FRM4GHG

Fiducial Reference Measurements for Greenhouse Gases

Deliverable D2 Phase 2

Technical note: Measurements and Retrieval evolution

Deliverable:	**2**
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1 Document change record

Issue	Date	Item	Comment
V0	2018-09-04	–	Initial version
V1	2018-09-05		
V2	2018-09-26		Comments added from MDM, DW, FH
V3	2018-10-24		Comments added from JN
V4	2019-03-27		Section 6 added on uncertainties
V5	2019-05-01		Added comments from DG on Allan Variance
V6	2019-05-09		Corrections/comments based on feedback from PC
V7	2019-05-14		Corrections/comments based on feedback from MS

2 Access list

This document is a deliverable “D2: Technical note: Measurements and Retrieval evolution" first version” created for the project FRM4GHG, and to 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 presents the deliverable for the Measurements and Retrieval evolution. The deliverable notes any additions/changes to individual participating instruments.

The deliverable addresses WP Data Measurements and Retrieval evolution Tasks T2.1: Automate, where possible, the instruments. Install automatic LN2 filling system for the Vertex7 0 instrument, and T2.2: Include measurements of H2C0 and if possible N20. If possible, use the same spectral regions as S5P/TROPOMI.

4 Document structure

Section 5: Describes action on Tasks T2.1 and T2.2

5 Technical note: Measurements and Retrieval evolution

The instruments and their respective retrieval methods are described in deliverable D2.3 from Phase 1

This technical note addresses two tasks identified for this deliverable, that is:

Tasks:

T2.1: Automate, where possible, the instruments. Install automatic LN2 filling system for the Vertex7 0 instrument, modify the InSb-detector for measurements of HCHO[R-8]

T2.1.1 EM27-SUN: As the extension phase is mainly intended to extend the observational period covered by phase 1 and for characterisation of the long-term stability of the device, instrumental changes should only be made if shortcomings or technical problems significantly hampering performance or reliability of measurements have been identified. As no issues with the EM27/SUN spectrometer were detected during phase 1, no instrumental modifications were done.

For demonstrating remotely controlled observations with the EM27/SUN, the operation in an enclosure provided by the Technical University of Munich (TUM) was foreseen for phase 2. Due to fabrication delay at TUM and time required for pretesting in Karlsruhe, the shelter was put into service only in September. First remote observation tests were performed successfully.

T2.1.2 Cube: the cube spectrometer is fully automated. There is an ongoing issue with the choice of the aperture (1.0mm) for the April-June measurement period. This aperture was chosen, instead of the 0.5mm aperture used in 2017, to address an identified issue with small potential non-linear effects. The 0.5 mm aperture produces an image of the sun that under-fills the detector. The large aperture would match the detector size (1mm^2). However the 1mm aperture produces instrument lineshape distortion, which is beyond the ability of the chosen software package, GFIT, to model in its current configuration. Work is progressing on using either or both Proffit-fast and SFIT4. Depending on the success of the required ILS modelling, either or both of these alternate analysis tools will be adopted.

T2.1.3 Vertex: The automatic LN filling system was tested at BIRA and then sent to Sodankyla. It has been installed and it works successfully. The InSb detector to be used with the LN-system was originally equipped with a cut off filter, installed inside the dewar, so the filter sits in an environment at the LN temperature. The filter has a cut-off at 3500 cm^{-1}, to be optimal for CO measurements. Since we decided to also measure CH_2O during phase 2, the detector was sent to Bremen, the detector was opened, the filter was dismounted, evacuated and sent back to Sodankyla. The InSb-detector will run with filters mounted on the filter wheel. Since no appropriate filter for that spectral region was available in Sodankyla, a filter covering the region around 2700 cm^{-1}, was sent to Sodankyla. It will arrive soon and will then be mounted on the filter wheel.

T2.1.4 LHR.

Instrument upgrade.

The LHR has been upgraded between phase 1 and phase 2 to include the incorporation of a second laser channel for CH_4 detection as well as corrective measures based on the experience learned from phase 1. The system has been further automated to be able to operate without local support in Sodankyla. The instrumental modifications have been fully described in the phase 2 D1[].

