FRM4GHG
Fiducial Reference Measurements for Greenhouse Gases

Description of measurement strategy to ensure comparable observations

Deliverable: **2.3**

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

Our ref.: **Proposal No. 1129/2015 –**

Proposal from February 16, 2016 plus comments from May 27, 2016

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1. Document change record

Issue	Date	Item	Comment
V0.0	2017-01-19	–	Initial version
V0.1	2017-08-14	–	Final version, included comments from ESA

2. Access list

This document is a deliverable "D2.3: Description of measurement strategy to ensure comparable observations" 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

The following report describes in details the measurement strategy which will be followed during the FRM4GHG campaign in Sodankylä, Finland. This will help us to ensure that we make comparable observations with the participating instruments.

4. Document structure

Section 5 Participating instruments – Presents a list of instruments and the corresponding responsible institutes which are taking part in the project.
Section 6 Instrument characterization – Describes the instrument characterization procedure to be followed by each instrument.
Section 7 Measurement setup – Describes the campaign measurement procedure to be followed by each instrument.
Section 8 Signal-to-noise determination – Describes the signal-to-noise requirements and optimization procedure.
Section 9 Detector linearity test – Describes the requirements to make a detector linearity test and report the results.
Section 10 & 11 Applicable and reference documents – Presents a list of all applicable and reference documents related to this deliverable.
Section 12 References for software/tool mentioned – Presents a list of all software/tool mentioned in this document.

5. Participating instruments

The comparison campaign will be executed with the participation of five different spectrometers and an AirCore system. The instruments and the associated groups which are taking part in the campaign are listed in Table 1.

Table 1: List of participating institutes and instruments in the FRM4GHG campaign

Instrument	**Institute**
Bruker IFS 125HR	Finnish Meteorological Institute (FMI)
Bruker Vertex70	University of Bremen (IUP) Royal Belgian Institute for Space Aeronomy (BIRA-IASB)
Bruker EM27/SUN	Karlsruhe Institute of Technology (KIT)
Bruker IR cube	University of Wollongong (UOW)
Laser Heterodyne Radiometer	Rutherford Appleton Laboratory (RAL)
AirCore system	University of Groningen (RUG)

6. Instrument characterization

All teams operating remote sensing devices will be asked to perform full functionality test of their respective instruments and accessories before shipping them to the campaign site in Sodankylä. During this functionality test it is recommended to do quality checks of the different components and perform instrumental line shape (ILS) measurements. These measurements will be used as a reference to check the effect (if any) of transportation on the instrumental properties and to ensure nominal operation in case of new setups. The ILS of our reference spectrometer the Bruker IFS 125HR should also be measured before the campaign. Although the ILS of the heterodyne radiometer can be predicted mathematically, cell target measurement will be made to detect any instrumental drifts. If the measured cell column is found to be equal to the actual cell column then it will confirm that the instrument suffered from no drift.

The same procedure should be applied regularly once the instruments are at the campaign site in Sodankylä. This will ensure that we start the campaign with quality controlled instruments. During the campaign period, lasting between March to November 2017, it is recommended to perform some instrumental line shape measurements for all participating instruments every two weeks. This will help to monitor the long term stability of the instrumental properties. If any instrument shows degradation of the instrumental properties then this should be taken into account during the analysis of the data. In case of serious degradation a restoration of instrument characteristic should be attempted.

At the end of the campaign after the instrument has been shipped back to their respective institutes, all groups are asked to do a final quality check of the instrument and perform instrumental line shape and atmospheric measurements. This will give us another reference measurement to see the effect (if any) of transportation on the instrument properties.

