# FRM4GHG

# Fiducial Reference Measurements for Greenhouse Gases

## Deliverable 4.3

## Recommendations for the instrument layout and settings, measurement procedures, retrieval algorithms and intercomparison protocols

**Deliverable:** 4.3

**Version:** 0

**Date:** 02/05/2018

**Lead Authors:** D.W.T.Griffith, N.B. Jones (UoW)

**Subject:** ESA-IPL-POE-LG-cl-LE-2015-1129

**Category:** ESA Express Procurement (EXPRO)

**Our ref.:** Proposal No. 1129/2015 –
Proposal from Feb 16, 2016 plus comments from May 27, 2016

# Table of contents

# 1 Document change record

| Issue | Date | Item | Comment |
|---|---|---|---|
| V0 | 2018-05-03 | – | Initial draft for review |
| V1 | 2018-05-22 | | Comments incorporated |
| V2 | 2018-05-25 | | Final comments incorporated |
| | | | |
| | | | |
| | | | |

# 2 Access list

This document is deliverable D4.3: "Recommendations for the instrument layout and settings, measurement procedures, retrieval algorithms and intercomparison protocols" created for the project FRM4GHG and will be submitted to ESA. The document will be a publicly accessible document and can be downloaded from the project webpage http://frm4ghg.aeronomie.be.

# 3 Purpose

This document reports on task T4.3: "Provide concrete recommendations for the harmonisation of the IR observation systems. This will address in particular the IR instrument layout and settings, measurement procedures, retrieval algorithms and intercomparison protocols [R-29]. While for the TCCON instrument and the EM27/SUN the instrumental layout and settings are well-established, for the other instruments recommendations will be given. »

# 4 Preamble

The original proposal « Fiducial Reference Measurements for Ground-Based IR Greenhouse Gas Observation (FRM4GHG) » envisaged a one-year campaign to compare mobile, low resolution infrared spectrometers against a TCCON-standard FTS and Aircore launches at Sodankyla, Finland though the sunlit months of 2017. Previous project reports and deliverables have described the site setup, instruments and results from the 2017 campaign. Since 2017-early 2018 the FRM4GHG project has been extended to a second year of measurements at Sodankyla in order to establish the improvements to measurements and analysis which resulted from the 2017 campaign, and to obtain a full year of further measurements in which instrument changes are minimised and from which relatively « clean » time series of measurements can be compared. This deliverable therefore is based on the campaign results from 2017 reported in D4.2 « System intercomparison and characterisation" and provides recommendations for improvements to be implemented for each instrument and analysis in the 2018 campaign.

# 5 Recommendations by instrument

The results reported in D4.2 and D3.2 show biases between individual instruments and the TCCON reference standard of the order of a few ppm for $X_{CO2}$, up to 20 ppb for $X_{CH4}$ and 1% for $X_{air}$. In addition all instruments show solar zenith angle dependence to some degree, sometimes small but greater than the measurement repeatability. In the following sections we provide a summary of the status of each instrument and recommendations for implementation in 2018.

## 5.1 TCCON standard

Sodankyla is a fully qualified station in the TCCON and its operation and data analysis follow standard TCCON precedures. The Sodankyla TCCON instrument and results act as the reference standard for all other test instruments in this study.

During 2017 a small non-linearity in the extended-range InGaAs detector response was identified of the TCCON instrument which leads to small biases in retrieved $X_{gas}$ values, for example < 0.5 ppm for $X_{CO2}$.

Recommendation:

- TCCON high resolution measurements should continue following standard TCCON operational procedures.
- In 2018 detector non linearity and its correction should be further investigated and corrected. However this effect does not have any impact on the routine measurement protocol for this instrument.

## 5.2 TCCON low resolution

The low spectral resolution of the FTIR test instruments potentially leads to biases due to effects such as different responses to a priori vertical profiles, atmospheric structure, interfering gases and through these effects, to different averaging kernels. To identify biases which may be due purely to the low resolution, measurements were also made by the TCCON FTS alternately with high resolution and the same low resolution, 0.5 $cm^{-1}$, as the low resolution instruments. The TCCON-LR data can be treated as an additional pseudo-instrument for the purposes of this study.

Recommendation:

- TCCON low resolution measurements should be continued in 2018. They provide useful analysis of resolution-only effects on retreived trace gas columns which can be compared with other instrument effects.

## 5.3 EM27/SUN

The Bruker EM27-sun is a mobile, integrated solar tracker and interferometer with parallel extended-range and narrow-range InGaAs detectors. It is the most-developed instrument in the comparison, having had several years of assessment, calibration and field studies (Frey et al., Building the COllaborative Carbon Column Observing Network (COCCON): Long term stability and ensemble performance of the EM27/SUN Fourier Transform spectrometer, submitted to AMTD May 2018). The EM27/SUN operated without configurational changes in 2017. Spectral analysis and retrieval methods are well established and were routinely applied using the retrieval software system PROFFIT from KIT.

