FRM4GHG 2.0
Fiducial Reference Measurements for Greenhouse Gases

Travelling standard EM27/SUN & calibration procedure

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1 DOCUMENT CHANGE RECORD

Issue	Date	Item	Comment
V1.0	2023-01-09	-	Initial version

2 ACCESS LIST

This document is a deliverable "D3.2.1: Travelling standard EM27/SUN & calibration procedure created for the project FRM4GHG 2.0 and will be submitted to ESA. The document can be downloaded from the project webpage http://frm4ghg.aeronomie.be.

3 PURPOSE

This document reports the progress on the Task 2 of the WP 3 of the ESA project "Fiducial Reference Measurements For Ground-based IR Greenhouse Gas Observations 2.0".

4 DOCUMENT STRUCTURE

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5 TRAVELLING STANDARD EM27/SUN

For the realization of the Travel Standard there are two main points to be considered.
First, the deployment to the visited TCCON sites is desired to be simple to maintain a high frequency of visited TCCON sites. Furthermore, it is desired to make it controllable fully remotely.
Second, it is desired to have a shelter to allow an operation of the spectrometer at a wide range of places around the world with different ambient conditions.

These requirements where fulfilled by a shelter which is built by the TU Munich (Heinle & Chen, 2018). The shelter is equipped with a PLC controlling the measurement dome. A small UPS is used to close the dome in case of a blackout to avoid e.g. rain coming into the shelter. An industrial computer used to control the spectrometer. A router designed for outdoor usage which can connect to the internet via LAN, WiFi or mobile data gives the possibility to access the shelter remotely.
To control the temperature in the enclosure it is equipped with a heater and a fan. A rain sensor mounted on top of the box closes the dome in case of rain to avoid any damage due to water.

The original shelter by TUM was designed to operate within Europe. Hence it could not handle voltages and frequencies different from the European standard. To make it compatible to the different voltages and frequencies in the different countries a large part of the electronic needed was replaced and rewired with a slightly different logic. In Figure 1 the electronic is shown and described. All new or modified parts are marked with ‘NEW’.

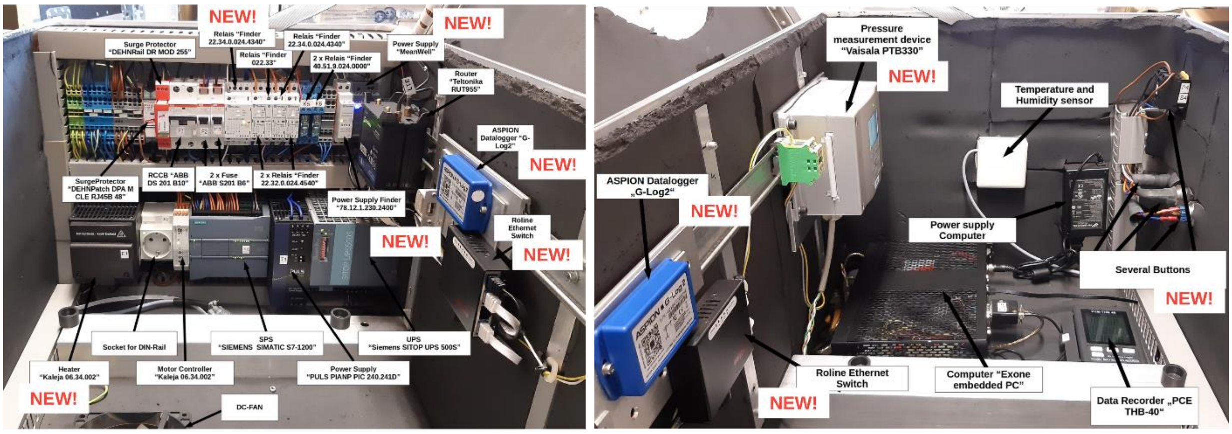

Figure 1: The electronics of the shelter created by TUM. The modifications by KIT for supporting wide power supply is marked with "NEW". In addition, a highly accurate pressure sensor “Vaisala PTB330” and a datalogger “ASPION G-Log2” to record shock events while transporting is added by KIT.