7. Measurement setup

All instruments should be set up at the campaign site and ready for performing atmospheric measurements at the latest by beginning of the third week of March 2017. The active measurement campaign is planned to take place between March and November 2017. The measurements will be recorded between sunrise and sunset, depending on the SZA limits set by the local scene and weather conditions (clouds, fog and strong winds). The recommended settings for the operation of the individual instrument are given in the table 2-7 below. The local team from FMI will monitor the operation of the instruments during the campaign period. It will be taken care that all spectrometers are operated continuously to cover the diurnal cycle and to improve measurement statistics, if weather conditions permit. This will be helpful in the comparison exercise among the instruments. The first phase of measurements will be used to perform a blind intercomparison of the different remote sensing instruments. As reference 10 good measurements days will be taken for the blind intercomparison. In total 8 AirCore balloon launches are planned during the campaign period. The vertical profiles of greenhouse gases derived from the AirCore flights will be feed as an input profile for the analysis done with the remote sensing instruments. It is recommended to perform a few AirCore balloon launches towards the beginning of the campaign when the RAL Heterodyne radiometer is also operating. These measurements can be used to calibrate the Heterodyne radiometer after the initial blind intercomparison study is finished. However, the exact launch dates will depend on the atmospheric situation, dynamics, which might lead to a shift of the launch dates. The exact launch date for the AirCore will be chosen after looking at the meteorological situation and discussion among the partners. Since the participating remote sensing instruments require solar light, launches will be performed during periods of sunny weather conditions and will avoid instrumental downtimes, if possible.

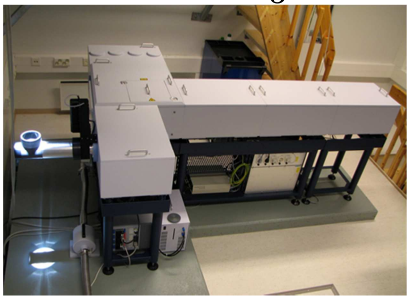
8. Signal-to-noise (SNR) determination

All instruments should be operated at the current optimized settings (see table 2) to get a good SNR. However after the first few days of measurements at the campaign site, the results from the individual instruments will be compared to the reference TCCON instrument (Bruker IFS 125HR). If needed the integration time or the number of individual measurement co-addition can be tuned to get the results comparable to the TCCON instrument. However, the individual PI's may also decide to continue running their instrument with their own well-known optimized settings and decide whether their time series are in good agreement with the reference TCCON data or their procedures need adjustment.

9. Detector linearity test

All instruments should perform detector linearity test and provide the information about the same. Special care should be taken if any instrument shows non-linearity behaviour of its detector during the test measurements.

Table 2: Instrument properties and settings used during the FRM4GHG campaign

<table>
<tr><td><u>Instrument type:</u> Bruker IFS 125HR</td><td rowspan="3">Bruker IFS 125HR
</td></tr>
<tr><td><u>Institute:</u> Finnish Meteorological Institute (FMI)</td></tr>
<tr><td><u>Responsible person(s):</u>
Rigel Kivi: +358 405424543
Pauli Heikkinen: +358 401806090</td></tr>
</table>

Instrument design	**Spectrometer type:** cube corner Michelson interferometer **Solar tracker type:** A547N by Bruker Optics, CamTracker included **Detector type:** InGaAs, Si and InSb detector **Beam splitter type:** CaF_2 **Entrance window:** CaF_2 **Filters:** red filter (Si), dichroic (Si/InGaAs), NDACC (InSb) **Mirrors:** gold coated **Temperature control of spectrometer:** ambient temperature **Temperature control of detector:** InGaAs and Si – amb. temp., InSb – LN2 cooled **Pressure control of spectrometer:** vacuum
Instrument performance	**Spectral range:** InGaAs – 4000-11000 cm^{-1}, Si – 9000-15000 cm^{-1}; InSb – 1800 –6000 cm^{-1} **Max OPD:** 45 cm (TCCON), 258 cm max **Spectral resolution**: 0.02 cm^{-1} (TCCON), 0.0035 cm^{-1} max **Tracking function:** camera based **Elevation angle capability:** all **Field of view:** $1.196x10^{-3}$ rad (internal semi FOV) **Typical scan duration:** 78 s (FWD-BWD) **Typical integration time:** 39 s (one interferogram) **Number of co-added measurements:** 1 **Instrument operation:** automated
Calibration/characterization procedures	**Line shape:** gas cell
Retrieval software	GFIT
Supporting measurements	camera, sun photometer, rain detector
Special needs/requests regarding logistics	**Power supply/consumption:** 230 V 3000VA UPS, vacuum pump 3PH 16A **Internet:** IP connection available **Space requirements**: installed in a dedicated lab **Maximum distance between sun-tracker and spectrometer:** 3 m **Local support:** operated by the FMI