One limitation of the EM27-sun is the current lack of weather protection, requiring the spectrometer to be covered and housed at night and manually set up by local staff or students on each measurement day. This requirement restricts the times for collection of spectra, often to the extent that data are collected only on "good" continuously clear days during working hours when local personnel are available. An automated weatherproof cover system that allows the EM27 to reside outside and not require manual actions is under development but was not ready for installation in 2017.

Recommendations:

- EM27 should continue as in 2017 as the most stable and consistent measurement set.
- The automated weather proof cover system should be installed and implemented as soon as practicable. This should significantly increase the temporal coverage of measurements.

## 5.4 IR-cube

The IRcube is based on a smaller version of the Bruker EM27 pendulum (“Rock-Solid”) inteferometer with 25mm rather than 50mm optics and consequently lower throughput. It uses a single extended range InGaAs detector. The IRcube system differs principally from the EM27 (and Vertex, below) in having a simple 400mm focal length Newtonian refractor telescope mounted on an external Eko tracker fibre-optic-coupled to the interferometer. The tracker is fully automated and located on the FRM4GHG container roof, while the IRcube and fibre-collimation optics are located inside and do not require weather protection. The IRcube collects data automatically whenever direct solar radiation is above a threshold (around 20% of a clear sky midday value). In 2017 there was an extended no-data period (March-May) due to a broken optic fibre soon after installation in March 2017. From May 2017 there were minimal changes in measurement configuration. A possible dependence of $X_{gas}$ values on solar intensity/detector signal level was identified, presumably due to the use of the extended range InGaAs detector which is known to have significant non-linearity characeristics. The instrument lineshape (ILS) of the IRcube is also less well defined than those of the larger instruments due to its compact short focal-length optics, and the impact of this ILS on $X_{gas}$ biases needs further attention.

Recommendations:

- Continue automated measurements as in 2017, with reduced throughput to avoid or at least minimise intensity-dependent bias
- Investigate the impact of ILS on retrieved total column amounts and $X_{gas}$ retreivals
- Investigate the potential impact, if any, of optical fringing effects in the fibre on the spectra and retrievals

## 5.5 Vertex70

The Bruker Vertex70 is a laboratory bench FTIR analyser located inside the container which accepts a parallel beam from the BIRA-designed and constructed tracker on the container roof through a port with $CaF_2$ window. It is built on the same pendulum interferometer design as the EM27. Data collection is fully automated and the system is routinely managed from BIRA in Belgium. In 2017 the FTS was equipped with an extended range InGaAs detector which led to identifiable non-linearity/saturation effects. Additional aperture stops were required to avoid or minimise saturation and improve the ILS, but a final optimised configuration has not yet been established.

Recommendations:

- Continue automated measurements as in 2017.
- Further assess the impact of detector non-linearity on retrieved trace gas columns.
- Investigate and implement the use and optimisation of a narrow band InGaAs detector to avoid detector saturation/non-linearity effects, trading off against measurement signal:noise ratio.

## 5.6 Laser Heterodyne Radiometer (LHR)

The RAL LHR was a new instrument under development in 2017 and not as mature as the other test instruments. The instrument operates in the thermal infrared and is based on a high resolution tunable laser-solar heterodyne which is tuned across individual spectra lines in the atmospheric transmission spectrum. The LHR thus does not have the broadband, multi-species characteristic of the FTS systems, but is small, compact and portable, and does not require a large solar beam. The 2017 instrument measured only $CO_2$, but not $CH_4$, CO or $O_2$. In the FRM4GHG project it utilised a 10 mm diameter solar beam pickedoff from the BIRA tracker before the Vertex. It showed larger scatter and larger biases than the FTS-based instruments and is being further refined and developed at RAL prior to the 2018 campaign. Following the 2017 campaign the instrument has been returned to RAL for a range of technical improvements and the addition of a $CH_4$ channel.

The LHR spectra are processed to produce vertical distribution of $CO_2$ and water vapour, which are then used to calculate the total columns. The retrieval approach is based on the well establish optimal estimation method minimizing the weighted difference between the measurement and a synthetic measurement calculated from a forward model, given an a-priori atmospheric state. The forward model used is based on the Reference Forward Model (RFM), a line by line radiative transfer code developed for the operational processing of MIPAS data and well suited for thermal infared modelling.

In summary, the current LHR data are not yet able to provide meaningful geophysical information but have proven invaluable to characterize and understand the LHR instrument during its first ever joint measurement campaign.

Recommendations:

- Make technical improvements to the LHR instrument and retrieval software to address the limiting issues of noise, diurnal variability and overall bias relative to the FTS-based instruments.
- Re-install and operate the $CO_2$ LHR with technical improvements.
- Expand the measurements to include a $CH_4$ channel.

