ACTRIS-2 TNA Activity Report

Calibration of FTIR instruments at MAIDO-OPAR laboratories using portable EM27/SUN spectrometer, FTIR-Cal-LaReunion

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- Introduction and motivation

The MAIDO-OPAR laboratory is equipped with two ground based high-resolution Fourier Transform Infrared (FTIR) spectrometers of the type Bruker IFS 125HR. The spectrometers are operated automatically or remotely by BIRA-IASB. These spectrometers perform quasi-continuous measurements, under clear sky conditions, in the mid-infrared (MIR) and the near-infrared (NIR) spectral range covering several gaseous compounds in the atmosphere. For the MIR data the special focus is on retrieving volatile organic compounds (VOC's) and biomass burning gases whereas for the NIR data the focus is set on greenhouse gases (GHG's). The NIR measurements are part of the Total Carbon Column Observing Network (TCCON) [1], where a scaling retrieval is performed to get the accurate and precise total column concentration of the target gases. The measurement station is a provisional TCCON station due to the fact that a calibration of the data could not yet be done as the remote location is difficult to be accessed with in-situ instruments on-board research aircrafts. This project aims at calibrating the TCCON data retrieved from the IFS 125HR NIR spectra with the help of a well-calibrated lightweight, portable, low-resolution spectrometer - EM27/SUN. This spectrometer has been proven to measure GHG's in the NIR spectral range with very high accuracy and precision meeting the TCCON requirements [2].

- Scientific objectives

There are two main scientific objectives for this project:

1) Calibration of the IFS 125HR spectrometer data retrieved in the NIR spectral window using a well calibrated portable EM27/SUN spectrometer,

2) Testing of the EM27/SUN spectrometer performance under tropical conditions at La Réunion.

- Reason for choosing station/ infrastructure

The MAIDO-OPAR laboratory (21° S, 55° E) is a unique atmospheric observatory in the Indian Ocean. The TCCON station at the laboratory is one of the few (5) TCCON stations in the southern hemisphere contributing to the world-wide observing system of the atmosphere. It provides an essential validation resource for the currently orbiting satellites measuring greenhouse gases, like the NASA's Orbiting Carbon Observatory – 2 (OCO-2) and JAXA's Greenhouse gases Observing SATellite (GOSAT), as well as for the future satellite missions like the ESA's Sentinel-5 Precursor, OCO-3, GOSAT-2. The data is also used for contributing to the evaluation and understanding of the global carbon cycle. The recent development of the EM27/SUN spectrometer with very high accuracy and precision has made it a suitable candidate for this study. One such EM27/SUN spectrometer, which was calibrated with respect to the Karlsruhe TCCON spectrometer, had been borrowed from the Karlsruhe Institute of Technology

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(KIT) and transported to La Réunion for the duration of the project to perform side-by-side measurements for the purpose of calibration of the TCCON spectrometer at Ile de La Réunion.

- Method and experimental set-up

We performed an intense measurement campaign between 21 October and 5 November 2015 with local support from the group of Jean-Pierre Cammas (UMS 3365, OSU). The transport of the EM27/SUN spectrometer to and back from the Reunion Island went well. The EM27/SUN (see Figure **1** left panel) was setup manually, on all days with good weather conditions, on the terrace next to the sun tracker of the Bruker IFS 125HR. That way it had a clear view of the sun during the whole day without any obstruction and both spectrometers were looking at the same atmospheric scene measuring side-by-side. During the period of the campaign both the high resolution IFS 125HR and the portable low resolution EM27/SUN spectrometer worked well, with the latter showing some data acquisition issues on the very first day. This problem was solved after restarting the spectrometer on the next day and it did not appear again. The data of the first day is therefore not considered for this study.

Figure 1: EM27/SUN spectrometer (left) and Bruker IFS 125HR spectrometer (right), both performing side-by-side measurements.