Compared to the instrument used in phase 1, the following additional data streams are recorded in the upgraded version:

- Quadrature signal from CO2 spectrum
- In phase and quadrature signals from CH4 spectrum
- Frequency of the chopper providing the amplitude modulation
- All the ancillary data associated to the CH4 laser operation (current, temperature, humidity)
- Laser optical switch status indicator
- Background shutter status indicator

All other instrumental parameters are identical to those described in the deliverable D2.3 of phase 1.

Figure RAL1 shows spectral data of the new CH_4 channel as well as the existing CO_2 channel to indicate wavelength coverage. The spectral window chosen (~1233.5 cm-1) for CH_4 also includes weak absorption lines of N_2O.

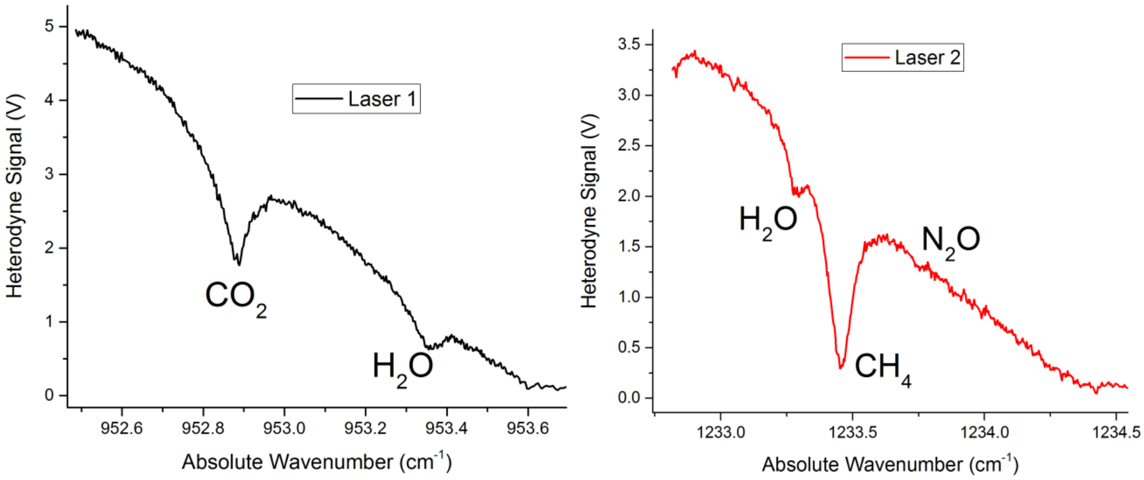

Figure RAL1. Raw spectral trace of the upgraded LHR configured for CO_2 (left) and for CH_4 (right) measurement.

Data processing.

Despite additional data streams required by the instrumental upgrade, the overall format and naming system is identical to that described in D2.4 of phase 1, but with additional new data appended. The overall goal in the development of an upgraded processor was to inherit as much as possible from the phase 1.

The existing L0 to L1 processor has been upgraded to include the new data and modified so that the L1 to L2 would not require modification. Figure RAL2 shows a flow chart of the new processors, from L0 to L2. The functions added or modified from phase 1 are highlighted in red. The most significant changes have been:

- Inclusion of a phase optimization routine. This routine determines the optimum phase for measurement of the in-phase signal, hence mitigating biases induced by phase drifts. The right-hand panel of Figure RAL2 shows the effects of optimising the phase angle to eliminate spectral information leaking into the quadrature (Y) channel.
- Inclusion of a background correction routine. Within the stability time of the instrument (determine by Allan variance analysis), a background measurement is periodically measured by obstructing the instrument input optical port. This spectral background signal is fitted to a polynomial, subsequently used to correct measured spectra.
- Inclusion of a “separation routine”, which split the L0 data into two separate L1 data sets, one related to CO2 and the other to CH4. Separated Level 1 NetCDF files are produced for each channel with the labels “CH4” or “CO2” appended to the file name. From this point on, the L2 retrieval process remain identical and L2 outputs are packaged as described previously (phase 1 D2.4) for each species.