# 6 Other recommendations

## 6.1 Aircore

Aircore in situ vertical profile measurements provide the essential link between remotely-sensed total column amounts of trace gases and the SI-traceable WMO calibration scales anchoring all global in situ measurements. The Aircore profiles cover from the surface to typically 30 km. They also provide measured a priori vertical profile shapes which can be used to improve retrievals from GFIT and PROFFIT and for diagnosing differences found between data derived from TCCON and the low-resolution spectrometers. Aircore profiles can also be used in the future for direct verification of mole fraction profiles derived from the LHR. Aircore remains an important core activity of the FRM4GHG project.

Recommendation:

- AirCore measurements at Sodankyla to be continued as often as is practical and affordable on clear sky days when all instruments are measuring in the best conditions.
- AirCore measurements at Sodankyla to be evenly distributed among different months of the year to capture the range of the variability of the vertical profiles, preferably a couple of profiles in the Spring.

## 6.2 Retrieval algorithms

Two well established independent retrieval software codes have been used in the analysis of different instrument data to retrieve total column trace gas amounts from spectra - GFIT and PROFFIT – as well as a new code developed at RAL. GFIT, developed at the Jet Propulsion Lab and Caltech, is the standard software used in the TCCON and in this project for retrievals from the IRcube and Vertex. PROFFIT, developed at KIT, is the standard software used for the EM27/SUN in the COCCON and here; PROFFIT has also been used to process the low resolution TCCON-LR spectra. GFIT and PROFFIT differ in the details of the spectrum fitting procedures and in the post processing, accounting for effects such as airmass dependent and independent bias corrections and indirect calibration to WMO in situ scales. There is clearly potential for bias due to the different analysis methods, even when applied to the same instrument dataset.

Recommendations:

- At least a subset, and preferably all, data should be processed with both GFIT and PROFITT to investigate and quantify analysis code dependent biases.
- The RAL retrieval system should be compared with GFIT and PROFITT to establish potential biases to LHR measurements.

## 6.3 Airmass/solar zenith angle dependences

All instrument/retrieval code combinations display airmass or zenith angle dependent biases to varying degrees, for example of the order of 0.5-3 ppm for XCO2. These manifest as both apparent diurnal and seasonal variability which is an artefact of the measurement-analysis system. This dependence is due to insufficiently accurate knowledge of spectral line parameters, spectral lineshapes, instrument lineshapes and the atmospheric state – as absorption depths increase at higher airmasses, errors in these quantities affect the retrieval in systematically different ways. This is a long-standing and ongoing issue in TCCON and relevant to FRM4GHG, but its complete resolution is beyond the scope of the FRM4GHG project.

Recommendation:

- Solar zenith angle or airmass depndences for each instrument/analysis code combination should be characterised so that empirical correction factors with quantified uncertainties can be applied to the retrievals to minimise the uncertainty in the final total column and $X_{gas}$ products.
- The unambiguous characterisation of each instrument's ILS through independent measurements of a cell or atmospheric water vapour should be continued.

## 6.4 Interferogram to spectrum conversion

Prior to retrieval of trace gas column amounts from spectra, spectra must be calculated by Fourier transformation of the measured interferograms. Variations in solar intensity during the scanning of an FTS modulate the amplitude of the interference in the interferogram and potentially affect the instrument lineshape. This can be corrected by measuring the interferograms in DC mode, thus including both the solar intensity (the DC level of the interferogram) and the interferogram itself (the AC interferogram). The DC component is then used to correct the amplitude of the modulation of the AC interferogram. This is important to correct two sources of intensity variation (1) measurements when the received solar intensity is modulated by atmospheric transmission via clouds and aerosols, and (2) in the pendulum corner-cube interferometers used in the EM27, IRcube and Vertex instruments, vignetting affects the throughput and DC level of the interferometer as a function of optical path difference. Conversion to spectra from interferograms is carried out by software codes developed in TCCON at both JPL and KIT for this purpose. It is important NOT to use Bruker's FT conversion software on DC interferograms because of the way the DC interferogram is padded out to the next $2^N$ number of points for Fourier transformation (equivalent to zero-filling for AC interferograms) - it may introduce a step in the DC interferogram which leads to artefact rippling in the spectra. In standard TCCON processsing this artefact is only apparent when solar intensity is variable, but it is always present in the spectra from the low resolution pendulum interferometer instruments.

Recommendations:

- All interferograms should be recorded as DC interferograms and converted to spectra using TCCON I2S or equivalent code and input parameters.

# 7 Applicable documents

Statement of Work: Fiducial Reference Measurements for Ground-Based FTIR Greenhouse Gas Observations (FRM4GHG)
Prepared by: T. Fehr/B. Bojkov (EOP-GMQ), Reference: ESA-EOPG-MOM-SOW-0007

# 8 Reference documents

FRM4GHG deliverable D4.2 : System intercomparison and characterisation document available via the project website **http://frm4ghg.aeronomie.be/index.php/outreach/deliverables**