Table 3: Instrument properties and settings used during the FRM4GHG campaign

<table>
<tr><td colspan="2"><u>Instrument type:</u> Bruker Vertex70</td><td rowspan="3">Bruker Vertex70
</td></tr>
<tr><td colspan="2"><u>Institute:</u> University of Bremen & Royal Belgian of Space Aeronomy</td></tr>
<tr><td colspan="2"><u>Responsible person(s):</u>
Justus Notholt: +49(0)421 218 62190
Christof Petri: +49(0)421 218 62173
Thorsten Warneke: +49(0)421 218 62177
Martine De Mazière: +32-(2)-37 30 400
Mahesh Kumar Sha: +32-(2)-37 30 389
Christian Hermans: +32-(2)-37 30 375</td></tr>
<tr><td>Instrument design</td><td colspan="2">Spectrometer type: Rock-solid pendulum interferometer
Solar tracker type: BIRA-IASB solar tracker based on two mirror concept
Detector type: InGaAs detector & InSb detector
Beam splitter type: CaF2
Entrance window: CaF2
Filters:
Mirrors: gold coated
Temperature control of spectrometer: ambient temperature
Temperature control of detector: InGaAs – amb. temp., InSb – LN2 cooled
Pressure control of spectrometer: ambient pressure, operated inside a container</td></tr>
<tr><td>Instrument performance</td><td colspan="2">Spectral range: InGaAs – 4000 - 14000 cm^{-1}, InSb – 3500 – 10000 cm^{-1}
Max OPD:
Spectral resolution: 0.16 cm^{-1} (enhanced res.), 0.4 cm^{-1} (nominal res.)
Tracking function: camera based
Elevation angle capability: all
Field of view: 0.005 °
Typical scan duration: 9 sec
Typical integration time:
Number of co-added measurements: e.g. 6 – 20
Instrument operation: automated</td></tr>
<tr><td>Calibration/characterization procedures</td><td colspan="2">Line shape: gas cell</td></tr>
<tr><td>Retrieval software</td><td colspan="2">GFIT / PROFFIT</td></tr>
<tr><td>Supporting measurements</td><td colspan="2">camera, sun photometer, rain detector</td></tr>
<tr><td>Special needs/requests regarding logistics</td><td colspan="2">Power supply/consumption:
Internet: 4 IP addresses
Space requirements: 80x50x30 cm^3
Maximum distance between sun-tracker and spectrometer: 3 m
Local support: occasionally</td></tr>
</table>