To compare the pressure measurements at the TCCON-sites, the enclosure is equipped with a “Vaisala PTB330”, a highly accurate pressure sensor. To check for possible shock events while transporting the Travel Standard, the transportation datalogger “ASPION Datalogger G-Log2” is added. Since the EM27/SUN used as the Travel Standard is equipped with a new Ethernet Camera, an additional ethernet switch is added to enable Gigabit ethernet within the enclosure (before the update only Megabit speed was available).

6 CALIBRATION PROCEDURE FOR THE TRAVELLING STANDARD EM27/SUN

In this section the calibration procedure of an EM27/SUN used as Traveling Standard (TS) for TCCON sites is described.
Specifically, the calibration to the Collaborative Carbon Column Observing Network (COCCON) reference device is described as well as the side-by-side measurements at a TCCON site and the subsequent analysis of the data as well as preliminary results of the comparison are shown.
All collected measurements have been processed with the PROFFAST2 software as required by COCCON.

We compare XGas measurements recorded with different spectrometers by using empirical relative bias correction factors. These correction factors are used to compare the XGas results of the different spectrometers which are under investigation in the context of this work.

The procedure for this is explained here: For two instruments x and y the bias correction factor for species i is denoted by $c_{\mathrm{x}}^{\mathrm{y}}(Gas_i)$. This is defined in a way that the gas abundances measured with instrument x reproduces the gas abundances measured by instrument y by calculating $c_{\mathrm{x}}^{\mathrm{y}}(Gas_i)$, so $XGas_i^y = c(Gas_i)_x^y \cdot XGas_i^x$. Here, $XGas_i^x$ denotes the abundance of a gas i measured with instrument x and $XGas_i^y$ denotes the abundance of a gas i measured with instrument y. Note that by definition $c_x^y(Gas_i) = 1/c_y^x(Gas_i)$.

To calculate the correction factors, XGas values of instrument x and y are both binned in intervals of 10 minutes, $\overline{\mathrm{XG}as_i^{x/y}}^{t_j}$ where t_j is enumerating the bins. Considering all coincident bins N of the intercomparison method of both instruments the correction factor is calculated by dividing the values of instrument y by the ones of instrument x and taking the average of it,

$$c_{\mathrm{x}}^{\mathrm{y}}(Gas_i) = \frac{1}{N} \sum_{j=\text{coincident bins}}^{N} \frac{\overline{XGas_i^y}^{t_j}}{\overline{XGas_i^x}^{t_j}}.$$

In a sequential comparison, involving the COCCON reference in Karlsruhe (which is empirically adjusted to the GGG2020 data set recorded with the TCCON-Ka spectrometer via the gas calibration factors assumed by PROFFAST), the TS, and the TCCON spectrometer in Japan (JP), we find

$$XGas_{JP} = c_{TS}^{JP} \cdot c_{Ref}^{TS} \cdot XGas_{Ref}$$

So the calibration bias factor between the TCCON spectrometer in Japan and the TCCON spectrometer in Karlsruhe (or, equivalently, the COCCON reference spectrometer operated in Karlsruhe), is the product of the calibration factor found for TCCON Japan with respect to the TS and the calibration factor for the TS with respect to the reference: $c_{TS}^{JP} \cdot c_{Ref}^{TS}$(for a graphical visualization see Figure 2).

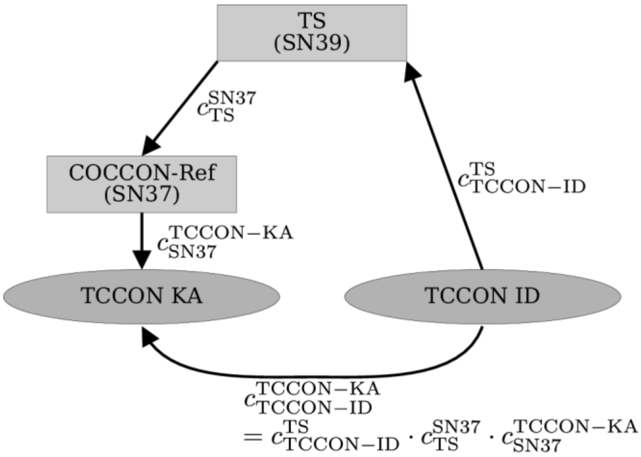

Figure 2: Scheme to calculate correction factors for comparing an arbitrary TCCON site to the KA-TCCON site

