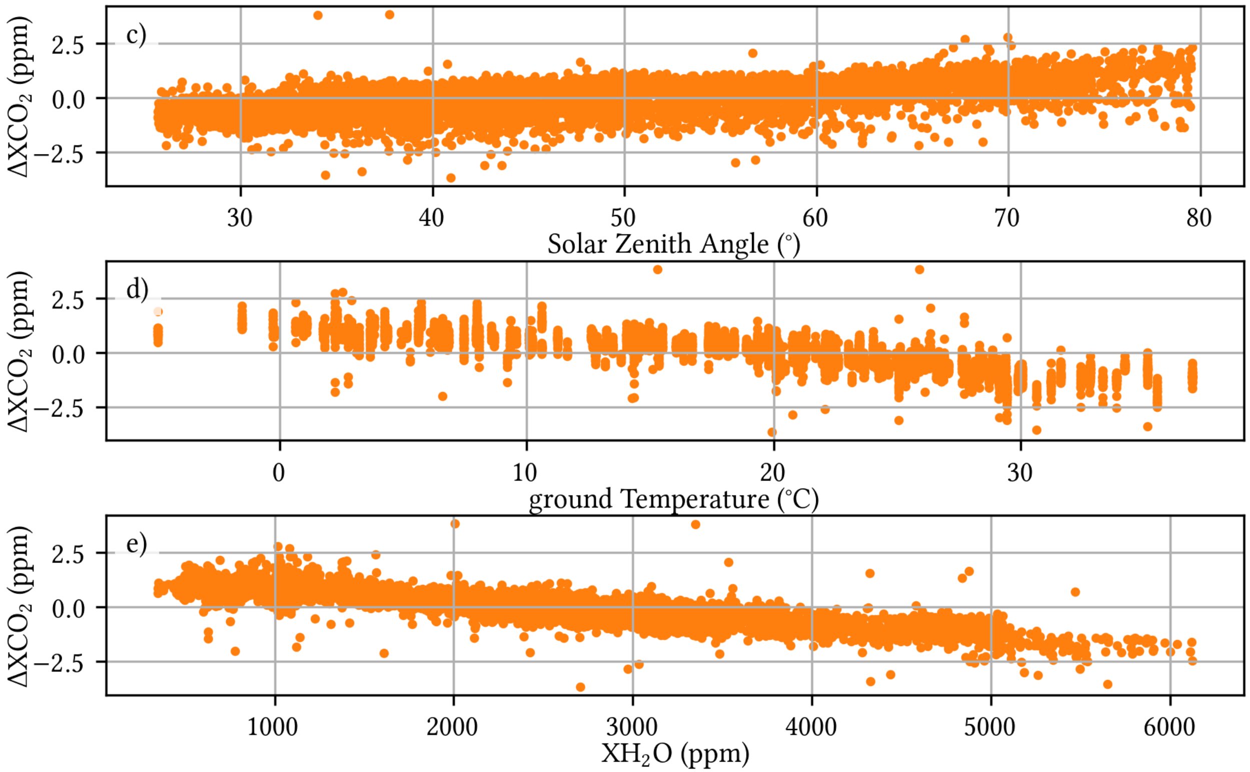
1) New Calibration: Determine ADCF

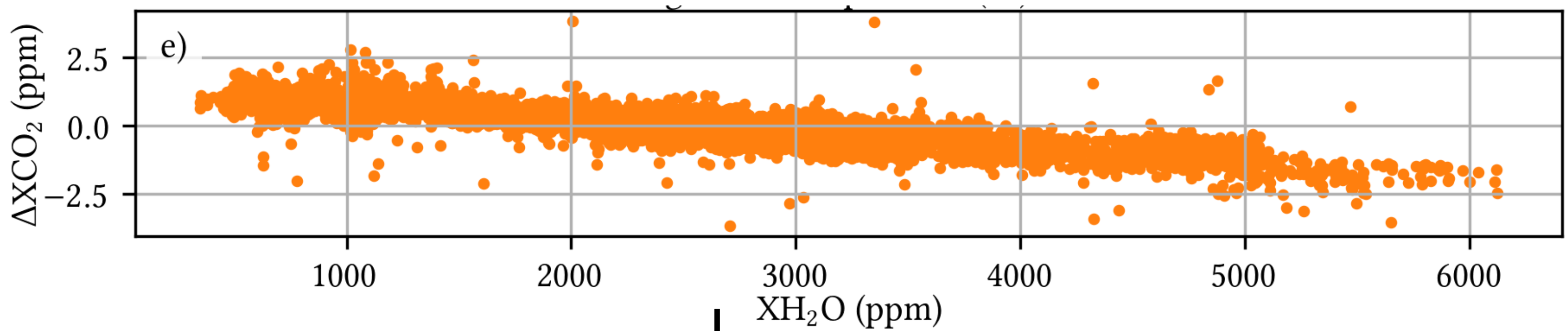


2) New empirical Correction Factor

Why choose XH_2O as the variable for the correction?

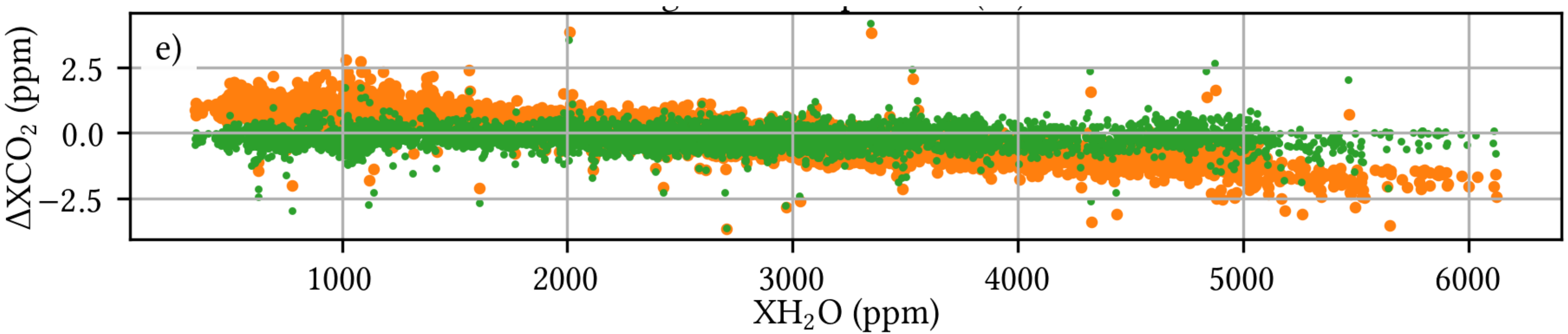


2) New empirical Correction Factor



Additional H2O correction on top of air-mass dependent correction.

$$\mathrm{XGas_{corr}} = \mathrm{XGas} \cdot \left[1 + CF_{\mathrm{XH_2O}}(\mathrm{XH_2O} - 2500)\right]$$