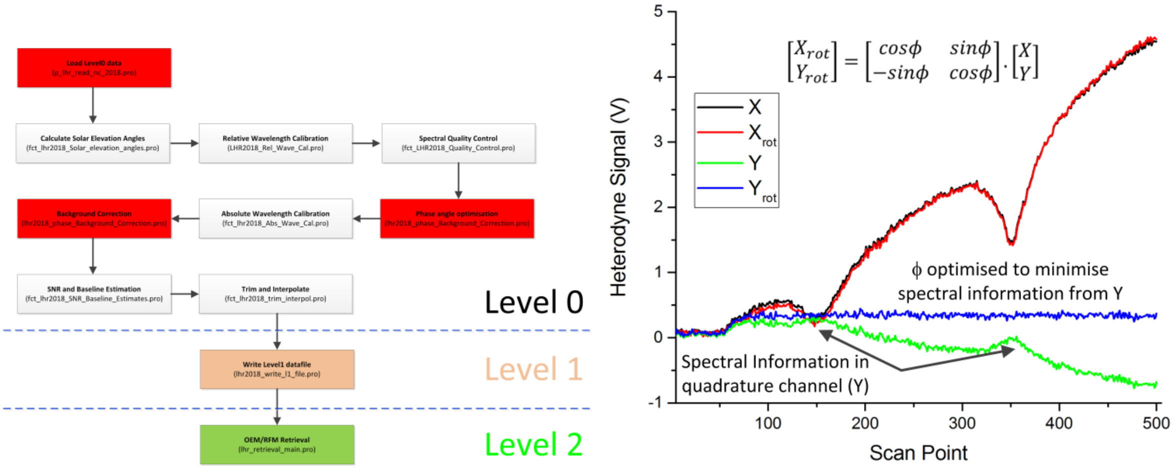

Figure RAL2. Left, schematic flow chart of the updated processor for the LHR. Red boxes indicate entirely new steps in the processing chain. Right, example of the optimisation of the phase angle in the phase sensitive detection process.

T2.2: Include measurements of HCHO and if possible N_2O. If possible, use the same spectral regions as S5P/TROPOMI [R-9, R- 10, R-11]

The addition of HCHO and N_2O products is relatively straightforward for high resolution spectrometers as part of the processing chain for either TCCON and NDACC (N_2O) or NDACC (HCHO). Other than the TCCON instrument, the Vertex spectrometer is the only low resolution instrument that has the ability to measure out to 3 microns. In the paper by Vigouroux et al (2018), it has been demonstrated that HCHO can be successfully retrieved at a resolution of 0.075 cm-1, but with larger uncertainties than the results with typical resolutions used within the NDACC for this molecule (0.006 to 0.02 cm-1). The feasibility of quantifying HCHO with spectra at 0.15 cm-1 has yet to be verified, but this is one of the purposes for phase 2 of the measurements at Sodankyla.

6 Uncertainty Estimation

This section addresses task “Tl .2: Give a detailed estimation of the uncertainty budget for each instrument [R-3, R-4]” from Work Package 1.

Here an outline of the work will be summarised on uncertainty estimation that is in preparation in Mahesh [2019,in preparation].

The basis to compare the low resolution precision will be based on the TCCON target repeatability as reported from Wunch et al xCO2 table 1, along with the 1 standard deviation statistics from table 3 of Mahesh et al 2019.

Molecule	Precision (Wunch, 2011)	Accuracy (Wunch, 2014)	WMO
CO2	~0.8 ppm	~1 ppm	0.1 ppm
CH4	~5 ppb	~9 ppb	2 ppb
CO	~0.5 ppb	~3 ppb	2 ppb

Figure 6-1 The precision and accuracy as reported by Wunch, (2011, 2014) for TCCON.

6.1 Method of precision estimation

The method used to estimate the precision of measurements that are presented in table 1 below is outlined in deliverable D3.1 phase 1 section 6, and also in the draft paper by Mahesh et al, FRM4GHG intercomparison campaign at Sodankylä TCCON site, paper in preparation, 2019.

The precision estimate used is a statistical one. Briefly, all data from the instruments were binned and averaged in 5 minute intervals. This was necessary due to the different acquisition times of each instrument. The timestamp of the reference dataset (TCCON) was matched with the timestamp of the respective low resolution instrument. From these resampled data, statistics of averages (bias), standard deviations, and correlation coefficients were computed.