Table 4: Instrument properties and settings used during the FRM4GHG campaign

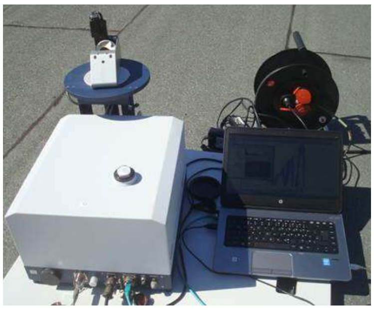
<table>
<tr><td colspan="2">Instrument type: Bruker EM27/SUN</td><td rowspan="3">Bruker EM27/SUN
</td></tr>
<tr><td colspan="2">Institute: KIT</td></tr>
<tr><td colspan="2">Responsible person(s):
Qiansi Tu: on site
Thomas Blumenstock: +49(0)721 608-22838
Frank Hase: +49(0)721 608-22434</td></tr>
<tr><td>Instrument design</td><td colspan="2">Spectrometer type: Rock-solid pendulum interferometer
Solar tracker type: Bruker tracker derived from KIT CamTracker
Detector type: InGaAs detectors
Beam splitter type: ZnSe
Entrance window: Schott RG
Filters: Silicon and Ge filter
Mirrors: gold coated
Temperature control of spectrometer: ambient temperature
Temperature control of detector: ambient temperature
Pressure and temperature control of spectrometer: the spectrometer will be operated outside of the container under ambient conditions (for demonstrating its operational capabilities under harsh campaign conditions)</td></tr>
<tr><td>Instrument performance</td><td colspan="2">Spectral range: 4000 - 10000 cm^{-1}
Max OPD: 1.8 cm (double sided IFG)
Tracking function: camera based
Elevation angle capability: all (non-accessible spot in immediate vicinity of zenith)
External field of view: ~0.6 x solar disc diameter
Typical scan duration: 6s
Typical integration time: 10 x 6s (coaddition of 10 interferograms)
Instrument operation: automated</td></tr>
<tr><td>Calibration/characterization procedures</td><td colspan="2">Line shape: open path</td></tr>
<tr><td>Retrieval software</td><td colspan="2">PROFFIT</td></tr>
<tr><td>Supporting measurements</td><td colspan="2">Low-cost pressure sensor
GPS sensor for accurate timekeeping (and position)</td></tr>
<tr><td>Special needs/requests regarding logistics</td><td colspan="2">Standard 220V power supply
Internet connection (if available)
Mechanical support for operation (any stable smooth base 1 – 1.5 m above ground elevation)</td></tr>
</table>

Table 5: Instrument properties and settings used during the FRM4GHG campaign

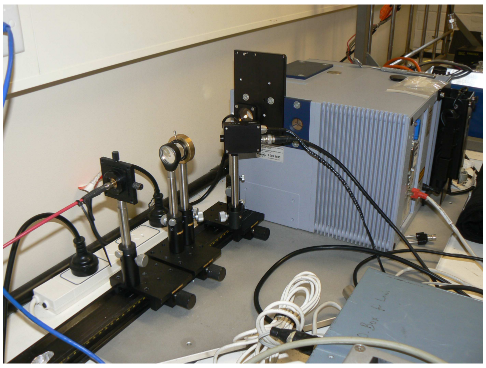
Instrument type: Bruker IR Cube **Institute:** UOW **Responsible person(s):** Nicholas Jones: +61 2 4221 5808 David Griffith: +61 2 4221 3515	Bruker IR Cube 
Instrument design	**Spectrometer type:** Rock-solid pendulum interferometer **Solar tracker type:** Eko-STR21G Sun tracker **Detector type:** InGaAs detector **Beam splitter type**: Quartz **Entrance window:** CaF2 wedged for reference solar signal (cloud filter) **Filters:** **Mirrors:** gold coated **Temperature control of spectrometer:** container temperature **Temperature control of detector:** container temperature **Pressure and temperature control of spectrometer:** the spectrometer will be operated inside the container
Instrument performance	**Spectral range:** 3800 - 11000 cm^{-1} **Max OPD:** 1.8 cm (single sided IFG) **Tracking function:** tracker precision (0.01 degree) **Elevation angle capability:** all (non-accessible spot in immediate vicinity of zenith) **External field of view:** 72 mrad **Typical scan duration:** 4s **Typical integration time:** 14 FWD 14 BWD x 4s (coaddition of 28 interferograms) **Instrument operation:** automated
Calibration/characterization procedures	**Line shape:** open path / Cell
Retrieval software	GFIT
Supporting measurements	pressure sensor
Special needs/requests regarding logistics	Standard 220V power supply Internet connection Mechanical support for tracker operation on roof of container Bi-Weekly cell measurements (if required)

