FRM4GHG 2.0
Fiducial Reference Measurements for Greenhouse Gases

Annuak Report Month T0+12

Deliverable:	**D4.1.3**
Date:	**03/09/2023**
Lead authors:	**Justus Notholt, Mahesh Kumar Sha and Martine De Mazière**
Subject:	**ESA-Contract No. 4000136108/21/I-DT-lr**
Category:	**ESA Express Procurement (EXPRO)**
Our ref.:	**Proposal, FRM4GHG 2.0 – Expro, ESA RFP/3-17031/21/I-DT-lr, revision from 27 August 2021 and 7 September 2021**

Table of contents

1 DOCUMENT CHANGE RECORD

Issue	Date	Item	Comment
V1.0	2023-09-03	-	Initial version

2 ACCESS LIST

This document is a deliverable "D4.1.3: Annual report Month T0+12 created for the project FRM4GHG 2.0 and will be submitted to ESA. The document can be downloaded from the project webpage http://frm4ghg.aeronomie.be.

3 PURPOSE

The document describes the progress of the WPs.

4 DOCUMENT STRUCTURE

The document gives the Power-Point-Files of the presentations for all partners. The presentations were shown at three regular monthly telecons on January 18, January 26 and February 9 . These presentations form the deliverable of the annual report D 4.1.3, including technical sections about the progress in WPs 1 to 3.

5 RESULTS

All WPs of FRM4GHG-2 make good progress. The talks were given in the following order:
1. University of Bremen, Germany
2. Royal Belgian Institute for Space Aeronomy, Belgium
3. University of Wollongong, Australia
4. Karlsruhe Institute of Technology, Germany
5. Rutherford Appleton Laboratory, Great Britain
6. University of Groningen, Netherland
7. Finnish Meteorological Institute, Finland

6 APPLICABLE DOCUMENTS

Statement of Work: Fiducial Reference Measurements for Ground-Based IR Greenhouse Gas Observations (FRM4GHG 2.0)
Prepared by: EOP-GMQ, Reference: ESA-EOPG-EOPGMQ-SOW-21

7 REFERENCE DOCUMENTS

none

3D prined solar tracker
and
125HR conversion for simultaneous InGaAs and InSb measurements

Christof Petri
Winfried Markert

wmarkert@uni-Bremen.de https://frm4ghg.aeronomie.be/

Objectives

- 3D printed solar tracker

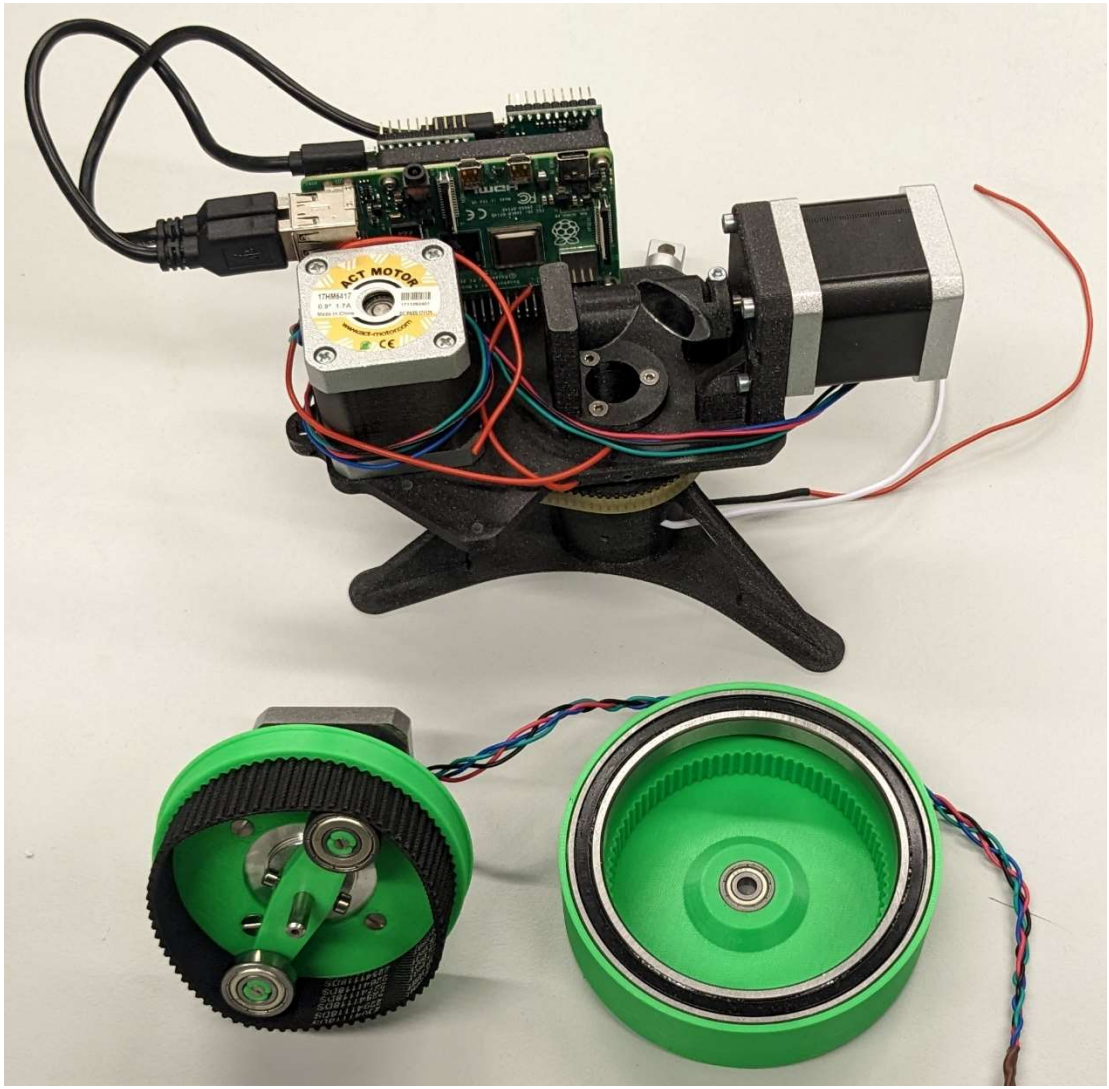
  Goals:

  - As simple as possible (no slip rings, no weather protection, no complicated mechanics, no Aux Systems)
  - Cheap, off shelf electronic components (Raspberry Pi, std. NEMA 17 steppers and stepper drivers)
  - Angular resolution <0.005° (100 steps = 1 sun diameter)
  - Able to operate in direct sun light on hot days

  Ideas:

  - All electronics at the turning Azimuth stage
  - Wireless data transmission
  - Power transmission through bearings
  - Mirrors directly mounted on the motor shaft
  - Angular resolution achieved by micro stepping (256 --> 0.0035°)
  - Printed from polycarbonates (temperature stable up to 90°C)

Objectives



Results:

- Test setup was build from PLA (no thermal stability under sun light)
- Micro stepping of 256 does not work with cheap stepper drivers --> mechanical gearing is necessary
- A low backlash strain wave gear was build for a reduction of 1 : 38.5

Objectives

- 125HR conversion for simultaneous InGaAs and InSb measurements

Thank you for your attention

Conversion of the detector chamber at the Nicosia TCCON site

Christof Petri, Winfried Markert, Justus Notholt

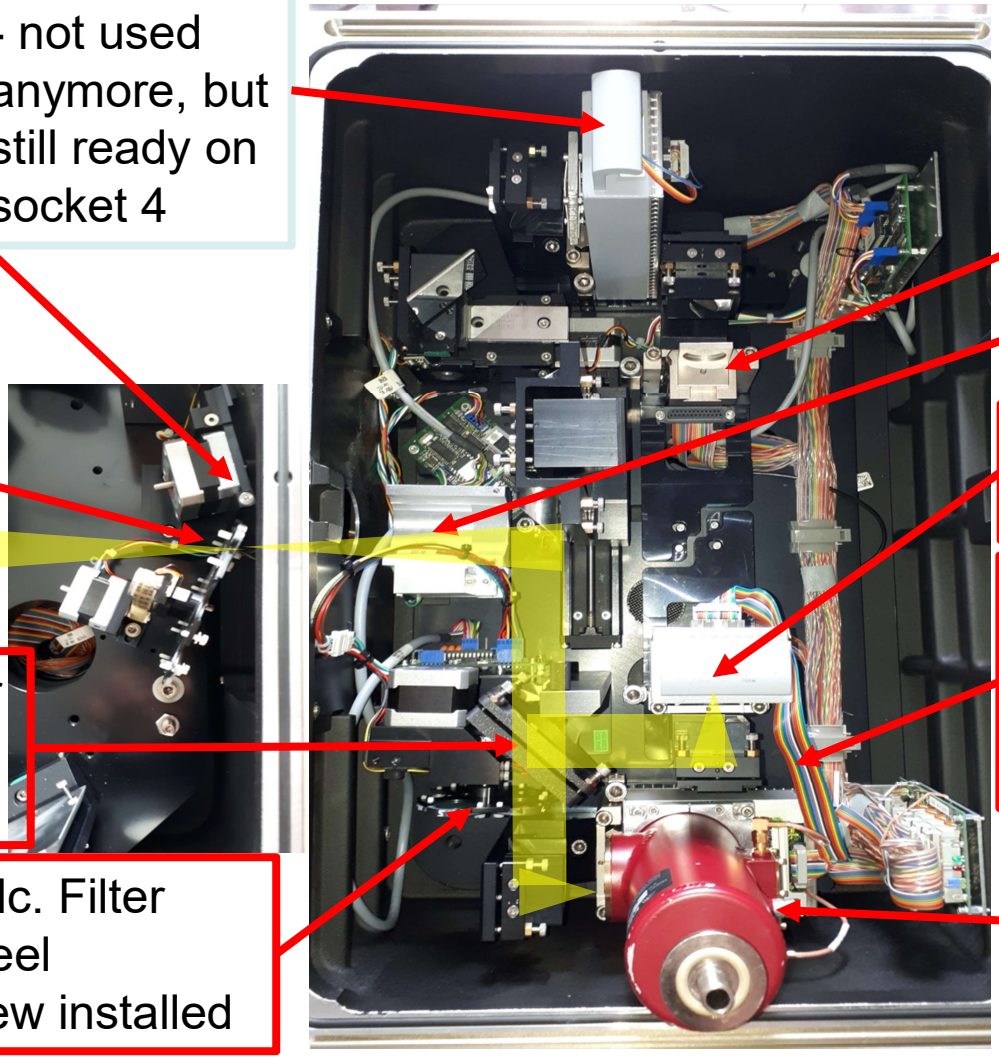
christof_p@iup.physik.uni-bremen.deid https://frm4ghg.aeronomie.be/

Nicosia TCCON site

Measurement Container on the roof of "The Cyprus institute"

Detector chamber

- **WP2 T3: Simultaneous measurements in NIR (InGaAs detector) and MIR (InSb detector) spectral domains**