6.1 Calibration to the COCCON Reference

Before each calibration campaign the TS (ID number SN39) spectrometer measures side-by-side with the COCCON reference instrument ID number SN37 operated continuously at Karlsruhe Institute of Technology (KIT). The ILS of the spectrometer is characterized by open path and gas

cell measurements (for monitoring the stability of ILS characteristics) (Alberti, et al., 2022) (Frey, et al., 2015).
The measurements were performed at two days each, before the Japan campaign in December 2021 and January 2022, so after the Japan trip and before the Canada campaign in June 2022 and lastly after the Canada campaign in October 2022.
The results of the side-by-side measurements are shown in Figure 3. The resulting correction factors are summed up in Table 1. The absolute change in the temporal mean values is for all gases less than the estimated error of the TCCON given in (Wunch, et al., 2015). From this it can be seen that the stability of the Travel Standard EM27/SUN instrument is sufficient for comparing TCCON stations (Wunch, et al., 2015).

Table 1: Correction factors for the TS instrument (SN39) to match the COCCON reference instrument (SN37)

Species	Date	K_{SN39}^{SN37}	ΔK_{SN39}^{SN37} [%]
XCO_2	January 2022	0.99886 ± 0.00038	–
	June 2022	0.99940 ± 0.00040	0.05380 %
	October 2022	0.99962 ± 0.00020	0.02266 %
XCH_4	January 2022	1.00034 ± 0.00032	–
	June 2022	0.99963 ± 0.00033	−0.07062 %
	October 2022	1.00068 ± 0.00018	0.10511 %
XCO	January 2022	1.00169 ± 0.00185	–
	June 2022	1.00176 ± 0.00405	0.00652 %
	October 2022	1.00106 ± 0.00160	−0.06949 %

The side-by-side measurements performed with the TS in Karlsruhe suggest an airmass-dependent XCO bias (see Figure 3). This was corrected using an empirical SZA dependent correction for XCO. The corrected XCO values are plotted in red and used to calculated the values in Table 1.

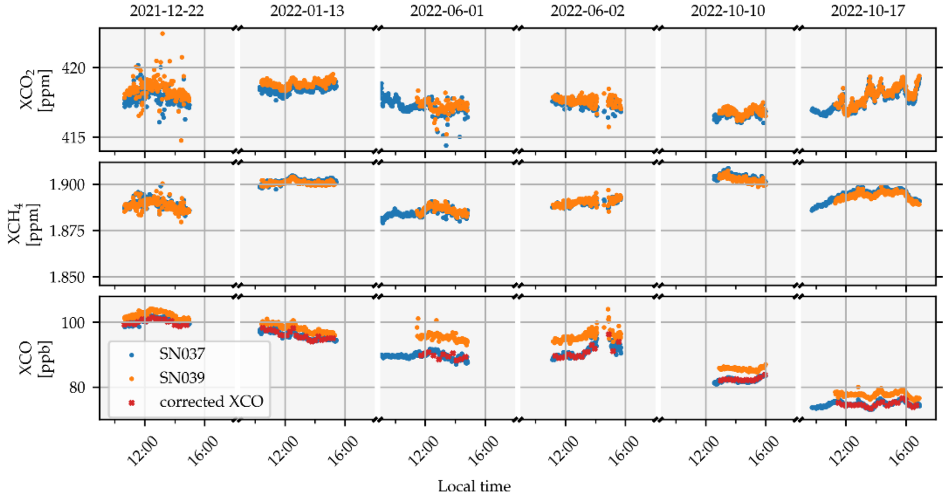

Figure 3: Results of the side-by-side measurements performed in Karlsruhe between the TS instrument (SN39) and the COCCON reference instrument (SN37).

Another tool to monitor the calibration of TS instrument is the measurement of the instrumental line shape (ILS). This is measured before each campaign. The results are shown in Figure 4.