Table 6: Instrument properties and settings used during the FRM4GHG campaign

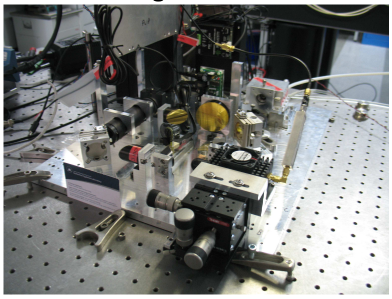
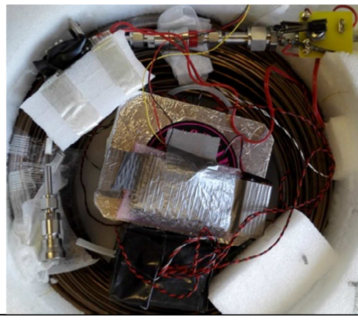
<table>
<tr><td colspan="2"><u>Instrument type:</u> Laser Heterodyne Radiometer (Research instrument)</td><td rowspan="3">Re-engineered LHR
</td></tr>
<tr><td colspan="2"><u>Institute:</u> Rutherford Appleton Laboratory</td></tr>
<tr><td colspan="2"><u>Responsible person(s):</u>
Alex Hoffmann: +44 (0)1235 445 367
Marko Huebner: +44 (0)1235 445 974
Damien Weidmann: +44(0)7771 682 702</td></tr>
<tr><td>Instrument design</td><td colspan="2">Spectrometer type: Quantum cascade laser heterodyne radiometer
Solar tracker type: Altazimuth with camera active feedback – Vertex 70 tracker to be used during the campaign (12 mm beam sampling).
Detector type: HgCdTe detectors
Beam splitter type: ZnSe
Entrance window: none
Filters: Ge bandpass filter
Mirrors: gold coated
Temperature control of spectrometer: ambient temperature
Temperature control of detector: Either -80C TEC or LN2
Pressure and temperature control of spectrometer: the spectrometer will be operated inside the container under ambient.</td></tr>
<tr><td>Instrument performance</td><td colspan="2">Spectral range: 952 – 955 cm^{-1}
Spectral Resolution: 0.002 to 0.02 cm^{-1}
Max OPD: N/A
Tracking function: N/A
Elevation angle capability: all
External field of view: ~0.45 x solar disc diameter
Typical scan duration: 90 s
Typical integration time: 90 s
Instrument operation: Manual</td></tr>
<tr><td>Calibration/characterization procedures</td><td colspan="2">Line shape: RF response measurements – Low pressure gas cell</td></tr>
<tr><td>Retrieval software</td><td colspan="2">OEM retrieval based on RFM</td></tr>
<tr><td>Supporting measurements</td><td colspan="2">Surface pressure
Temperature and pressure profiles for retrievals</td></tr>
<tr><td>Special needs/requests regarding logistics</td><td colspan="2">Standard 220V power supply
Internet connection
Mechanical support for operation
Dry nitrogen or zero air gas line
Potentially LN2</td></tr>
</table>

Table 7: Instrument properties and settings used during the FRM4GHG campaign

Instrument type: AirCore	AirCore 
Institute: University of Groningen	
Responsible person(s): Huilin Chen: +31 50 363 8638 Marcel de Vries: +31 50 363 7145 Bert Kers: +31 50 363 7144	