Si-detector
- not used anymore, but still ready on socket 4

Outgoing aperture-wheel

8-plc. Filter wheel
- placed in the interferometer chamber

50-50 beamsplitter in self constructed holder

5-plc. Filter wheel
- new installed

Empty socket 3

Holder for HCl cell

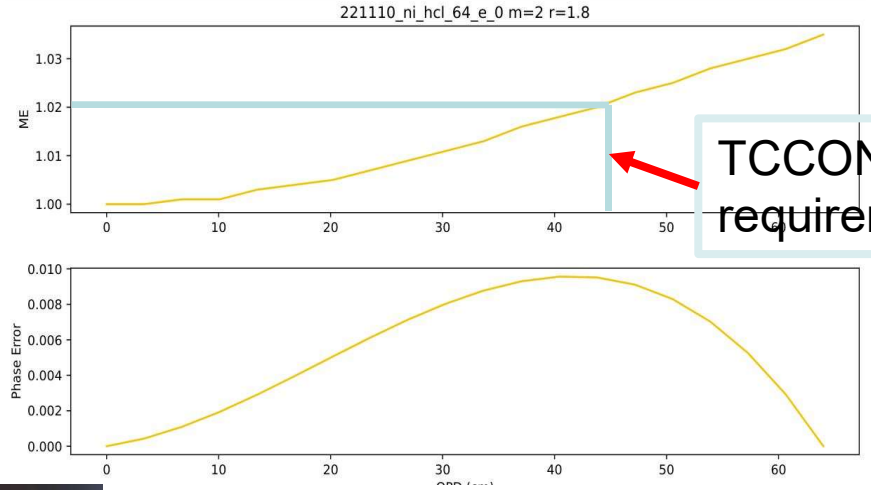
InGaAs-detector on socket 2

Connection cable for dual channel recordings on socket 1 and 2

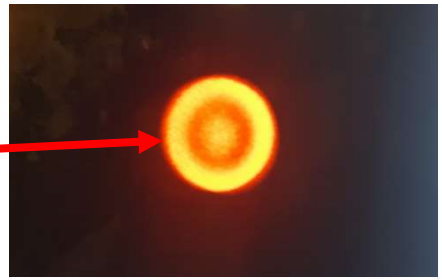
InSb-detector -new installed on socket 1

Instrument status

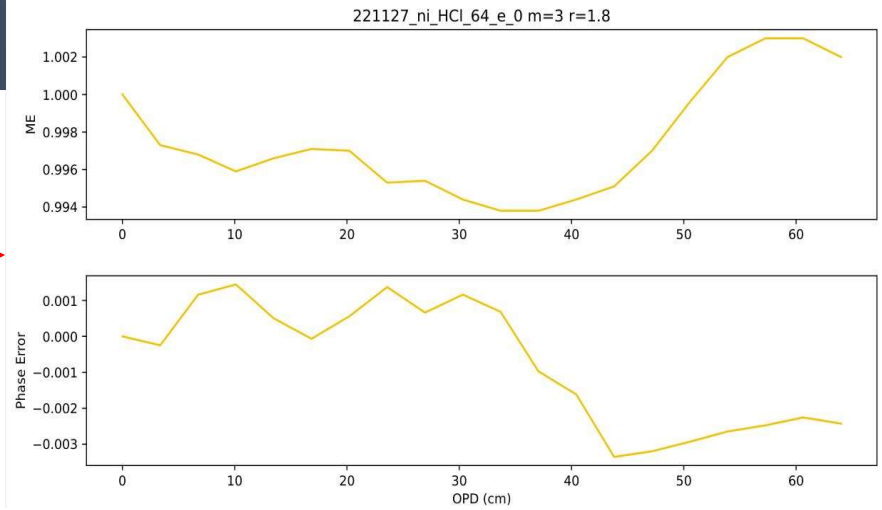
Instrument status before alignment:
- just inside TCCON requirements



Centered fringes as seen with the new alignment tools



Instrument status after alignment:
- almost perfekt



Thank you for your attention

BIRA-IASB progress in WP 1 – 4 until Jan 2023

BIRA-IASB team – Mahesh Kumar Sha*, Martine De Mazière, Sophie Berkenbosch, Pepeijn Cardoen, Filip Desmet, Lars Jacobs, Nicolas Kumps, Corinne Vigouroux, Minqiang Zhou

*mahesh.sha@aeronomie.be https://frm4ghg.aeronomie.be/

WP 1: Instrumental improvements to low-resolution spectrometers for GHG observations

Contractor: UBremen

WP Manager: **UBremen**

Start Event: Month 1 Planned Date: September 2021
End Event: Month 48 Planned Date: September 2025

Inputs:

- EM27/SUN, Vertex70, IRcube and LHR in their final configurations assessed in the FRM4GHG projects Phases 1 and 2
- All results of FRM4GHG-1

Tasks (Responsible partners; lead in bold):

T1 (**BIRA**, UBremen, UoW, KIT):

Develop a more mobile, stand-alone version of the Bruker Vertex70 instrument for deployment in the field. The envisaged adaptations are:

- Embedding the Vertex spectrometer in a thermally isolated, waterproof enclosure, including a rain sensor and compact solar tracker mounted to the spectrometer, and an automatically controlled cover of the tracker.
- Testing the use of an alternative detector to replace the Liq. N2 cooled InSb detector (e.g., TE-cooled MCT detector).

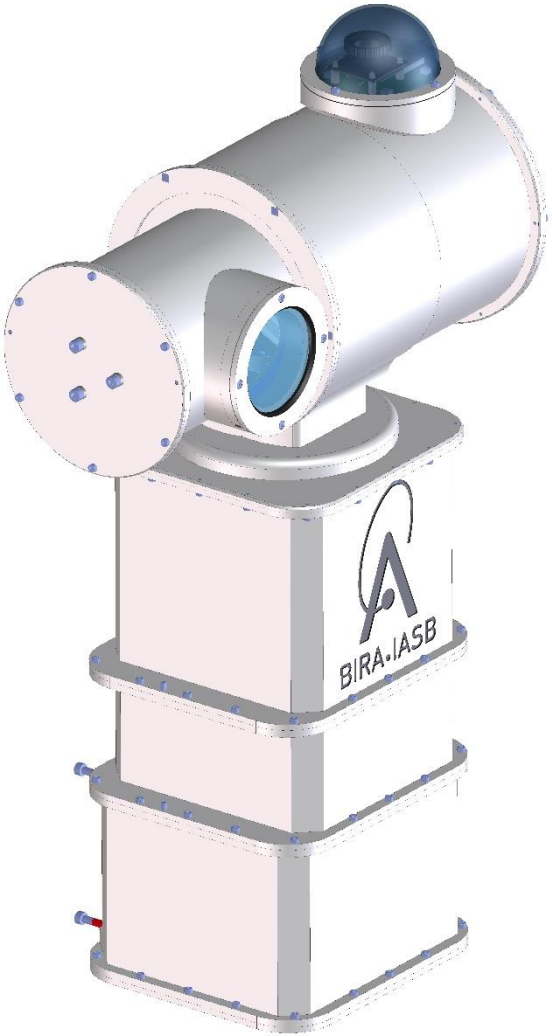
Current situation and planned work for the short term:

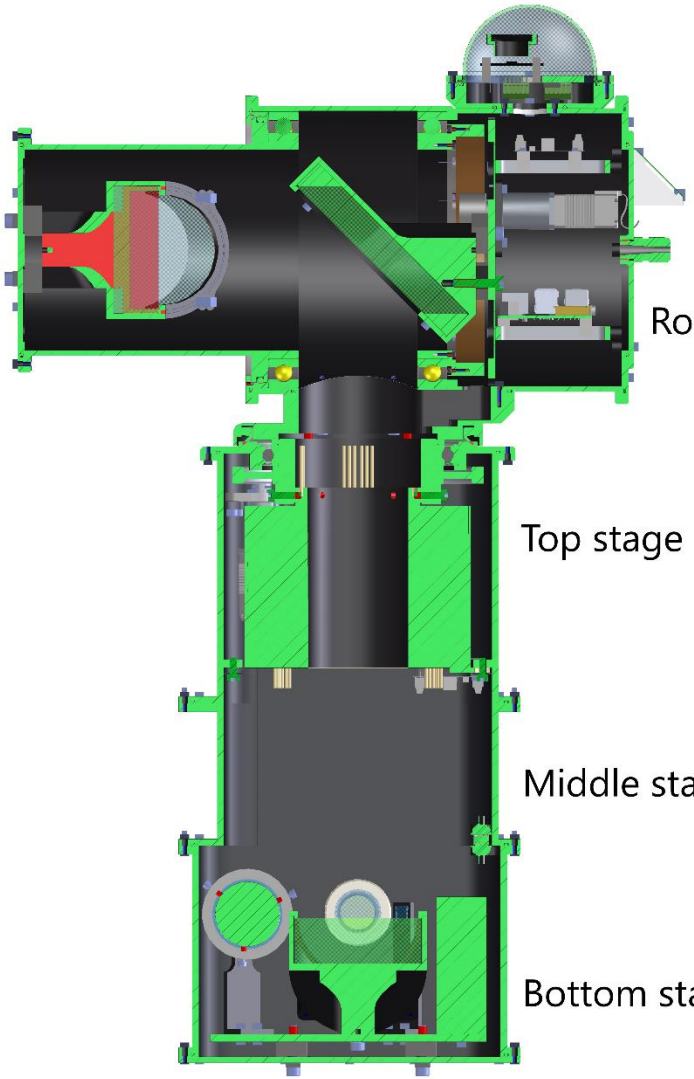
Status – BIRA-IASB

- Design and testing of components of the compact solar tracker is ongoing
- Design of the enclosure is done, currently in production
- Next step is assembly and testing

Mechanical design and realisation

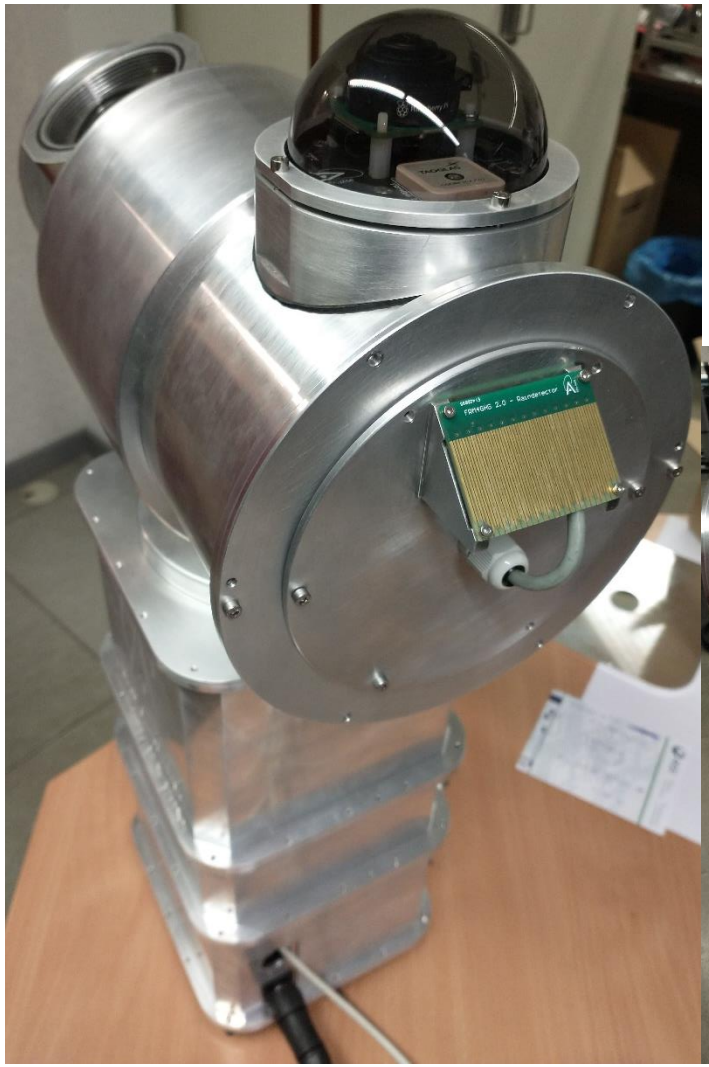
The design of the tracker tower was finalized and put into production