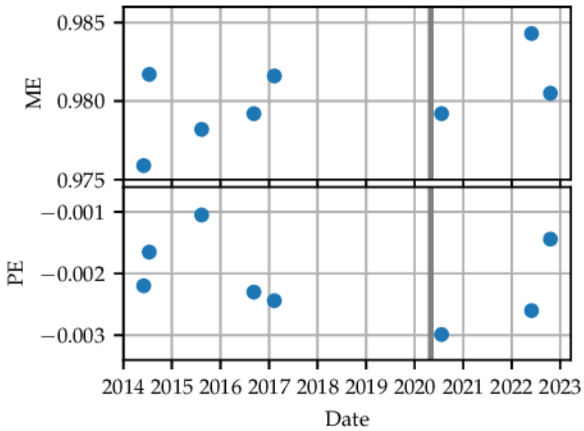

Figure 4: Modulation Efficiency (ME) and Phase Error (PE) of the TS-instrument measured using open path measurements. The ME and PE determine the ILS of an instrument.

The values before the grey line are given to provide a comparison with the historical data of the ILS measurements. They are not used for the Travel Standard campaigns.
As a measure of the stability, the mean and the standard deviation of the ME and the PE are calculated over all measurements in Figure 4. For the ME the result is 0.98008 ± 0.002555, for the PE the result is -0.00208 ± 0.00065. As a comparison, the values for ME and PE of the reference instrument SN037 as published in (Alberti, et al., 2022) are $\mathrm{ME} = 0.98361 \pm 0.00267$ and $\mathrm{PE} = 0.00145 \pm 0.00122$. These values are in the same order showing that the Travel Standard instrument operates within the normal range of an EM27/SUN.

6.2 TCCON site visits

During each visit of the TS to the TCCON site, the TCCON instrument records the standard, high-resolution TCCON interferograms (TCCON-HR) and additionally low-resolution (LR) double-sided interferograms matching the records of the EM27/SUN (TCCON-LR). TCCON and low-res interferograms are recorded in an alternating way. The HR data are the source of the official TCCON-product and hence retrieved using GGG2020. The LR data are retrieved using PROFFAST2.

The first site visited with the TS was Tsukuba, Japan. There, 8 days of measurements were collected. The data are visualized in Figure 5.

XAIR can be used as a quality check of the data: it basically compares the column of dry air derived from the spectrum with the column of dry air theoretically calculated from the ground pressure. For a perfect aligned spectrometer XAIR should be unity. Small deviations as given here are due to imperfections of any measurement performed.
The reason for XAIR having different shapes for the LR and HR data is that its calculation in GGG2020 and PROFFAST2 is implemented different (basically the it is implemented inverse, i.e. PROFFAST2 devides the retrieved dry air by the theoretical amount, while GGG2020 does it vice versa).

For XCO_2 and XCH_4 the agreement is well. For XCO the agreement varies from day to day. To exclude an error in the PROFFAST2 algorithm XCO is also retrieved by using GGG2020 to process the LR data, which shows the same variation. The difference for XCO likely is the result of an unrealistic a-priori CO profile shape reported in the TCCON mod file (which serves as a-priori profile for both the GGG2020 and the PROFFAST retrieval. The quality of the CO a-priori profile is not well represented for high polluted sites and is a known GGG2020 issue (D. Wunch, priv. comm.), (Lambert, et al., 2022) in combination with different column sensitivities of high- and low-resolution measurements. For more details see (Herkommer, et al., 2023).

