

FRM4GHG

Fiducial Reference Measurements for Greenhouse Gases



Data protocol

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1 Document change record

Issue	Date	Item	Comment
Vo.0	2017-05-08	–	Initial version, for completion by D. Weidmann and H. Chen
Vo.1	2017-08-16	–	Input added by D. Weidmann + Huilin Chen

2 Access list

This document is a deliverable “D2.4: Data protocol” 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 protocol describes the data files which will be archived, made available within the consortium and finally to the public, as result of the campaign observations in Sodankylä, Finland.

4 Document structure

Section 5 Participating instruments – Presents a list of instruments and the corresponding responsible institute which are taking part in the project.

Section 6 Data and measurement device classification – Describes the different categories of instruments which are taking part in the project. It also describes the different categories of data which is generated by the participating instruments.

Section 7 Data format and contents – Describes the data format for each instrument and the content of the data which will be reported within this project.

Section 8 Data dissemination – Describes the strategy used for the dissemination of the data, plots and reports generated from the project.

Section 9 & 10 Applicable and reference documents – Presents a list of all applicable and reference documents related to this deliverable.

Section 11 Reference 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. More information about these instruments can be found in the FRM4GHG deliverable D2.2 ‘Instrumental Overview’.

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 Royal Belgian Institute for Space Aeronomy (BIRA-IASB)
Bruker EM27/SUN	Karlsruhe Institute of Technology (KIT)
Bruker IR cube	University of Wollongong (UOW)
Heterodyne spectrometer	Rutherford Appleton Laboratory (RAL)
AirCore system	University of Groningen (RUG)

6 Data and measurement device classification

The measurement devices can be classified in different categories:

- (A) FTIR spectrometers manufactured by Bruker
- (B) Laboratory-built research Laser heterodyne spectrometer
- (C) In situ / aircore system

The data of each measurement device also belong to different categories:

- (1) Housekeeping data
- (2) Data for instrument characterisation (ILS and non-linearity/out-of-band artefacts)
- (3) Atmospheric measurements (for the trace gas analysis)
- (4) Auxiliary information defining the atmospheric state (ground pressure, p/T profiles, VMR profiles)
- (5) Retrieved data resulting from the quantitative spectral analysis (for the spectrometers) or from the PICARRO analysis (for the AirCore system)

7 Data format and contents

FTIR spectrometers manufactured by Bruker

All participating FTIR spectrometers use the same operating software (OPUS from Bruker) which generates files in the OPUS format (these contain the recorded interferograms and also the housekeeping data). Therefore, raw FTIR measurements (called as level 0 data) of any kind will be archived at the BIRA-IASB server as OPUS files.

The spectra used for the quantitative spectral analysis are the result of the pre-processing of spectra. Although these are derived data (they can be regenerated from the raw measurements when needed), it seems useful to archive these calibrated spectra (called as level 1 data) also as part of the documentation. The file format depends on the retrieval software used: GFIT uses a format derived from the OPUS format, whereas PROFFIT uses a self-constructed binary format (open format, commented FORTRAN source code for reading and writing will be enclosed).

The files containing the auxiliary atmospheric information are self-explaining ASCII table files, named in PROFFIT *.prf files, in GFIT *.mod files. The GFIT ground p, T data are collected in *.grl files.

The primary files containing the retrieval results (called as level 2 data) are ASCII tables: GFIT generates a single large *.eof file containing results from all processed spectra, whereas PROFFIT generates several ASCII ? files per retrieval, which are combined in a *.zip folder and stored in a unique subfolder assigned to each measured spectrum. Additional PROFFIT tools allow to collect the primary retrieved and auxiliary data in ASCII tables, the resulting tables will also be submitted.

In the process of the quantitative analysis, static spectroscopic input files are required: these line lists (including the solar line lists) will be made available as ASCII files.

Auxiliary measurements recorded for instrument characterisation (ILS, nonlinearity) will be made accessible as raw data (OPUS files). The results from the associated data analysis

(e.g. ILS retrievals using LINEFIT) will be provided in form of a document, the LINEFIT input and output files will also be archived.