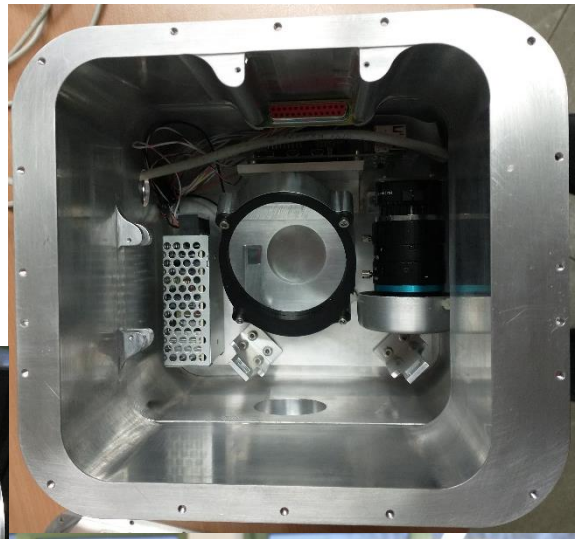


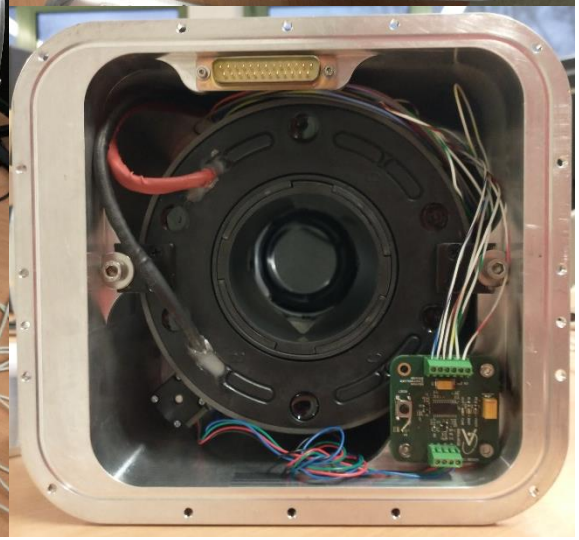


Mechanical design and realisation

The current status Tracker : All mechanical parts are finished, electrical & software integration is ongoing