Table 6.1: Table 6, page 2, from Mahesh et al: **FRM4GHG_intercomparison_results_all_20190510.pptx.**

Species	XCO_2 / ppm	XCH_4 / ppm	XCO / ppb	XAir
Bias (mean ± standard deviation) and correlation coefficient (r) Measurement period: Full year in 2017				
LHR	-18.891±5.342 (0.4990)	-	-	-
VERTEX70	1.464±1.633 (0.9836)	0.023±0.013 (0.5131)	3.572±2.568 (0.9469)	0.009±0.009 (0.0772)
IRCUBE	-5.023±1.040 (0.9714)	-0.008±0.004 (0.9321)	-	-0.015±0.002 (0.5564)
EM27/SUN	-0.727±0.474 (0.9957)	0.000±0.004 (0.9725)	4.384±1.361 (0.9926)	0.020±0.002 (0.2205)
HR125LR	-1.207±0.662 (0.9905)	-0.008±0.004 (0.9702)	-0.124±1.021 (0.9962)	0.029±0.002 (-0.2601)
Measurement period: 06 July 2017 – 12 September 2017				
LHR	-19.019±4.437 (0.4616)	-	-	-
VERTEX70	-0.160±0.574 (0.9328)	0.010±0.002 (0.9576)	1.335±1.035 (0.9905)	0.000±0.002 (0.4543)
IRCUBE	-5.034±0.809 (0.9007)	-0.010±0.004 (0.9282)	-	-0.017±0.002 (0.7393)
EM27/SUN	-0.382±0.389 (0.9731)	-0.002±0.002 (0.9742)	3.981±1.178 (0.9879)	0.021±0.002 (-0.1643)
HR125LR	-0.785±0.555 (0.9412)	-0.009±0.002 (0.9695)	-0.639±0.997 (0.9925)	0.028±0.002 (-0.0110)
Measurement period: Full year in 2018				
LHR	-28.616±16.752 (0.1816)	0.015±0.039 (0.2335)	-	-
VERTEX70	-1.201±0.838 (0.9710)	0.009±0.004 (0.9503)	0.633±0.762 (0.9947)	0.005±0.003 (0.0821)
IRCUBE	-6.064±1.142 (0.8275)	-0.002±0.005 (0.9042)	-	-0.010±0.004 (0.4134)
EM27/SUN	-0.580±0.489 (0.9918)	-0.001±0.004 (0.9389)	5.092±1.234 (0.9963)	0.021±0.002 (0.2452)
HR125LR	-0.287±0.607 (0.9863)	-0.009±0.004 (0.9592)	-0.350±1.231 (0.9961)	0.030±0.002 (-0.1755)

Table 6-1 is a statistical estimate of the precision and accuracy (with respect to the collocated HR125) of each instrument. The values from the measurement period after 6-July 2017 will be used in the following discussion of accuracy and precision (unless stated otherwise) after the significant improvement to the Vertex.

Accuracy (bias): the TCCON targets are xCO2 (1ppm), xCH4 (9ppb), and xCO (3 ppb). The EM27/Sun performs to this level of bias for xCO2 and xCH4 and is slightly high for xCO. It is noted that the EM27/SUN has been scaled to TCCON previously in Karlsruhe, while this process has yet to be done for the other participating instruments which is the goal of this campaign. Therefore the following observations are made for the IRCube, Vertex, and HR125LR with this caveat. The IRCube (5ppm) is high with respect to the target TCCON xCO2 bias. In the case of the IRCube, its compact optical configuration and single sided interferograms result in a less than perfect ILS (ME of 0.97 from lab measurements) which accounts for most of the xCO2 bias. It is not clear why the IRCube does not have quite the same issue with xCH4. The IRCube is higher at 10ppb than the TCCON xCH4 value of 9ppv, but it is noted that for the full 2017 year the IRCube meets this target at 8ppb, and easily meets this in 2018 at 2ppb. The assumption is that the IRCube, analysed by GFIT, is more sensitive to averaging kernel and apriori differences than the EM27/Sun and HR12LR using PROFFAST, while the Vertex's higher resolution removes this sensitivity. There is also the assumption in GFIT, that the airmass dependent and independent correction factors (0.0263 and 0.989 respectively for xCO2) is the same for both high and low resolution instruments, which is most likely not the case. The Vertex meets TCCON accuracy for xCO2 and xCO, but is high for xCH4. The HR125LR meets the criteria for all gases for the dataset post 6 July 2017. The pre July 2017 data for the HR125LR was affected by non-linearity of the measured spectrum.