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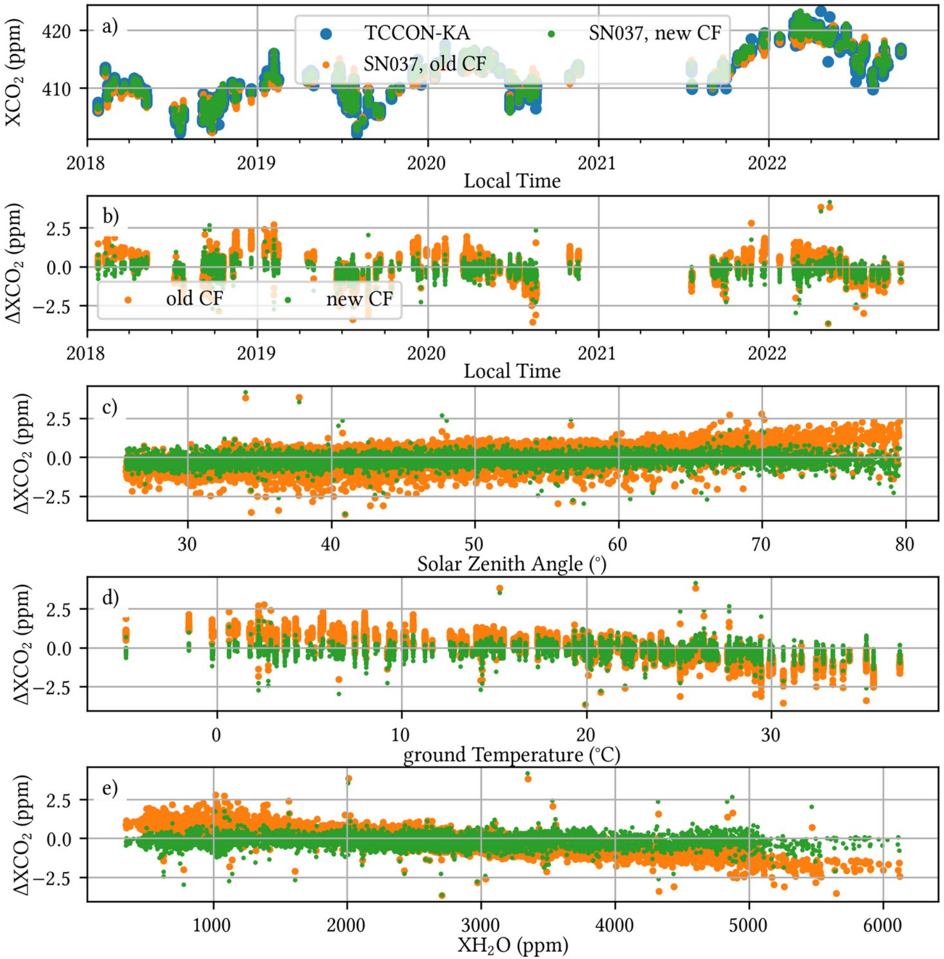
2) + 3) XH2O correction + AICF



Assessment of Calibration

The table shows the relative deviations and the relative standard deviation in %

Species	Average of (SN37, SN39, SN122) (%)
XCO_2	0.02840 ± 0.11337
XCH_4	-0.01310 ± 0.19023
XCH_4^{S5P}	-0.03920 ± 0.26753
XCO	-0.27420 ± 1.60327
XH_2O	-1.20523 ± 1.88773
XAIR	0.00020 ± 0.25413

Conclusion

1. The **new calibration** is based on several COCCON and TCCON spectrometers and results in an **excellent adjustment** of **COCCON with PROFFAST2** and **TCCON with GGG2020**.

2. In the **future**: **confirm** the calibration using an **additional** souther hemisphere **TCCON site** (Wollongong?)