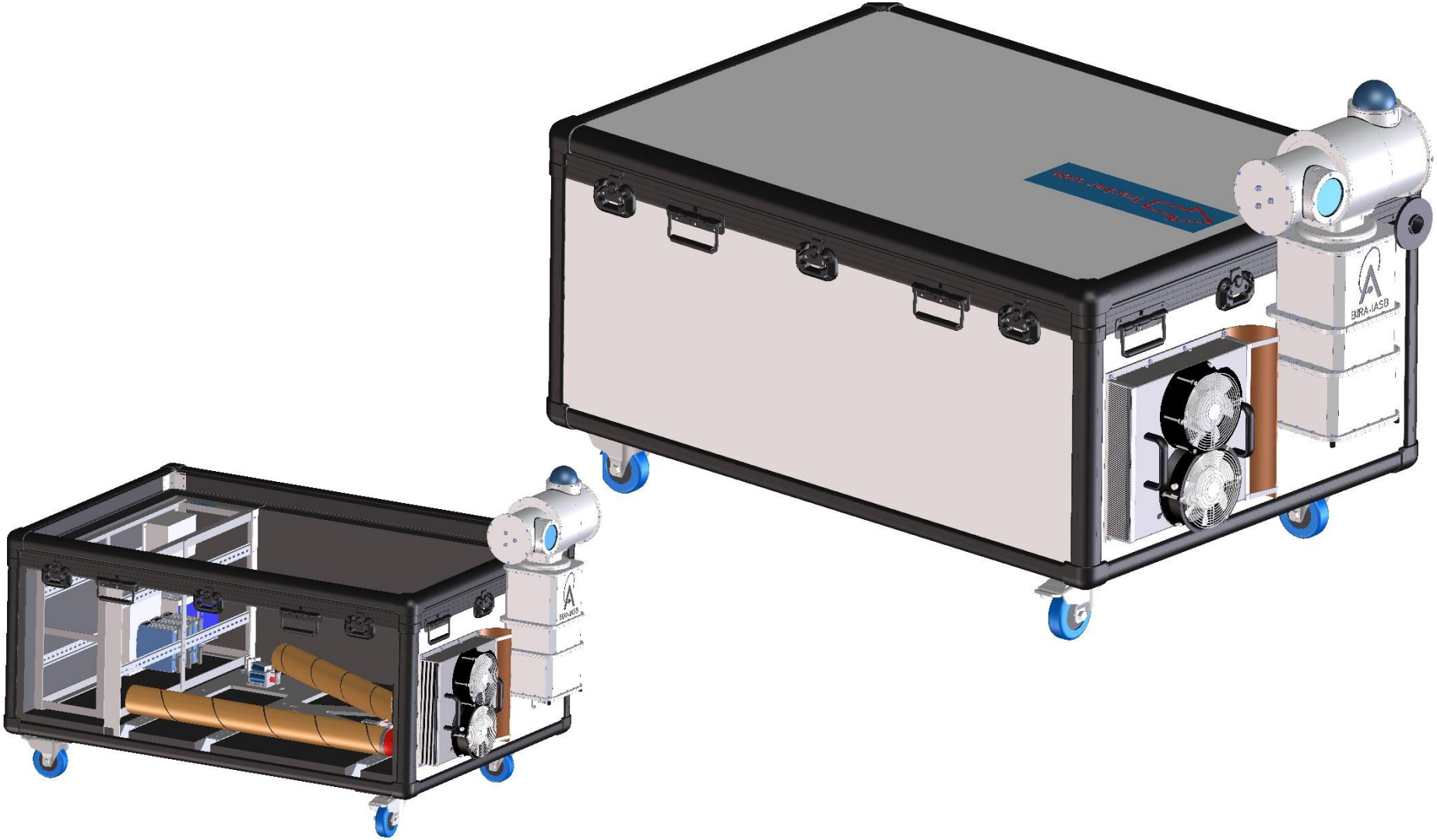




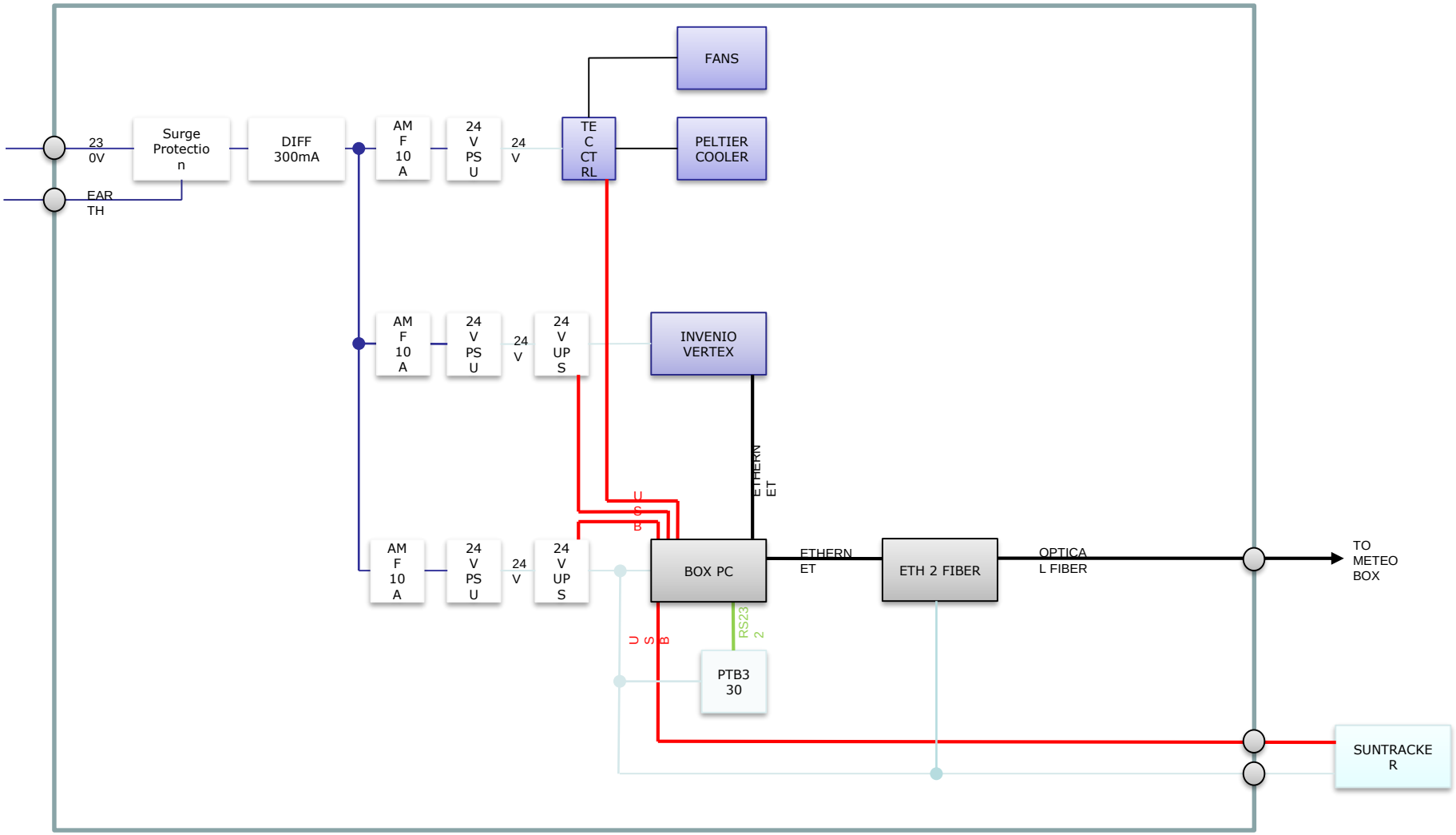


Mechanical design and realisation

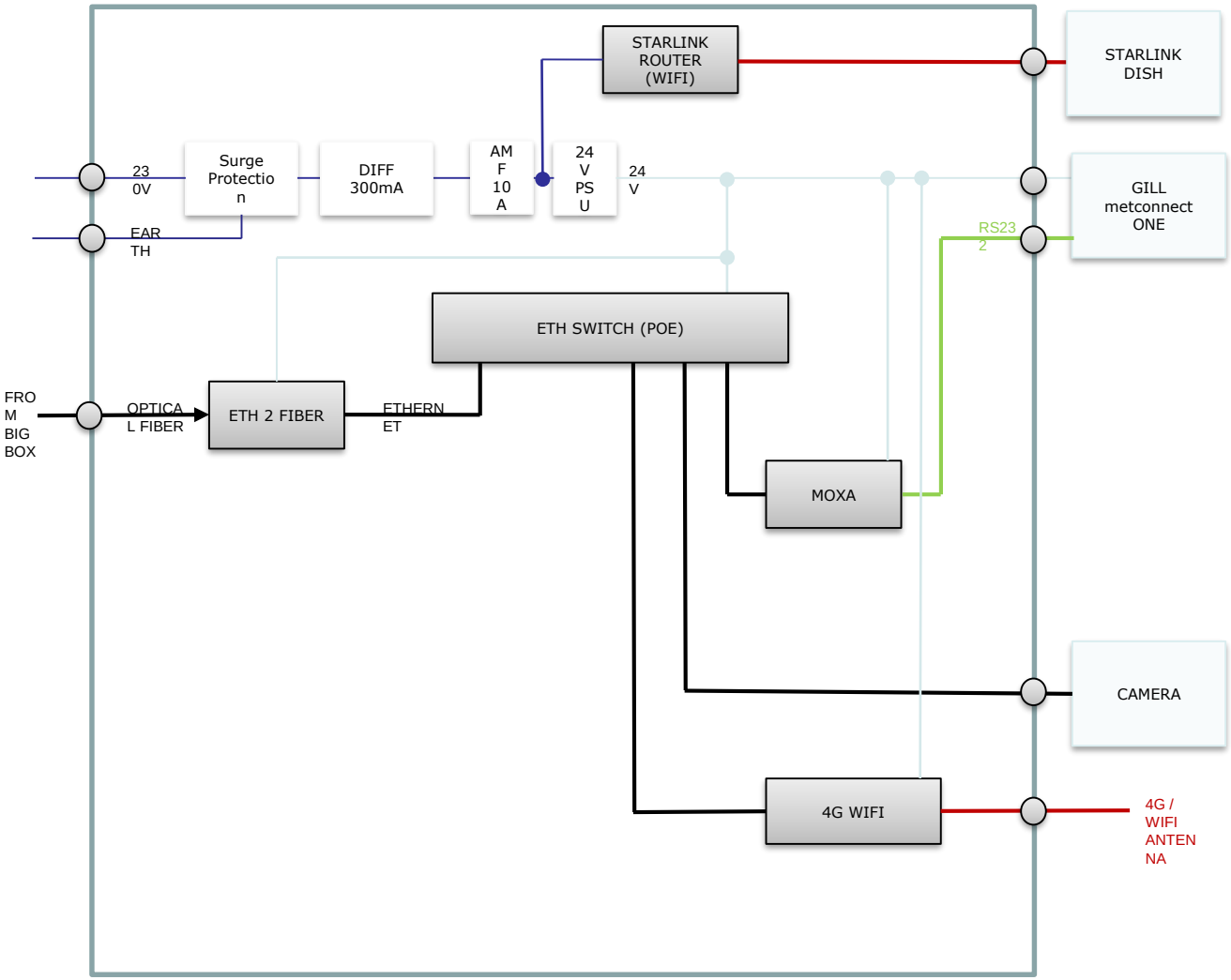
The design of the instrument enclosure is finished. Production has started and all parts should be ready for integration by mid February



Electronics design and realisation



Electronics design and realisation



WP2: Improvements to retrieval algorithms for GHG and additional species from low-resolution and TCCON spectrometers

T3 (**UBremen**, BIRA, UoW, FMI, KIT):

Further development of GHG profiling using NIR and MIR spectra, for CO_2, CH_4, CO and N_2O

- Perform (quasi-)simultaneous measurements in NIR (with InGaAs detector) and MIR (with InSb detector) spectral domains at Cyprus, Wollongong, Sodankyla, Karsruhe and St Denis/La Réunion. 'Simultaneous' points to InSb measurements at TCCON standard resolution (0.02 cm^{-1}); 'quasi- simultaneous' points to InSb measurements at NDACC standard resolution with the TCCON instrument. (All)
- Develop strategies for profile retrieval of the target GHG, and determine spectral resolution that enables retrieval of partial column information for the target GHG gases:
  - CH_4 (BIRA):
    - optimise CH_4 profile retrieval from standard TCCON NIR spectra (using SFTI4NIR);
    - investigate CH_4 profile retrieval from the InSb MIR spectra recorded simultaneously with the standard TCCON measurements, i.e., at the standard TCCON spectral resolution of 0.02 cm^{-1}
    - investigate to what extent CH_4 partial column information can be retrieved from the low-resolution spectrometer data in the NIR and MIR spectral domains (0.2 to 0.5 cm^{-1}).
  - CO (UBremen):
    - verify improved CO column retrievals from the NIR TCCON spectra (with GGG) using vertical profile information from the MIR spectra (retrieved with SFIT4, at TCCON and NDACC resolutions).
    - investigate the feasibility of retrieving CO from the low-resolution (Vertex) spectrometers in the MIR domain
  - N_2O (UBremen):
    - Investigate the possibility of retrieving the N_2O tropospheric column from standard TCCON spectra
- Validate these 'enhanced' retrieval products using collocated independent data (e.g., available AirCore or aircraft data, in-situ data, …) (BIRA for CH_4, UBremen for CO and N_2O)

Current situation and planned work for the short term:

Status – BIRA-IASB

CH_4 & N_2O retrieval from Bruker Vertex70 and mid-infrared spectra from Bruker IFS 125HR at Sodankylä – for details see slides presented during the meeting on 17 November 2021 and publication submitted to AMT with title "Atmospheric N2O and CH4 total columns retrieved from low-resolution FTIR spectra (Bruker Vertex 70) in the mid-infrared region"

Nothing new to report now

WP2: Improvements to retrieval algorithms for GHG and additional species from low-resolution and TCCON spectrometers

T4a (**BIRA**, UoW):

Optimize retrieval of HCHO for low-resolution instruments (Vertex70, HR125LR) that include measurements in the MIR spectral domain.

T4b (UBremen)

Investigate feasibility of retrieving OCS from the low-resolution MIR spectra using SFIT4.

T5 (**FMI**, RUG):

- Perform additional AirCore launches during the 4 years of the project to have enough statistical coverage
- Improve retrieval of CO and CH_4 profiles in the stratosphere from AirCore measurements based on dual launches and LISA launches at Sodankyla.
- Reprocess all 2017-2019 Aircore data at Sodankyla

T6 (**BIRA**, KIT, UBremen, UoW, FMI, RAL):

Update FRM4GHG dataset based on latest version of PROFFAST and GGG.

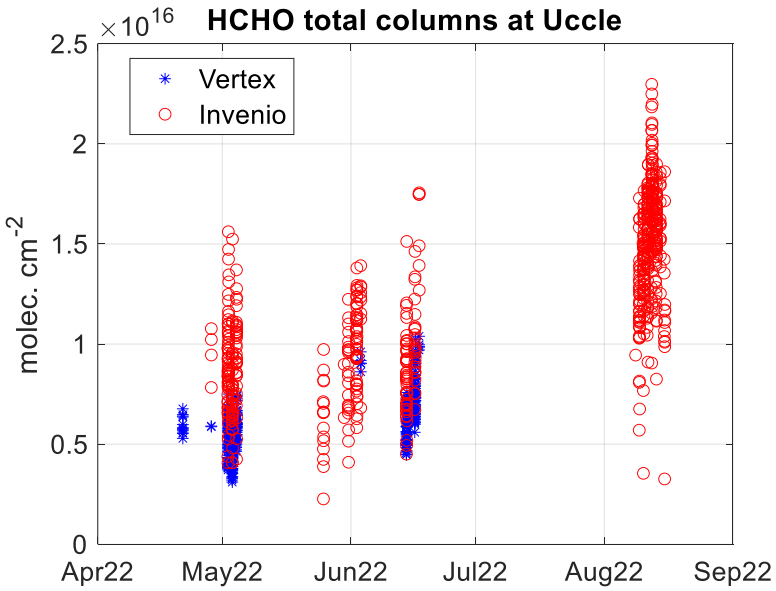
- All partners will re-process their own data with latest version of GGG / PROFFAST/ LHR retrieval algorithm
- BIRA will re-do the intercomparison exercise to validate the results.

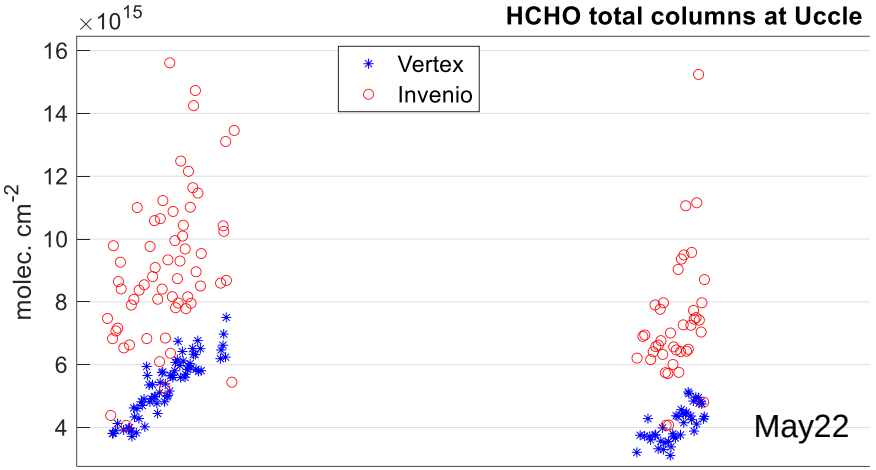
Current situation and planned work for the short term:

Status – HCHO – BIRA-IASB – Vertex70 setup at Uccle (BIRA campus)

WP2: Improvements to retrieval algorithms for GHG and additional species from low-resolution and TCCON spectrometers

- **Formaldehyde (HCHO) retrievals at Uccle from Bruker Vertex70 and Invenio measurements.**