Precision: The 1-σ error will be used as the estimate of the respective instrument precision error. With respect to figure 6-1 that reports the precision of TCCON for xCO2 (0.8ppm), and xCH4 (5ppb), the Vertex ([0.6,0.8]ppm xCO2, [4,4] ppb xCH4), EM27/Sun ([0.4,0.5]ppm xCO2, [2,4] ppb xCH4), and IRCube ([0.8,1]ppm xCO2, [4,5]ppb xCH4) are all near equal to or less than these target values. The values in the square brackets represent post 6-July 2017 and 2018 respectively. The IRCube has precision marginally higher in 2018 that reflects an issue with the choice of aperture. This produced noisier spectra so the original of this reduction in precision is understood. The TCCON precision for xCO (0.5ppm) is not currently reached by any of the instruments. Note that the IRCube precision is apparently worse in general than the other instruments, but the reported precision for the IRCube does not combine the forward and reverse scans so potentially the precision values are a factor of 0.7 less which brings it in line with the Vertex and EM27/SUN.

6.2 The Allan Variance

In FRM4GHG – D4.2 phase 1, section 6.3, the measurement precision was computed using Allan Variance from a single clear day measurement. In this section an interpretation of this estimation of error will be given.

If only random noise, η, is present in the measurement, the Allan Variance ($\eta/(t)^{0.5} + \alpha t$, where t is the time and α the drift), decreases as $t^{0.5}$. The drift, α, (airmass dependence for example), at some point will dominate the random error.

Considering figure 15 from D4.2 phase1, one can make the following observations:

1) TCCON-LR, EM27, and the IRCube have low η
2) The EM27 has lower α (drift), than both the IRCube and the Vertex, so that the EM27 noise can be further improved with averaging for longer periods
3) The Vertex has relatively both higher η and α, than the EM27, probably as a result of the small aperture introduced to help reduce non-linear effects of the detector.
4) The IRCube is currently operating as its best η given its larger α. Improvements in its airmass dependence, if this is the dominating drift factor, will mean potentially longer averaging times and improvement in its random noise.

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

CCN1 Statement of Work: Extension of Fiducial Reference Measurements for Ground-Based IR Greenhouse Gas Observation.
Prepared by: EOP-GMQ, Reference: ESA-EOPG-MOM-SOW-0005

8 Reference documents

FRM4GHG deliverable D1 Phase 2 Campaign site and instrument definition

FRM4GHG deliverable D2.3 Phase 1: Description of measurement strategy to ensure comparable observations
FRM4GHG deliverable D3.1 Phase 1: Preliminary datasets & results distributed among partners via project Web portal (Semi-blind intercomparison)

FRM4GHG deliverable D4.2 Phase 1 : System intercomparison and characterisation document, made available via the project website **http://frm4ghg.aeronomie.be/index.php/outreach/deliverables**

Mahesh et al., FRM4GHG intercomparison campaign at Sodankylä TCCON site, manuscript in preparation, 2019

Vigouroux, C., et al. (2018). "NDACC harmonized formaldehyde time series from 21 FTIR stations covering a wide range of column abundances." Atmos. Meas. Tech. **11**(9): 5049-5073.

Wunch, D the TCCON Science Team, The Total Carbon Column Observing Network, Noble Lecture, University of Toronto, March 21, 2011

Wunch, D, GC Toon, V Sherlock, NM Deutscher, C Liu, DG Feist, and PO Wennberg. 2015. "The Total Carbon Column Observing Network's GGG2014." Data Version 43, doi:10.14291/tccon.ggg2014.documentation.R0/1221662.