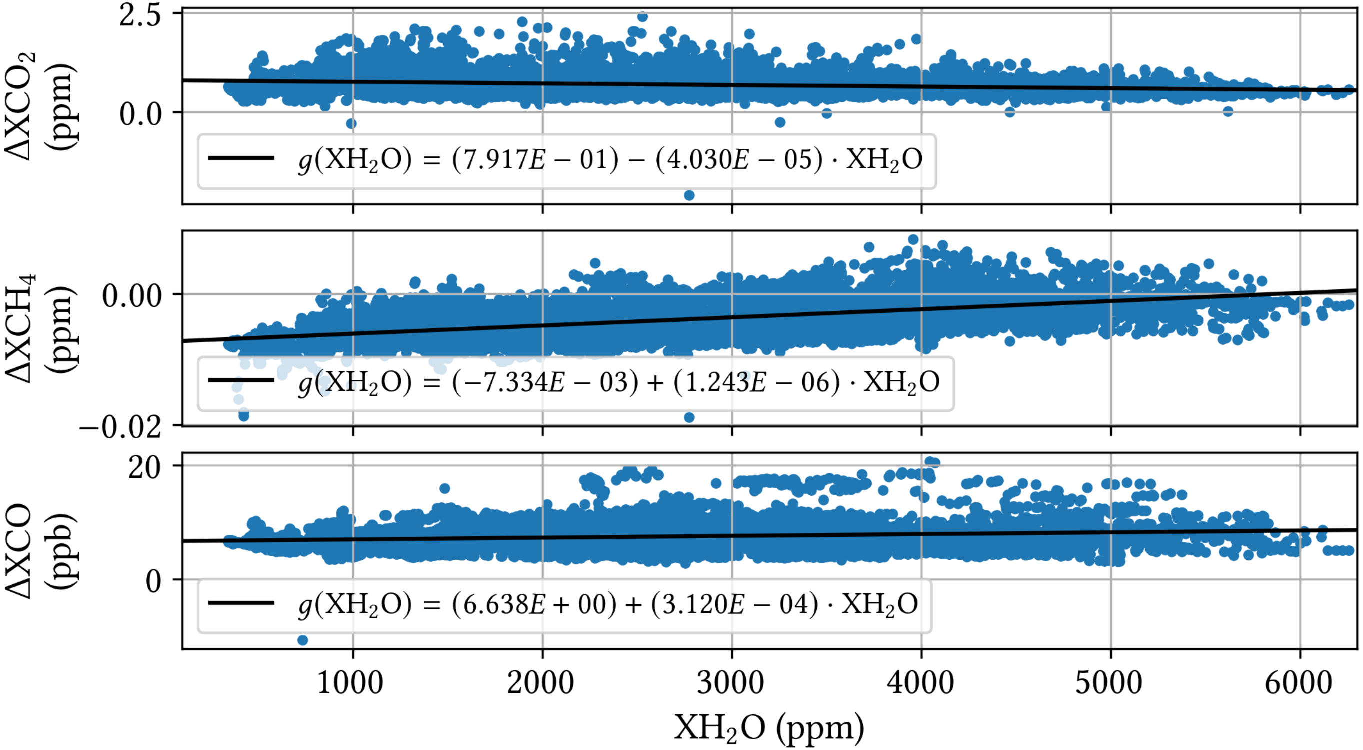
3. It is **surprisingly** that the $C_{\mathrm{XH_2O}}$ are **this consistent** across different species.