The Bruker IFS 125HR (see Figure **1** right panel) was operated in the standard TCCON mode with high spectral resolution (0.02 cm^{-1}) for investigating the first scientific objective; it was also operated in the low resolution mode (0.5 cm^{-1}), at the same spectral resolution as the EM27/SUN, for investigating the second scientific objective. The TCCON measurements have been analyzed with the standard retrieval software GGG2014 used by the TCCON community. The column averaged dry air mole fraction for the target gas (Xgas) is calculated using a scaling retrieval with respect to a model a priori vertical profile for each day. The EM27/SUN data analysis has been performed with the standard retrieval software PROFFIT used by the COCCON and NDACC communities. A scaling retrieval is performed with respect to a modeled climatological a priori vertical profile (WACCM) for that site, to deliver the resulting Xgas, i.e., the column averaged dry air mole fraction for the target gas. In the usual retrieval procedures for the TCCON and the COCCON data, the resulting Xgas values are then scaled ('corrected') in a second step by a calibration factor corresponding to the target gas to calibrate the results with respect to the WMO standards. In TCCON, this calibration factor is identical for all sites and is obtained from comparisons between the retrieved Xgas and the comparable values obtained from in-situ vertical profile measurements onboard aircrafts overpassing easy to access TCCON sites. In COCCON, this calibration factor for each target gas is obtained for each instrument from a comparison between the Xgas value retrieved from the EM27/SUN and from a collocated standard TCCON calibrated measurement. The retrieval of the low resolution measurements from the Bruker IFS 125HR has been performed with the PROFFIT software and using WACCM a priori. A comparison of these two datasets ensures that we have the same measurement conditions (resolution, atmospheric scene), same retrieval conditions (software, a priori) such that we compare purely the two instruments.

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- Preliminary results and conclusions

The TCCON measurements are performed with automatic routines under good meteorological conditions. We had good weather conditions during the first three days. After that the sky was overcast and the frequent rain made it impossible to record data on a continuous basis. During the last week of the campaign we got some days of data. The EM27/SUN data (red points in Figure **2**) starts always a bit later than the TCCON data (black points in Figure **2**) because the automated weather controlled operational system of the TCCON starts to record spectra with the first light of the sun falling on the sun tracker in contrast to the daily manual start of the EM27/SUN. Each TCCON measurement requires about 3.5 min of acquisition time whereas each EM27/SUN measurement requires about 1 min. As a result, when both instruments are operational, there are more EM27/SUN measurements than TCCON measurements. Also under variable cloud or light overcast conditions there are more opportunities for good EM27/SUN measurements than for good TCCON measurements due to the EM27/SUN's shorter acquisition time.