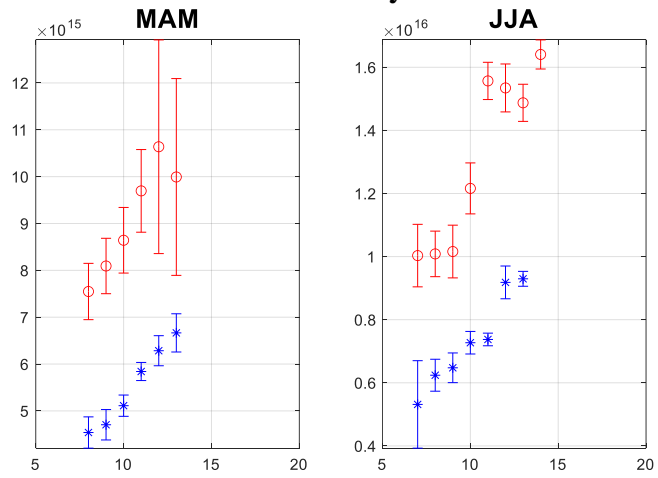




- **7 days of coincidences.**

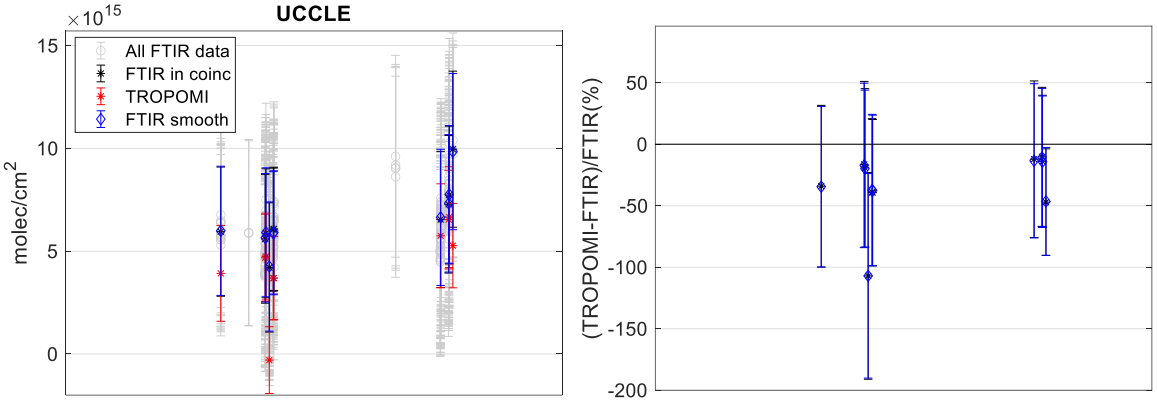
- **Larger scatter for Invenio (18% vs 9.5% for daily std)**
- **Invenio biased high (about a factor 2 !)**

Diurnal cycle



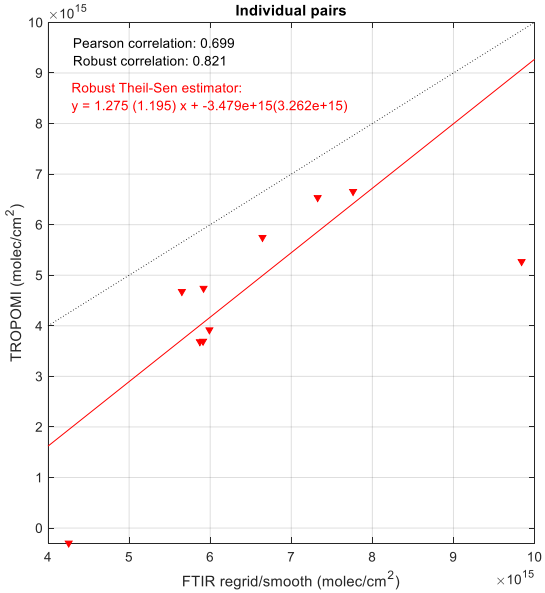
WP2: Improvements to retrieval algorithms for GHG and additional species from low-resolution and TCCON spectrometers

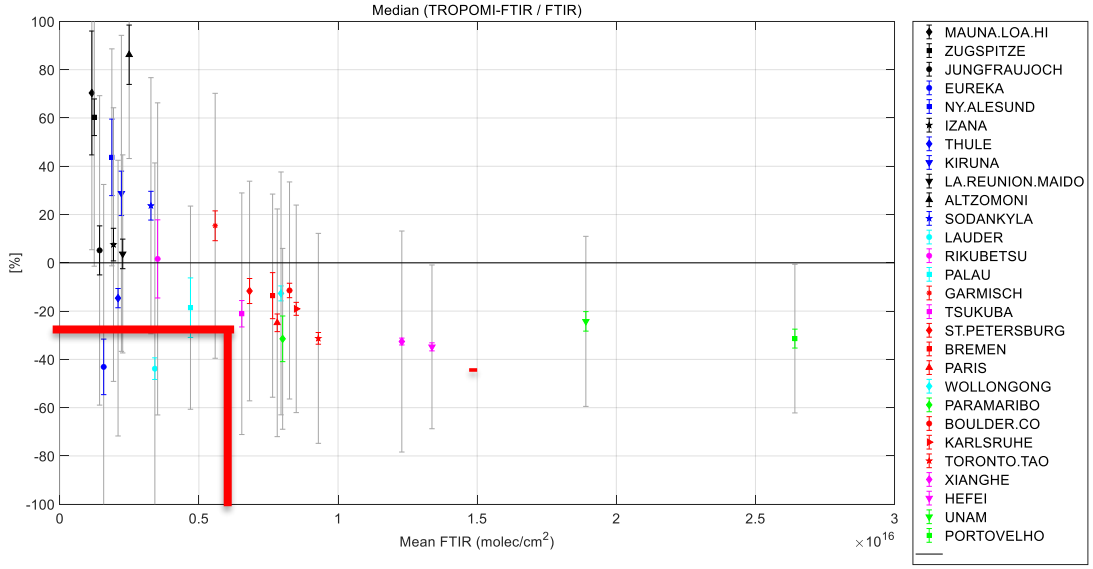
- **Comparison Vertex HCHO with TROPOMI.**



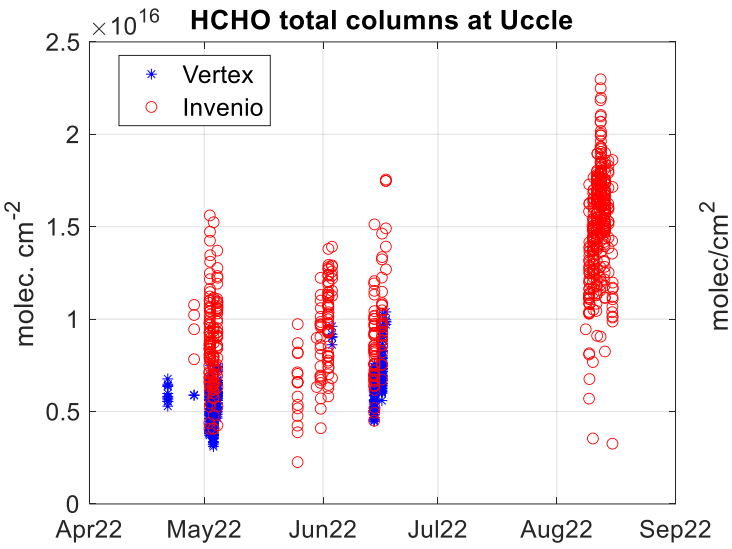
- Median BIAS TROPOMI vs Vertex = -27%
  This is in rather agreement with validation using NDACC data for the mean HCHO levels in Uccle. (6.3E15 molec/cm2)
  Need more coindicences…

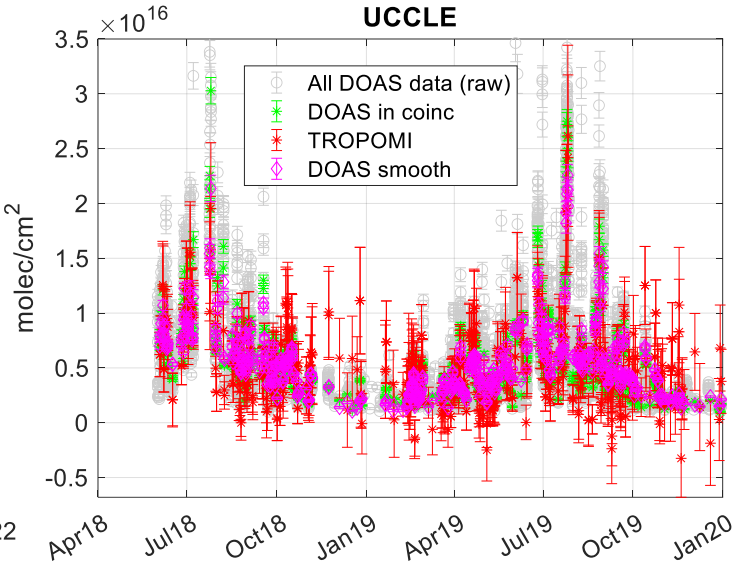
- BIAS TROPOMI vs Invenio= -52%
  Invenio high bias to be investigated…





WP2: Improvements to retrieval algorithms for GHG and additional species from low-resolution and TCCON spectrometers

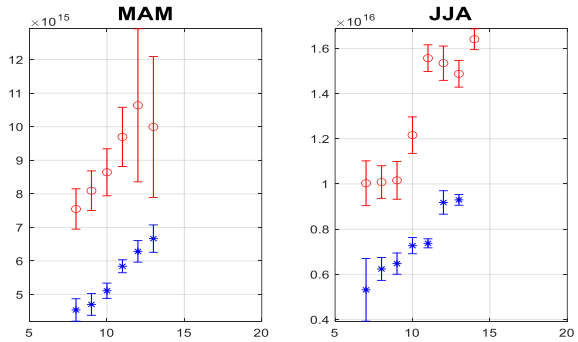


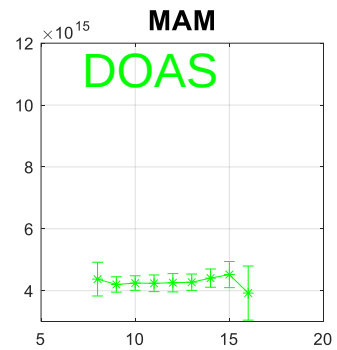


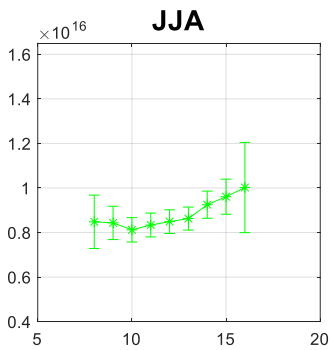
- **Seasonal cycle in agreement with MAX-DOAS at Uccle: maximum in (July) - August**

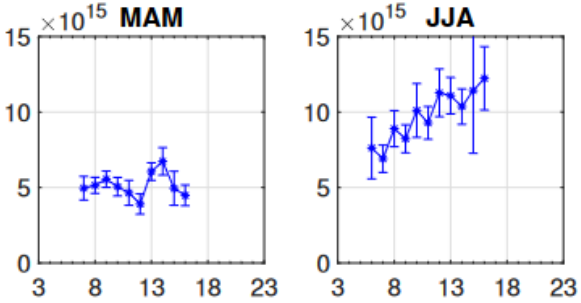
- **Stronger diurnal cycle with vertex / invenio than with MAX-DOAS**

- **To be investigated, but similar stronger diurnal cycles in JJA can be observed with 125HR as well for similar areas (e.g., Bremen here)**









Bremen

WP 3: Improvements to TCCON and COCCON network operations, consistency and data delivery

Contractor: UBremen

WP Manager: **KIT**

Start Event: Month 1 Planned Date: September 2021
End Event: Month 48 Planned Date: September 2025

Inputs:

- GGG2020 with updated TCCON a priori profiles
- Prototype EM27/SUN travelling standard instrument
- Agreement with ECMWF for facilitating delivery of ECMWF/CAMS data

Tasks (Responsible partners; lead in bold):

T1 (**BIRA**, KIT, UBremen):

Develop rapid delivery of GHG data for satellite validation from low-resolution NIR spectra:

- Establish and implement procedure for procuring NRT ECMWF P/T profiles and providing them to partners
- Implement dual option to either use NCEP or NRT ECMWF P/T profiles in PROFFAST
- Verify the improvements of the retrieval products using the updated TCCON a priori profiles in PROFFAST
- Investigate the benefits of using CAMS data provided by ECMWF as a priori profiles for the target gases in PROFFAST
- Coordinate with TCCON chairs and GGG developers for using NRT ECMWF P/T profiles in GGG
- Plan and implement, for Vertex70 and IRCube, all the proper actions and procedures aimed at pursuing harmonisation with COCCON

Current situation and planned work for the short term:

Status
3.1.1 – ECMWF P/T profiles (ERA5 – reanalysis*) will be provided for the target TCCON / COCCON, latency of 5 days, monthly files are available on 6th of every month, lat-lon 0.25 degree, 37 pressure levels (1000 hPa to 1 hPa) – BIRA-IASB
3.1.2 – KIT
3.1.3 – BIRA-IASB
3.1.4 – CAMS (O-suite – changes in time with model updates, **reanalysis** – stable in time, produced using 4DVar data assimilation in Cycle 42r1 of ECMWF's Integrated Forecasting System (IFS), with 60 hybrid sigma/pressure (model) levels in the vertical, with the top level at 0.1 hPa, 3-hourly, 3-dimensional, time-consistent atmospheric composition daily means or monthly means of daily means for the month as a whole, CO2, CH4, CO data, public data till 2020, private data to be discussed, working on an opendap database to distribute the data to the project partners.
3.1.5 – UBremen
3.1.6 – UBremen, UoW, KIT
COCCON plan for Vertex and IRCube yet to start.
*https://cds.climate.copernicus.eu/cdsapp#!/dataset/reanalysis-era5-pressure-levels-monthly-means?tab=overview

T2a (BIRA, all partners)
Outreach:

- Throughout the whole project duration: regularly update FRM4GHG Webpages including internal documents repository (building upon FRM4GHG-1 Website); track communications/ publications including results from the project
- Coordinate/ monitor involvement in Sentinel validation efforts

T2b (BIRA, all partners)
Disseminate FRM4GHG-2.0 dataset (see D4.2.3) and PROFFAST source code via Webpages; the FRM4GHG-2.0 relevant datasets will also be made available to the ESA Validation Data Centre (EVDC) in GEOMS HDF

Current situation and planned work for the short term:

Status – BIRA-IASB

D4.2.1 Dynamic FRM4GHG Website (BIRA, continuously)
D4.2.2 Technical Report about Sentinel validation results using FRM4GHG-2.0 data (BIRA, continuously)
D4.2.3 Provision of FRM4GHG-2.0 datasets (BIRA, M48)
Dissemination of all measurement data [Level 1] and corresponding retrieved data [Level 2] collected during the project, as well as of all re-processed (during the project) datasets [Level-2], including a Digital Object Identifier DOI, through the EVDC [RD-9] in GEOMS HDF format [RD-10] as well as through the FRM4GHG project webpages.

frm4ghg.aeronomie.be website update of several pages

Twitter: #frm4ghg
Link to @ESA_EO, @CopernicusEU, @Sentinel5P, …

Write on Campaign Blog

Update pictures on website from campaigns, instrument development, site visits of traveling standard, team meetings, conference / workshop presentations, …

Thank you for your attention

Progress Report - Wollongong

Nicholas Jones*, David Griffith, Nicholas Deutscher

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https://frm4ghg.aeronomie.be/

Objectives

Fiducial Reference Measurements for Ground-Based Infrared Greenhouse Gas Observations (FRM4GHG 2.0)

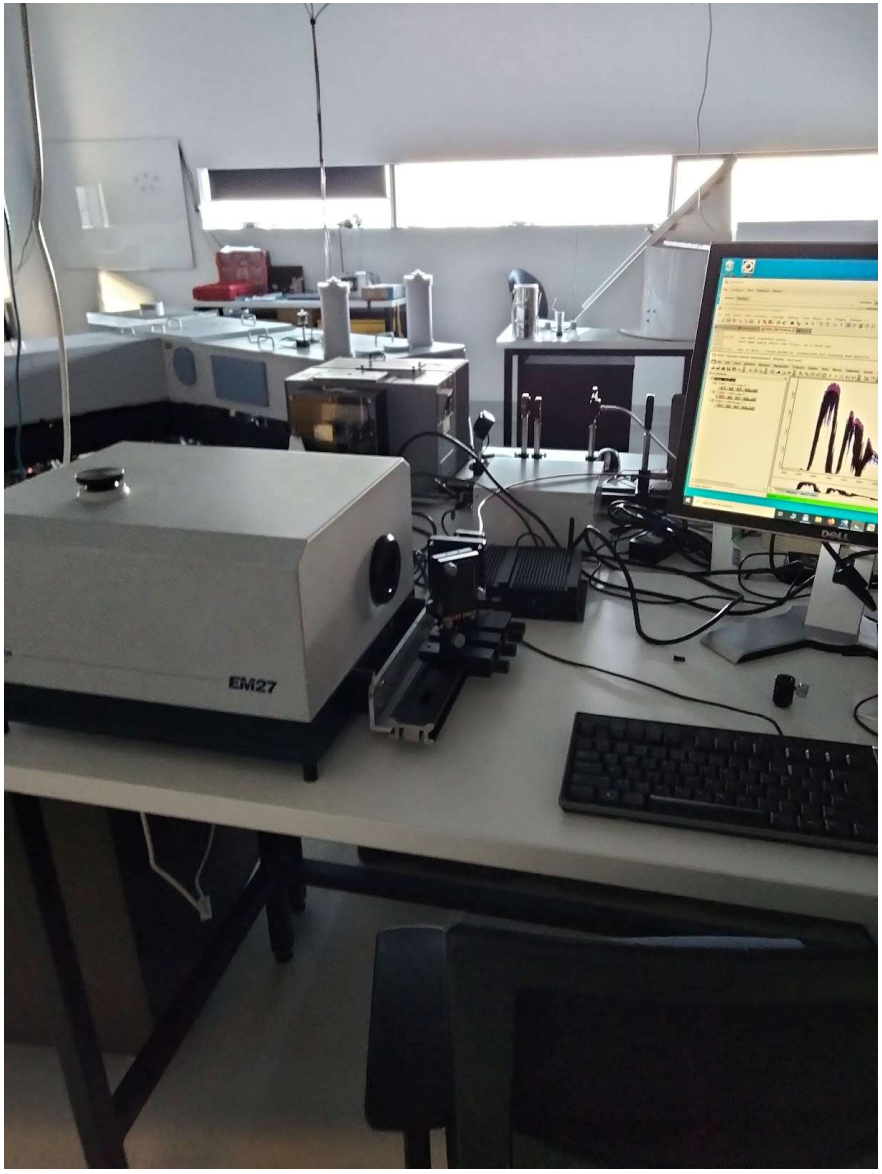
- Spectrometers (NJ)
  - IRCube and EM27 moved to new building
  - Currently running EM27/SUN in "tracker mode" alongside 3 visiting EM27/SUN's including the travelling standard
  - IRCube is running with the "old" fibre as the replacement was broken after the AirCore Campaign

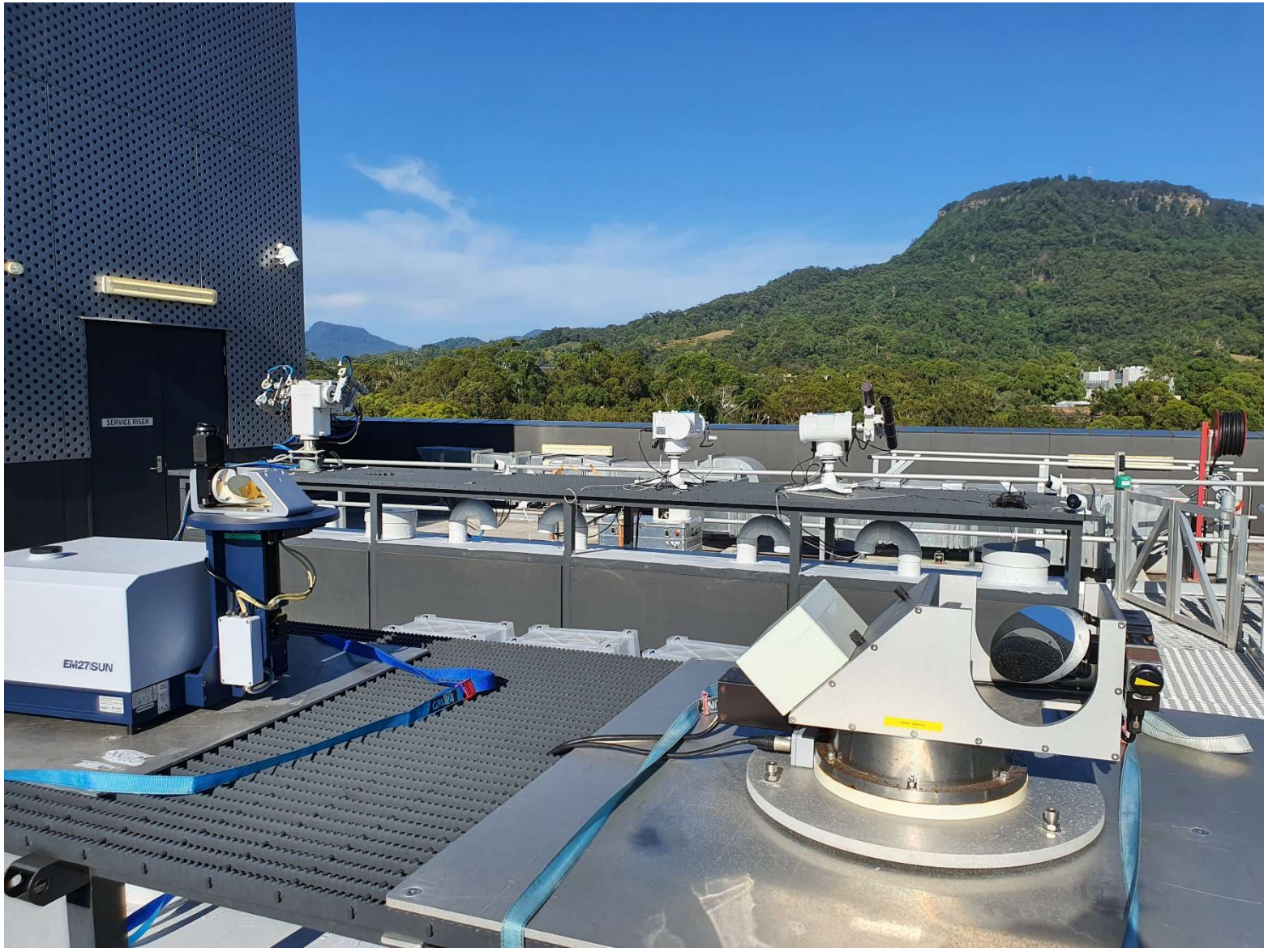
- Analysis of IRcube spectra 2021-2022 (NJ)
  - GGG-2016 nearly complete (up to June 2022)
  - GGG-2020 ongoing