Laser Heterodyne Spectrometer (LHR)

The LHR activity produces 3 different datasets: raw instrument outputs (Level 0 data – L0), calibrated transmission spectra (Level 1 data – L1), and atmospheric retrieval data output (L2). These three datasets are described hereafter.

Level 0:

The level 0 data are outputted in the NetCDF format and can be read by standard NetCDF interface (for instance, Panoply). The following example shows a typical filename and the way it is constructed.

SOD30LHR.ao.20170710.071903.nc,

SOD	30	LHR	.ao	.20170710	.071903	.nc or .sun_nc
geographical location code	Total acquisition time	Instrument code	File processing level	Year, month, day aggregated	Time stamp of first spectrum in hour minute second	File extension

The “.sun_nc” file extension indicated that the file also contains 2D images of the solar disk taken during measurements.

The L0 data files contains all the raw data recorded by the various sensors part of the instrument, as well as all the relevant instrument settings. The figure below gives the lists of the different fields.

Name	Long Name	Type
▼ SOD30LHR.a0.20170701.034252.nc	SOD30LHR.a0.20170701.034252.nc	Local File
▼ ancillary_means	ancillary_means	—
air_temperature	air_temperature	1D
etalon_in	etalon_in	1D
laser_current	laser_current	1D
laser_relative_humidity	laser_relative_humidity	1D
laser_TEC_temperature	laser_TEC_temperature	1D
source_azimuth_pointing_deviation	source_azimuth_pointing_deviation	1D
source_camera_exposure	source_camera_exposure	1D
source_camera_gain	source_camera_gain	1D
source_diameter	source_diameter	1D
source_elevation_pointing_deviation	source_elevation_pointing_deviation	1D
source_intensity_max	source_intensity_max	1D
source_intensity_mean	source_intensity_mean	1D
source_intensity_min	source_intensity_min	1D
source_intensity_standard_deviation	source_intensity_standard_deviation	1D
source_pixel_position_X	source_pixel_position_X	1D
source_pixel_position_Y	source_pixel_position_Y	1D
▼ ancillary_spectra	ancillary_spectra	—
laser_current	laser_current	2D
laser_temperature	laser_temperature	2D
source_azimuth_pointing_deviation	source_azimuth_pointing_deviation	2D
source_elevation_pointing_deviation	source_elevation_pointing_deviation	2D
source_intensity_mean	source_intensity_mean	2D
source_intensity_standard_deviation	source_intensity_standard_deviation	2D
▼ spectra	spectra	—
etalon_channel_voltage	etalon_channel_voltage	2D
heterodyne_voltage	heterodyne_voltage	2D
photomixer_DC_voltage	photomixer_DC_voltage	2D
time	time	1D

Level 1

The L1 data are derived from LO. The raw spectra undergo the following steps:

- Calibrated in absolute wavenumbers via etalon signals
- Offset correction
- Edge trimming
- Interpolation onto regular wavenumber grid

In addition, from the time stamp and the location the solar coordinates are calculated, the SNR over the spectra is estimated, and a first guess of the second order polynomial baseline is determined.

From a LO file (e.g. “SOD30LHR.a0.20170710.071903.nc”) the corresponding L1 file is produced (e.g. “SOD30LHR.l1.20170710.071903.nc”) which includes the additional data derived from LO.

Level 2

Level 1 data are next used as input into the optimum estimation retrieval code. At this stage, other inputs data are required:

- Spectroscopic data (Hitran 2012) provided on the FRM4GHG website.
- ILS data in the form of an ascii file containing the ILS direct measurements, also provided on the FRM4GHG website.
- An atmospheric profile of minor constituents (O₃, N₂O, NH₃, COF₂) from the daytime midlatitude MIPAS profiles.
- WACCM a priori and covariance matrices for CO₂ profiles.
- NCEP T and p profiles shared with the other FRM4GHG partners
- Surface T and p from the Sodankyla AWS, also shared with other FRM4GHG partners.