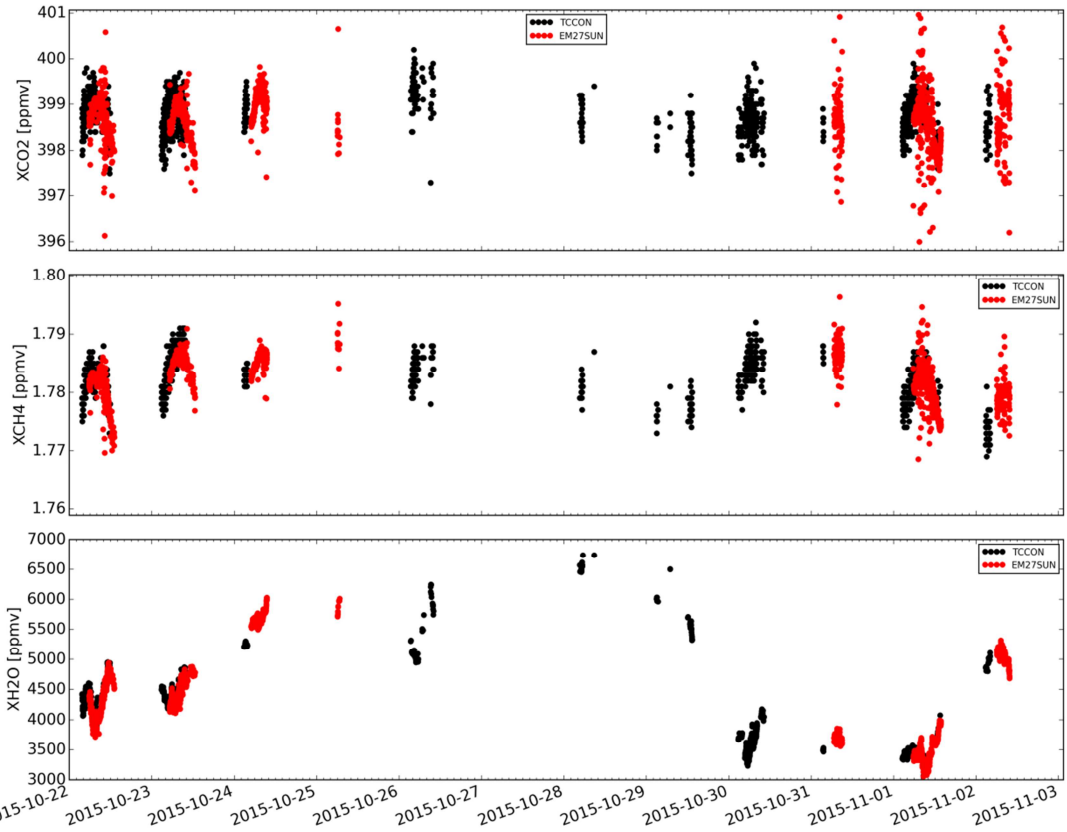

Figure 2: Time series of XCO2, XCH4 and XH2O from TCCON (black) and EM27/SUN (red) measurements at Ile de La Réunion site.

The XCO2 (upper panel), XCH4 (middle panel) and XH2O (bottom panel) time series for the TCCON spectrometer (black points) and EM27/SUN spectrometer (red points) are shown in Figure **2**. The plots show a good match of the two datasets with no significant bias. However, the EM27/SUN data shows a high scatter on cloudy days (example: 2015-10-31). This is because cloud detection criterion is not very strict. A better cloud detection algorithm based on detector DC fluctuation and the signal-to-noise ratio variation is required, which will then filter out the outliers. On 2015-10-25 few EM27/SUN data are retrieved whereas there are no TCCON data on this day. The TCCON Xgas standard calibration factors for the different gases are: CO2 – 0.9898; CH4 – 0.9765, H2O – 1.0183, respectively and used for the data in Figure **2**.. The EM27/SUN spectrometer was calibrated with respect to the TCCON spectrometer at the Karlsruhe site before and after the measurement campaign at La Réunion. The calculated calibration factors before and after the measurement campaign was stable and did not show any drift.

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The values are: CO2 – 0.9928, CH4 – 0.9937, H2O – 0.8380, respectively. These calibration factors were used to calculate the Xgas values for the EM27/SUN measurements at Ile de La Réunion.

A detailed analysis of the dataset is done taking into account the co-incident measurements between the TCCON and the EM27/SUN data sets to quantify the residual bias. The TCCON dataset was taken as reference; for each of the TCCON measurements, all co-incident EM27/SUN measurements were sorted and averaged. A new set of data pairs matching the TCCON and the corresponding averaged EM27/SUN measurement is constructed and plotted in Figure **3**.