- MIR operation of IRcube with TE-MCT detector and CaF2 BS (DG)
  - Planned work over the next few months

- Aircore campaign Broken Hill September/October 2022 (NJ, DG, ND)


DANGER

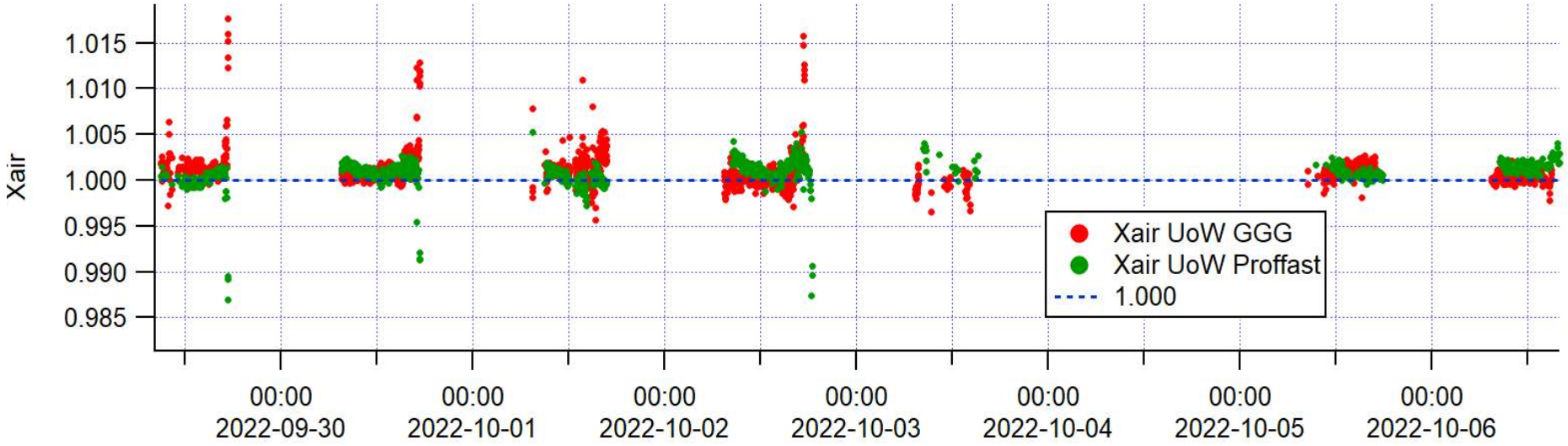

EM27


SERVICE RISER
EM27/SUN

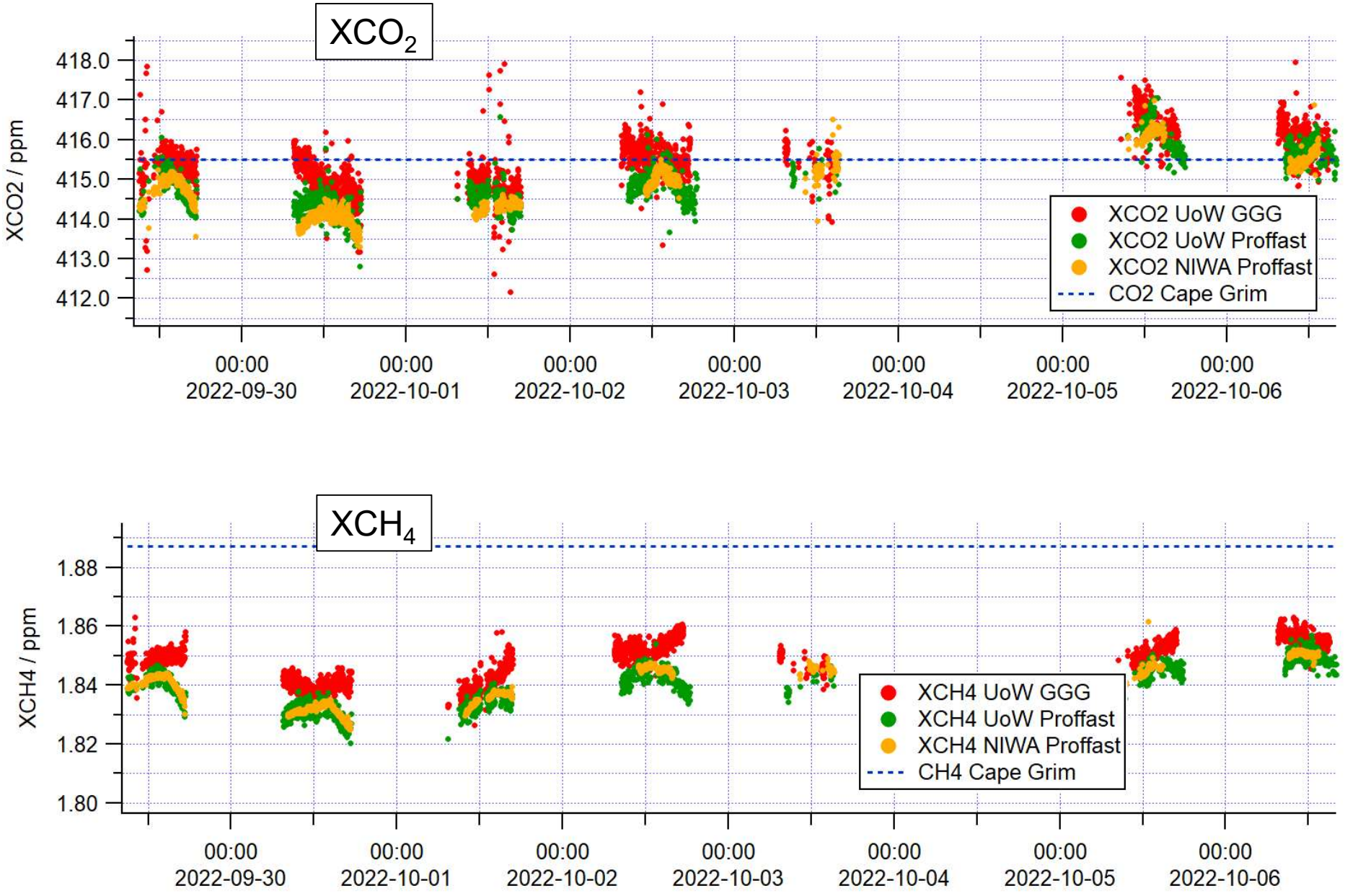
Xgas measurements

Xgas = total column mean mole fraction of gas X

- Two independent retrieval codes
  - GGG (Toon, TCCON), PROFFAST (Hase, COCCON)
- Xgas = column gas / column O_2 x 0.2095
- Xluft (Xair) = pressure / O_2 x 0.2095
  - Reality check: Xluft = 1.00 if O_2 retrieval is perfect



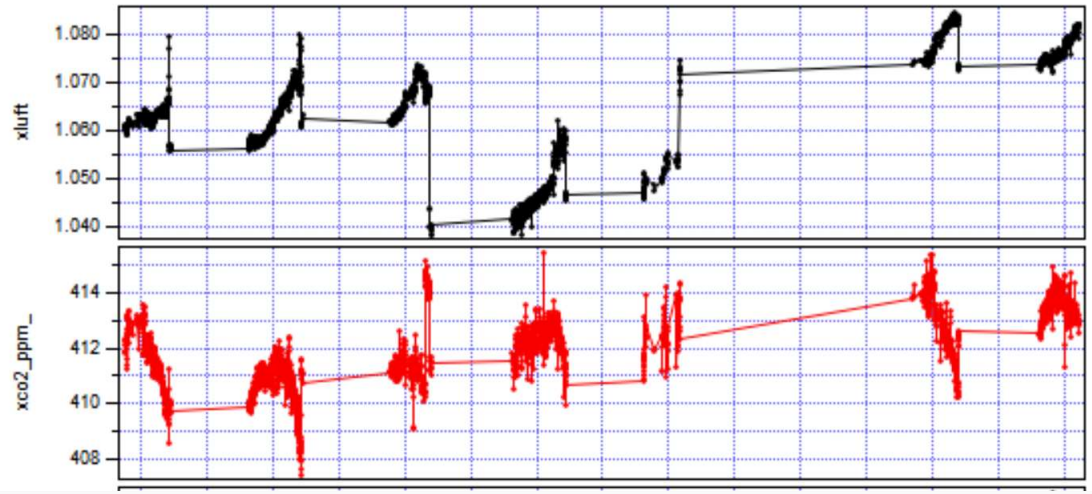
Griffith et al, ACCOMC, Melbourne, 2022



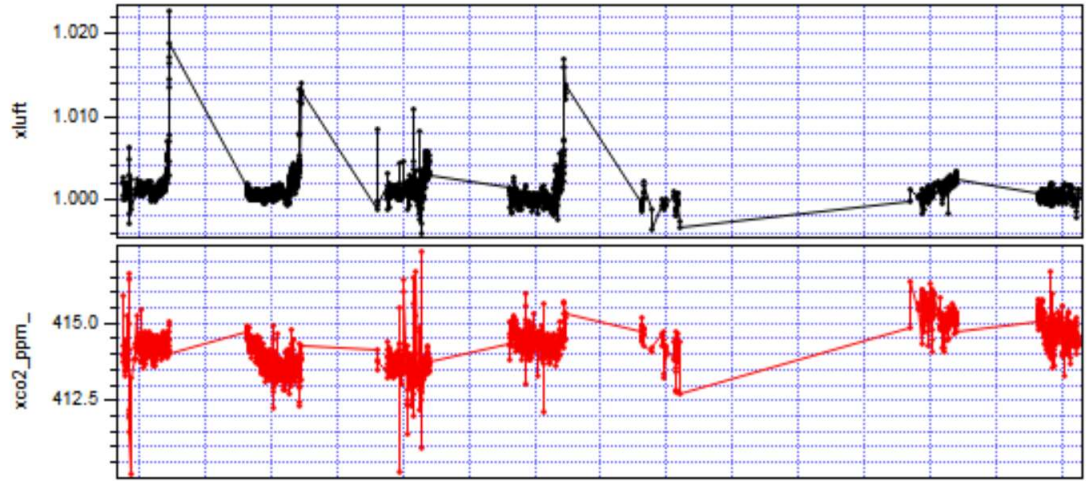
Griffith et al, ACCOMC, Melbourne, 2022

Broken Hill IRCube and EM27/SUN

IRcube:



EM27:



Planned activities 2023

Fiducial Reference Measurements for Ground-Based Infrared Greenhouse Gas Observations (FRM4GHG 2.0)