The retrieval outputs are currently archived as Excelis IDL save files (.sav). The L2 outputs include:

- Vertical distribution of H₂O and CO₂
- Total, smoothing, and measurements errors on H₂O and CO₂ profiles
- Total columns and errors for CO₂ and H₂O
- Averaging kernels
- Information contents, DFS, and retrieval diagnostics data
- Individual modelled fitted spectra
- Individual residuals

The plan is to build an L2 netCDF file generator for final data archival.

LO, L1, and L2 data in the NetCDF format will be transferred to the BIRA server for open access along with file descriptors, following the data dissemination plan described below.

Aircore system

The aircore system collects air samples that are analysed by a Picarro analyser (G2401) to obtain mole fractions of CO₂/CH₄/CO.

The raw data are the reported mole fractions of CO₂/CH₄/CO from Picarro as ASCII files *DataLog_User.dat.

The auxiliary data include

- 1) datalogger ASCII files *.Bo1 or *.Bo2, which contain temperature measurements of AirCore during flight, automatic valve control signal
- 2) Radiosonde ASCII files *.tsv, which contain profiles of ambient pressure, temperature, altitude, wind speed, and wind direction

The calibrated mole fractions of CO₂/CH₄/CO are output as intermediate files (equivalent to Lib processed) as ASCII files *.csv.

The final profile retrievals of CO₂/CH₄/CO are output as ASCII files, in the NASA Ames format *.naf.

Table 2: data generated for atmospheric observations by different devices

Instrument (Institute)	Raw data	L1b processed	Auxiliary data	Retrieval results
IFS 125HR (FMI)	OPUS format interferograms	calibrated spectra (OPUS)	Daily *.mod, and map *.map files. *.grl file	*.eof file
Vertex70 (UIP + BIRA)	OPUS format interferograms	calibrated spectra (OPUS / *.BIN)	Daily *.mod, and map *.map files. *.grl file (+pTn.prf files + daily clim. files)	*.eof file
EM27/SUN (KIT)	OPUS format interferograms	calibrated spectra (*.BIN)	pTn.prf files, a-priori VMR files in daily vmr_clim folder	Result.zip files and overview tables
IR cube (UoW)	OPUS format interferograms	calibrated spectra (OPUS)	Daily *.mod, and map *.map files. *.grl file	*.eof file
Heterodyne (RAL)	NetCDF raw outputs	NetCDF L1 data	.hit HITRAN files .ils instrument lineshape file .atm file of minor constituents WACCM a priori files NCEP T and p profiles Surface T and p	Currently IDL .sav NetCDF planned.
AirCore (RUG)	ASCII file *.dat	ASCII file *.csv	ASCII file *.tsv ASCII file *.Bo1 or *.Bo2	ASCII file *.naf

8 Data dissemination

The raw spectra, all other data listed in Table 2, and the measurements performed for instrumental characterization, are made accessible among the consortium after the blind phase.

Before closure of the project in January 2018, all data files listed in Table 2, and the files describing the atmospheric state, the line lists used and the spectra recorded for instrumental characterisation will be made publicly available via the project webpage as well as EVDC (ESA Validation Data Center). Furthermore, two DOI's will be created by BIRA-IASB, one DOI pointing to the level 0 and level 1 data and the second DOI pointing to the level 2 data and all other documentation, deliverables and reports generated during the project.

The results of the intercomparisons are available on the project website, as well as the plots and the reports are also made available on the project webpage. The data used for

every comparison plots generated are frozen and saved separately on the project webpage. The Correction factors used to calculate the Xgas values should also be documented.

Data sets and intercomparison plots are made available via the project website

<http://frm4ghg.aeronomie.be/index.php/documents/results>

9 Applicable documents

FRM4GHG deliverable D2.2: Instrument overview, made available via the project website
<http://frm4ghg.aeronomie.be/index.php/documents/results>

10 Reference documents

N/A

11 Reference for software / tool mentioned

The GGG user's manual, Tech. report, Available as [ggg_manual.pdf](https://tcon-wiki.caltech.edu/Publications_and_Presentations/Technical_Documents) from https://tcon-wiki.caltech.edu/Publications_and_Presentations/Technical_Documents

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.