Instrument design	**Instrument type:** AirCore **Dryer:** Magnesium perchlorate, $Mg(ClO_4)_2$ **Valve:** automated **Length:** 100 m **Volume:** 1400 mL
Instrument performance	**Gas analyzer:** Picarro G2401-m **Trace gases:** CO_2, CH_4, CO **Precision:** $\mathbf{CO_2}$**:** 0.05 ppm; CH_4: 0.5 ppb; CO: 8 ppb; **Accuracy:** $\mathbf{CO_2}$**:** 0.1 ppm; CH_4: 1 ppb; CO: 3 ppb;
Calibration/characterization procedures	
Retrieval software	Custom-made RUG
Supporting measurements	Radiosonde ambient pressure, temperature; AirCore temperature
Special needs/requests regarding logistics	Table for the Picarro G2401 and two cylinders

10. 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

11. Reference documents

FRM4GHG deliverable D2.2: Instrument overview, made available via the project website http://frm4ghg.aeronomie.be/index.php/outreach/deliverables

TCCON Sodankylä site: https://tccon-wiki.caltech.edu/Sites/Sodankyla

Kivi, R. and Heikkinen, P.: Fourier transform spectrometer measurements of column CO2 at Sodankylä, Finland, Geosci. Instrum. Method. Data Syst., 5, 271-279, doi:10.5194/gi-5-271-2016, 2016. Available from: http://www.geosci-instrum-method-data-syst.net/5/271/2016/

Gisi, M., F. Hase, S. Dohe, T. Blumenstock, A. Simon, and A. Keens: XCO2-measurements with a tabletop FTS using solar absorption spectroscopy, Atmos. Meas. Tech., 5, 2969-2980, doi:10.5194/amt-5-2969-2012, 2012.

Griffith, D. W. T., N. M. Deutscher, C. G. R. Caldow, G. Kettlewell, M. Riggenbach and S. Hammer (2012). "A Fourier transform infrared trace gas and isotope analyser for atmospheric applications." Atmos. Meas. Tech., 5, 2481–2498, 2012, doi:10.5194/amt-5-2481-2012

Vertex70: Bruker spectrometer: https://www.bruker.com/products/infrared-near-infrared-and-raman-spectroscopy/ft-ir-research-spectrometers/vertex-series/vertex-7070v/overview.html

D. Weidmann, T. Tsai, N.A. Macleod, G. Wysocki, Atmospheric observations of multiple molecular species using ultra-high-resolution external cavity quantum cascade laser heterodyne radiometry, Optics Letters, 36, 11, 1951-1953 (2011)

Chen, H., J. Winderlich, C. Gerbig, A. Hoefer, C. W. Rella, E. R. Crosson, A. D. Van Pelt, J. Steinbach, O. Kolle, V. Beck, B. C. Daube, E. W. Gottlieb, V. Y. Chow, G. W. Santoni and S. C. Wofsy: "High-accuracy continuous airborne measurements of greenhouse gases (CO2 and CH4) using the cavity ring-down spectroscopy (CRDS) technique." Atmos. Meas. Tech. 3: 375-386, doi:10.5194/amt-3-375-2010, 2010

12. Reference for software/tool mentioned

Standard GFIT software tool has been used for processing of FTIR data. The description of the software can be found in the following reference

Wunch, D., G. C. Toon, J.-F. L. Blavier, R. A. Washenfelder, J. Notholt, B. J. Connor, D. W. T. Griffith, V. Sherlock, and P. O. Wennberg (2011), The total carbon column observing network, Philosophical Transactions of the Royal Society - Series A: Mathematical, Physical and Engineering Sciences, 369(1943), 2087-2112, doi:10.1098/rsta.2010.0240. Available from: http://rsta.royalsocietypublishing.o.../2087.full.pdf

Standard PROFFIT software tool has been used for processing of FTIR data. The description of the software can be found in the following reference

Hase, F., J.W. Hannigan, M.T. Coffey, A. Goldman, M. Höpfner, N.B. Jones, C.P. Rinsland, S.W. Wood: Intercomparison of retrieval codes used for the analysis of high-resolution, ground-based FTIR measurements, Journal of Quantitative Spectroscopy & Radiative Transfer 87, 25–52, 2004.