4. **But**: are we confident that **GGG2020** is **correct** in this respect?

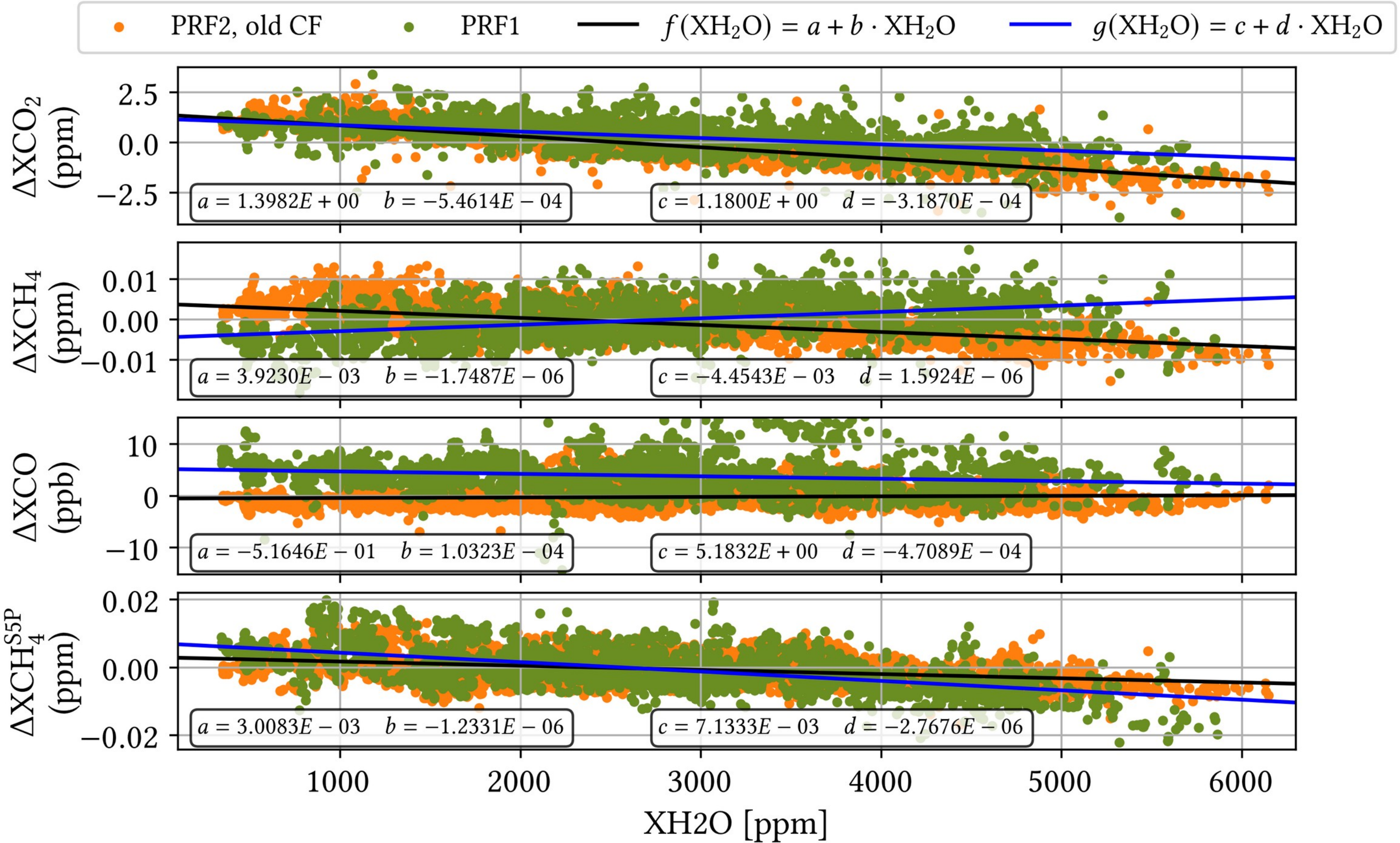
   → We are in discussion with the TCCON board!