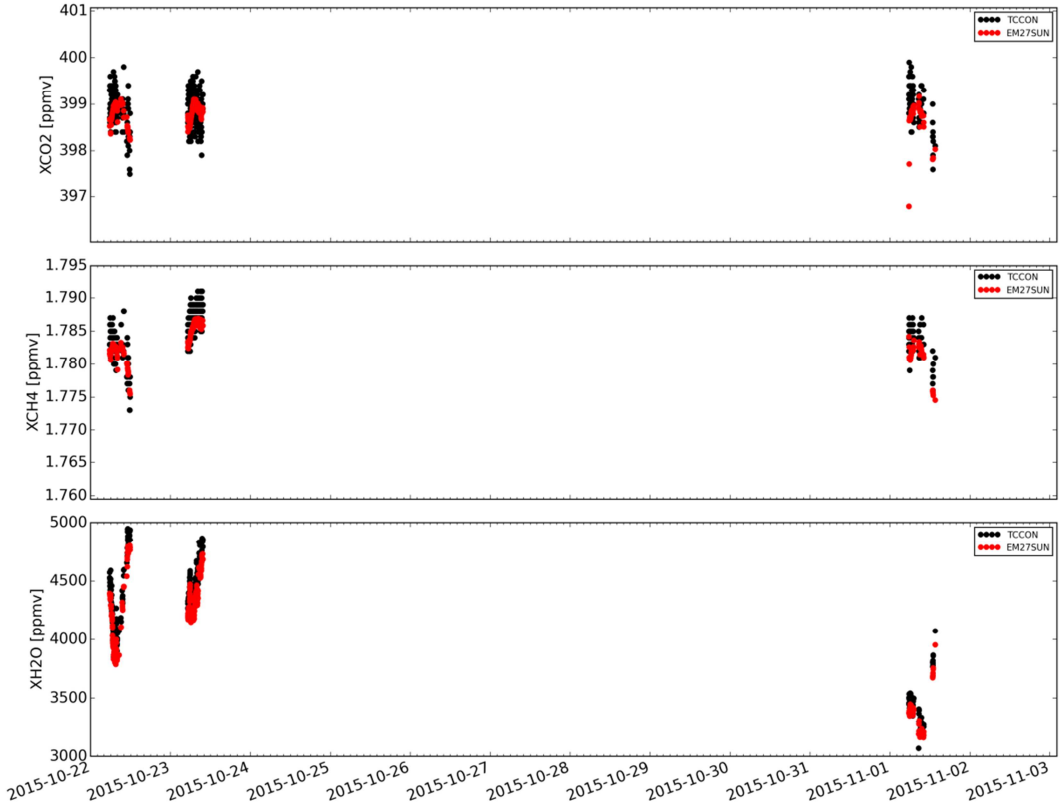

Figure 3: Time series of collocated TCCON (black) and EM27/SUN (red) measurements for XCO2, XCH4 and XH2O at the Ile de La Réunion site.

The Xgas values in Figure 3 show very good match between the TCCON and the coincident EM27SUN data set. The bias in the Xgas values between the TCCON and the EM27/SUN for the three days shown in Figure 3 are the following (mean ± standard deviation):

XCO2 = 0.053718843 ± 0.55640101 ppm, 0.056615856 ± 0.36132389 ppm, 0.3842575 ± 0.60366291 ppm.
XCH4 = 0.0010091368 ± 0.003321099 ppm, 0.0013881801 ± 0.001692988 ppm, 0.00173939 ± 0.001882578 ppm.
XCO2 = 102.45102 ± 57.655605 ppm, 91.32444 ± 52.885715 ppm, 66.207008 ± 41.547447 ppm.

The small difference in the Xgas values can be due to the instrumental effects like modulation efficiency (ME), choice of a priori. During the campaign period, the ME of the TCCON instrument was slightly over modulated by about 3.5%, this would cause the measured Xgas value to deviate from the true Xgas, which makes a good contribution to the small difference seen by the EM27SUN spectrometer. In general, the bias for the good day of measurement is much lower than the precision requirement of TCCON (0.25% for XCO2, 0.5% for XCH4 and 1.3% for XH2O). Therefore from the preliminary analysis of the data we can conclude that the TCCON standard calibration factors for the network are also applicable for the Ile de La Réunion site.

Low resolution (LR) TCCON measurements were performed on two days during the campaign. The EM27/SUN calibration factors for the respective gases have been used for the LR TCCON data. This will give a first impression of the data quality. The actual calibration factor for the resp. gas has to be calculated (or verified) for the LR TCCON measurements from a longer time series in the future. The

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time series of the collocated Xgas values for the two instruments (see Figure **4**) match well. This shows the good performance of the EM27/SUN in tropical conditions at Ile de La Réunion.