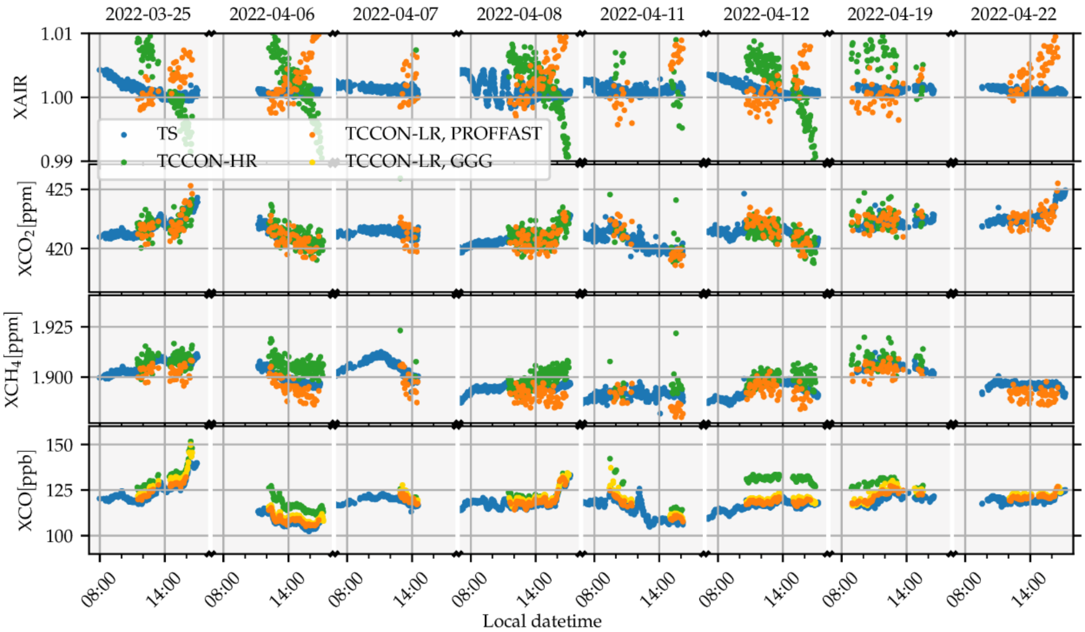

Figure 5: The XGas data measured in Tsukuba, Japan with the Travel Standard and the TCCON spectrometer. XAIR are calculated in a different way in GGG2020 and PROFFAST resulting in the different shapes of XAIR for the TCCON-HR and TCCON-LR data.

For both, the HR and the LR data, a bias correction factor to the TS data is calculated using the scheme described above. By multiplying the correction factors of the different spectrometers, it is possible to calculate a pseudo-factor which let us compare the data of a remote station to the Karlsruhe TCCON-station. This scheme is depicted in Figure 2.

Using the formula

$$\begin{aligned} \Delta_{\%}\mathrm{XGas}_{\text{TC-TK}}^{\text{TC-KA}} &= \frac{\overline{\mathrm{XGas}}_{TC-KA} - \overline{\mathrm{XGas}}_{TC-TK}}{\overline{\mathrm{XGas}}_{\text{TC-KA}}} \cdot 100 \\ &= \frac{1 - c_{\text{TC-TK}}^{\text{TC-KA}}}{c_{\text{TC-TK}}^{\text{TC-KA}}} \cdot 100\,. \end{aligned}$$

it is possible to calculate a deviation in % of a XGas value between the Tsukuba and the Karlsruhe TCCON station using the calculated pseudo-factors $c_{\text{TC-TK}}^{\text{TC-KA}}$. TC-KA and TC-TK stand for TCCON Karlsruhe and Tsukuba, respectively. The results of this evaluation for the Tsukuba data is given in Table 2. For details on the calculation of the given errors see (Herkommer, et al., 2023).

Table 2: Deviation of the Tsukuba TCCON site to the COCCON reference device in percentage

Species	$\Delta^{\mathrm{SN37}}_{\mathrm{XX\text{-}LR}}$ [%]	$\Delta^{\mathrm{SN37}}_{\mathrm{XX\text{-}HR}}$[%]
XCO2	$0.14417 \pm 0.08254 - 0.05414\%$	$0.10812 \pm 0.09331 - 0.05412\ \%$
XCH4	$0.18642 \pm 0.08277 + 0.07111\%$	$-0.24248 \pm 0.09318 + 0.07080\ \%$
XCO	$7.07261 \pm 0.40896 - 0.00748\%$	$1.19027 \pm 0.41081 - 0.00707\ \%$

As a conclusion, an excellent agreement on the 0.1% level for XCO_2 is found, very good agreement (0.2% level) is found for XCH_4. The high bias for XCO in the comparison of high-resolution with low resolution measurements very likely indicates a problem with the a-priori CO profile shape in the agglomeration area of Tokyo resulting in the large deviation for the low-res data.

7 APPLICABLE DOCUMENTS

Statement of Work: Fiducial Reference Measurements for Ground-Based IR Greenhouse Gas Observations (FRM4GHG 2.0)
Prepared by: EOP-GMQ, Reference: ESA-EOPG-EOPGMQ-SOW-21

8 REFERENCE DOCUMENTS

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Wunch, D., Toon, G., Sherlock, V., Deutscher, N., Liu, C., Feist, D., & Wennberg, P. (2015). The Total Carbon Column Observing Network's GGG2014 Data Version. doi:10.14291/TCCON.GGG2014.DOCUMENTATION.R0/1221662