Thank you for your attention!

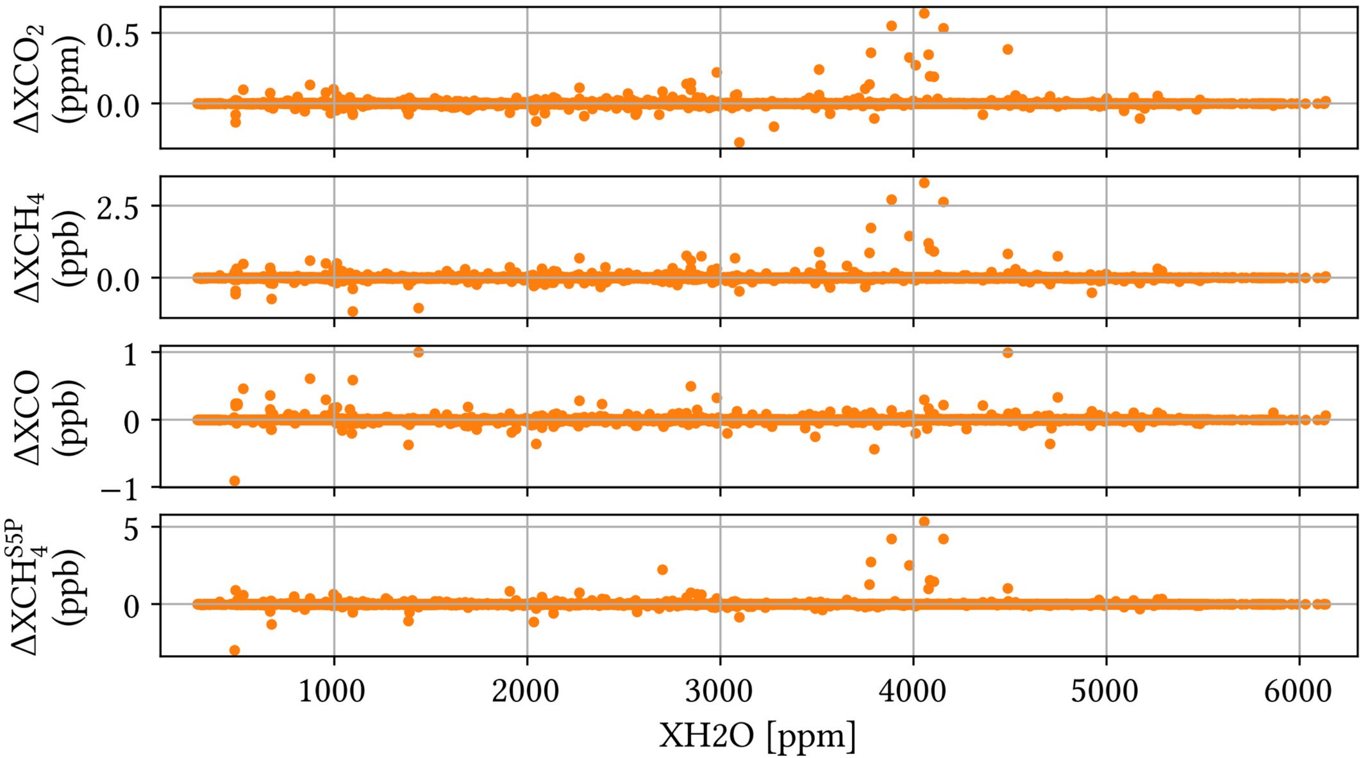
Comparison GGG2020 vs GGG2014



Comparison PRF1 and PRF2 vs GGG2020



Comparison PRF 2 with PRF 1 H_2O line list



Final Calibration Factors

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XGas	$ADCF_1$	$ADCF_2$	$ADCF_3$	AICF	CF_{XH_2O}
XH_2O	0.00000	0.0000	0.0000	1.0000	–
XAIR	−0.0075	−0.0072	0.0000	0.9910	0.00
XCO_2	0.00040	0.0020	0.0000	0.9975	−1.50
XCH_4	0.00275	0.0100	0.0000	0.9884	−0.72
XCH_4^{S5P}	−0.0008	0.0025	0.0000	0.9950	−0.72
XCO	0.07150	0.0060	0.0000	1.0000	−0.30

Assessment of Calibration

The table shows the relative deviations and the relative standard deviation in %

Species	SN37 (%)	SN39 (%)	SN122 (%)	Average of (SN37, SN39, SN122) (%)
XCO_2	-0.0429 ± 0.0949	0.0464 ± 0.0861	0.0817 ± 0.1591	0.02840 ± 0.11337
XCH_4	0.0006 ± 0.1596	0.0184 ± 0.1536	-0.0583 ± 0.2575	-0.01310 ± 0.19023
XCH_4^{S5P}	0.0342 ± 0.2403	0.0110 ± 0.2252	-0.1628 ± 0.3371	-0.03920 ± 0.26753
XCO	0.9157 ± 2.3268	-0.8551 ± 1.1736	-0.8832 ± 1.3094	-0.27420 ± 1.60327
XH_2O	-1.5683 ± 2.5825	-1.1757 ± 1.6904	-0.8717 ± 1.3903	-1.20523 ± 1.88773
XAIR	-0.1759 ± 0.1410	0.0823 ± 0.3581	0.0942 ± 0.2633	0.00020 ± 0.25413

How to calculate the deviations in percent

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1) Calculate the difference of 10 minute bins: $\Delta XGas_i = \overline{XGas_i}^{TC} - \overline{XGas_i}^{CC}$

2) Calculate the average of the differences: $\overline{\Delta XGas} = \frac{1}{N}\sum_{i=1}^{N} \Delta XGas_i$

3) Calculate the standard deviation of the differences.

4) Calculate the timely average Xgas value of the TCCON-Site over the whole comparison period.

5) Calculate the relative difference and standard deviation:

$$\widehat{\overline{\Delta XGas}} \pm \widehat{\sigma_{\Delta XGas}} = \frac{\overline{\Delta XGas}}{\overline{XGas_{TCCON}}} \pm \frac{\sigma_{\Delta XGas}}{\overline{XGas_{TCCON}}}$$