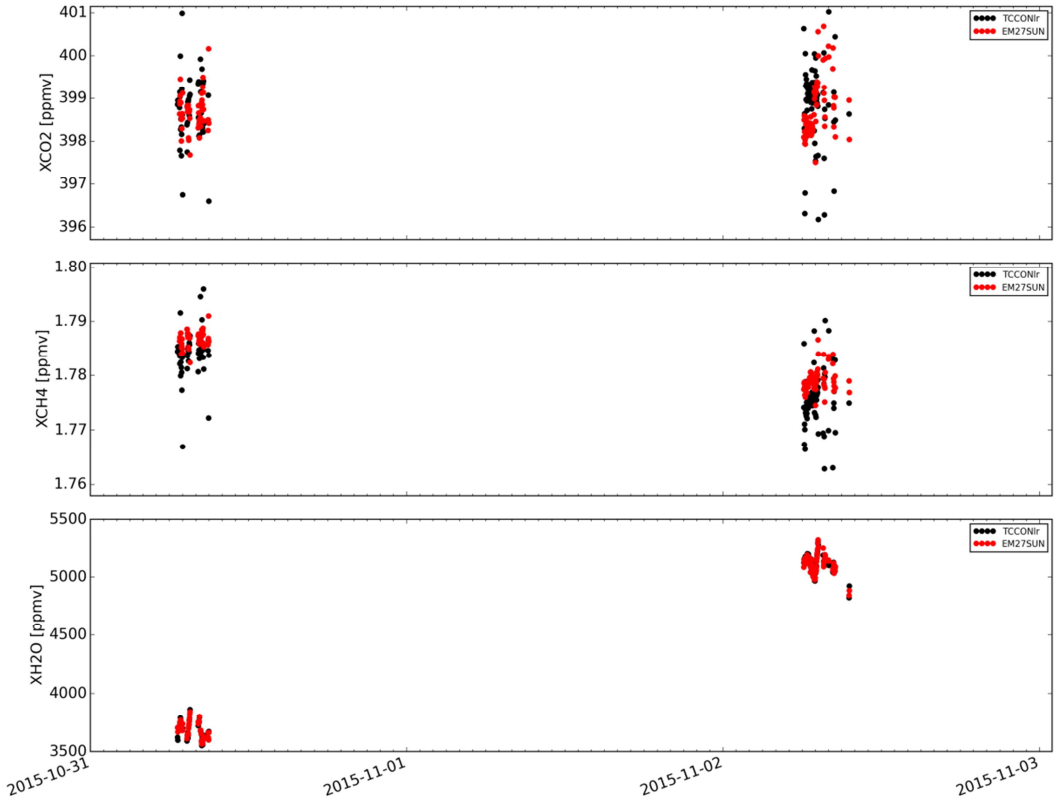

Figure 4: Time series of collocated low resolution TCCON (black) and EM27SUN (red) measurements for XCO2, XCH4 and XH2O at the Ile de La Réunion site.

- Outcome and future studies

The campaign facilitated us to obtain EM27/SUN measurements at the tropical TCCON site on the Reunion Island. These measurements from a well calibrated EM27/SUN are useful for the calibration of the Bruker IFS 125HR spectrometer in the NIR spectral window. Furthermore, we have made a direct comparison of the two spectrometers using the same resolution and retrieval conditions. The first results show comparable values for the EM27/SUN with respect to the low resolution measurements performed with the IFS 125HR. The detailed results will be published in Sha et al. 2016. A longer time series is needed to determine the stability of the calibration factors. The EM27/SUN operated very well under tropical conditions and is suitable to be used as a traveling calibration standard for the TCCON network.

- References

[1] D. Wunch, G. C. Toon, P. O. Wennberg, S. C. Wofsy, B. B. Stephens, M. L. Fischer, O. Uchino, J. B. Abshire, P. Bernath, S. C. Biraud, J.-F. L. Blavier, C. Boone, K. P. Bowman, E. V. Browell, T. Campos, B. J. Connor, B. C. Daube, N. M. Deutscher, M. Diao, J. W. Elkins, C. Gerbig, E. Gottlieb, D. W. T. Griffith, D. F. Hurst, R. Jiménez, G. Keppel-Aleks, E. A. Kort, R. Macatangay, T. Machida, H. Matsueda, F. Moore, I. Morino, S. Park, J. Robinson, C. M. Roehl, Y. Sawa, V. Sherlock, C. Sweeney, T. Tanaka, and M. A. Zondlo. Calibration of the total carbon column observing network using aircraft profile data. *Atmospheric Measurement Techniques*, 3(5):1351–1362, 2010.

[2] M. Frey, F. Hase, T. Blumenstock, J. Groß, M. Kiel, G. Mengistu Tsidu, K. Schäfer, M. K. Sha, and J. Orphal. Calibration and instrumental line shape characterization of a set of portable FTIR spectrometers for detecting greenhouse gas emissions. *Atmospheric Measurement Techniques*, 8(7):3047–3057, 2015.

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