- Spectrometers (NJ)
  - IRCube and EM27 continued operation in new building
  - Place instruments back into their "normal" configuration (IRCube with replacement FO, and EM27/SUN old FO)
  - Investigate IRCube's XLUFT sensitivity with respect to FO rotation
- MIR operation of IRcube with TE-MCT detector and CaF2 BS (DG)
  - Planned work over the next few months
- Analysis of IRcube spectra 2021-2022 (NJ)
  - GGG-2016 complete to end of 2022
  - GGG-2020 cover same tim eperiod as GGG-2016
  - Reanalysis of Sodankyla and Darwin campaigns with GGG2020
  - Proffast analysis

Thank you for your attention

Aircore Broken Hill 2022
Total column remote sensing with solar FTS

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https://frm4ghg.aeronomie.be/

Aircore Broken Hill 2022

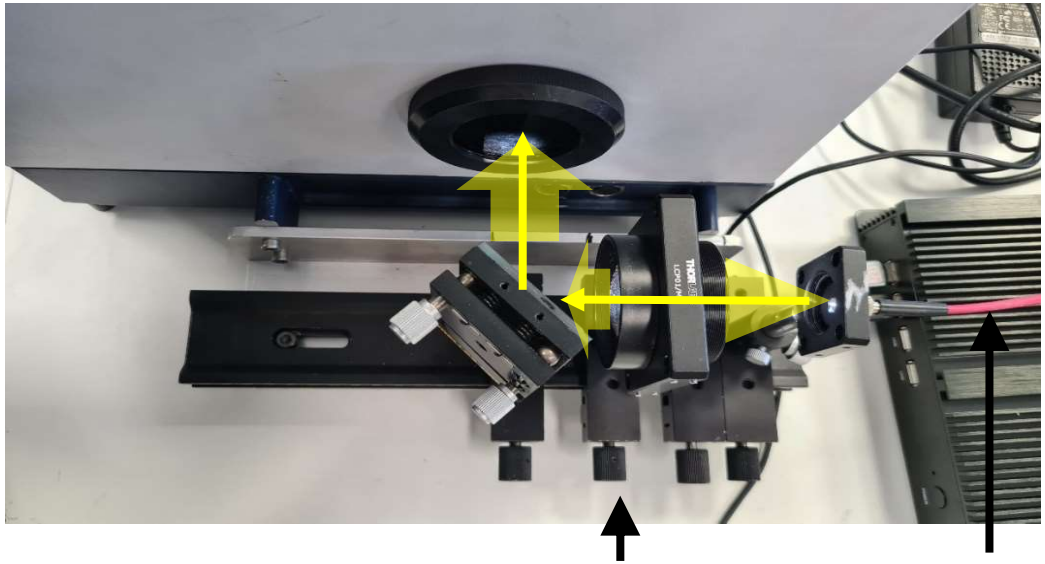
Total column remote sensing with solar FTS

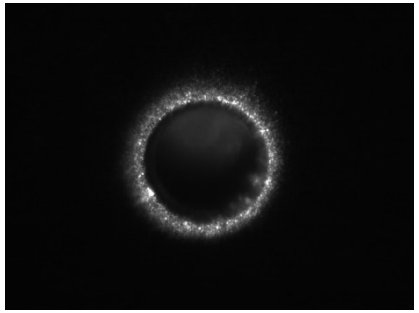
David Griffith, University of Wollongong

- UoW – Aircore and solar FTS remote sensing
  - Nick Deutscher, David Griffith, Clare Murphy, Jack Simmons, Travis Naylor, Nicholas Jones
- NOAA – Aircore
  - Bianca Baier, Tim Newberger, Jack Higgs
- NIWA, U Auckland – EM27/Sun remote sensing
  - Dave Pollard, David Noone (i.a.)

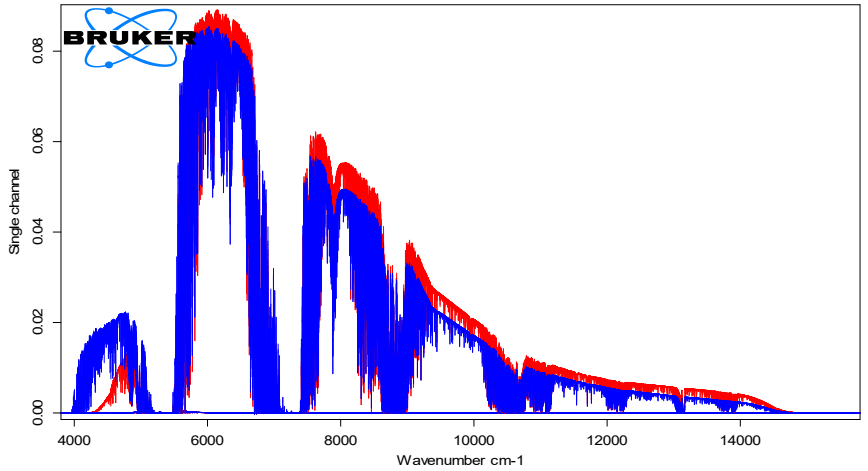
To remind you:

EM27 / IR cube with fibre optic solar tracker coupling



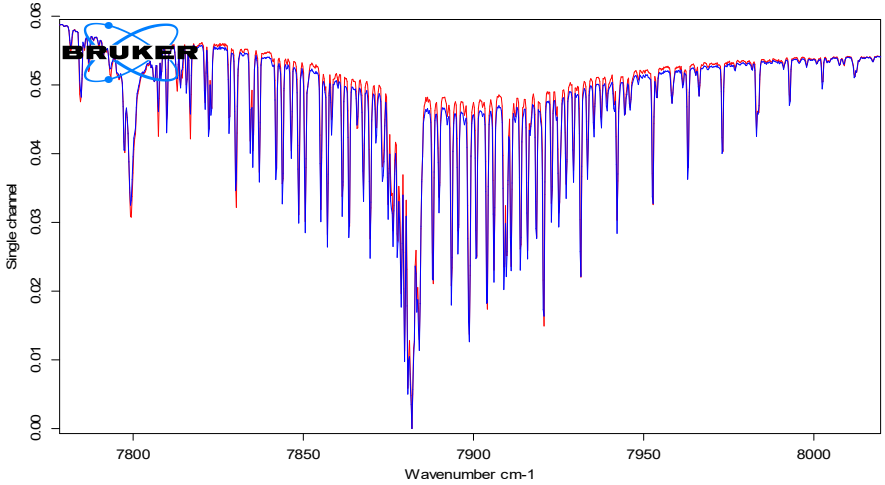


Comparative spectra
cam tracker & fibre-optic



O:\Data\EM27\FO\220607_142234samp.0	EM27SUN setup	2022-06-07
O:\Data\EM27\FO\220617_130020samp.0	EM27SUN setup	2022-06-17
O:\Data\EM27\FO\220607_142234samp.0	EM27SUN setup	2022-06-07
O:\Data\EM27\FO\220617_130020samp.0	EM27SUN setup	2022-06-17

Page 1/1

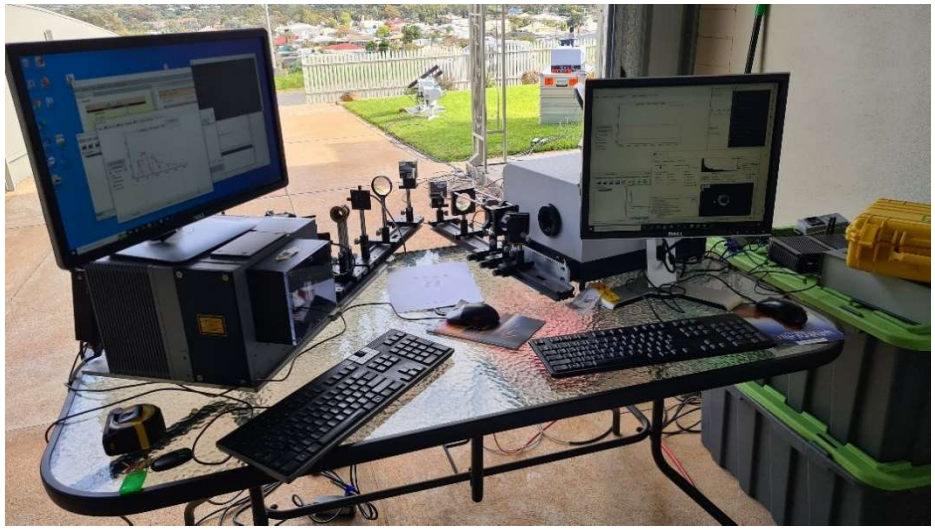


O:\Data\EM27\FO\220607_142234samp.0	EM27SUN setup	2022-06-07
O:\Data\EM27\FO\220617_130020samp.0	EM27SUN setup	2022-06-17

Page 1/1

EM27 and IRcube remote sensing measurements at Broken Hill

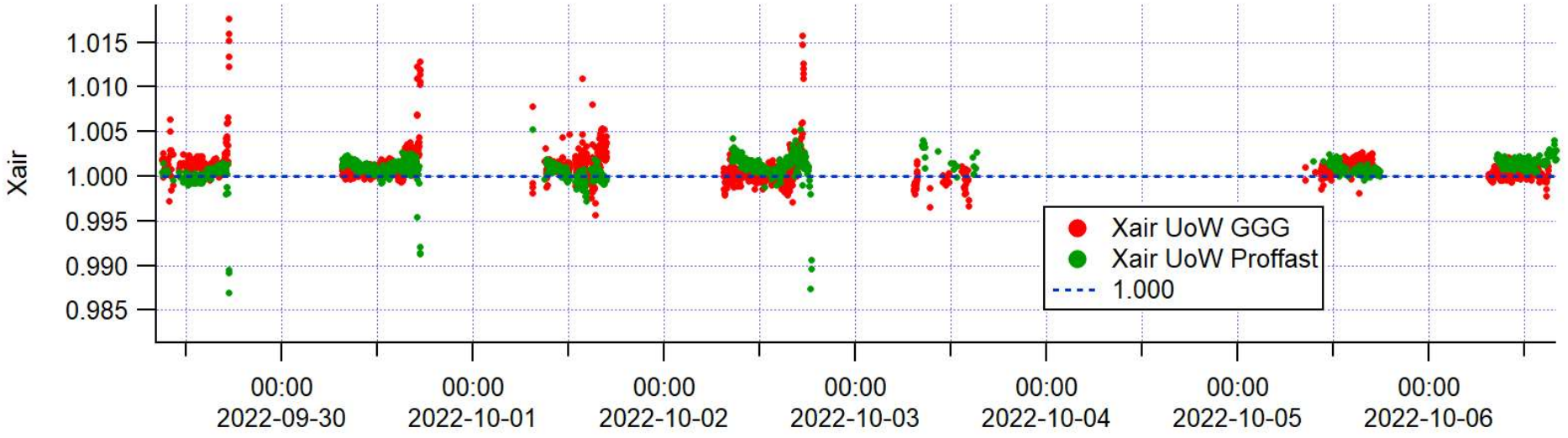
- 4 independent low resolution solar FTS instruments
  - 2 x EM27/Sun with camtracker (NIWA, Uni Auckland, COCCON standard)
  - 1 x EM27 FTS with fibre-optic coupling to tracker (UoW – in development)
  - 1 x IRcube FTS with fibre-optic coupling to tracker (UoW)
- 7 days of measurements, including all aircore flight days

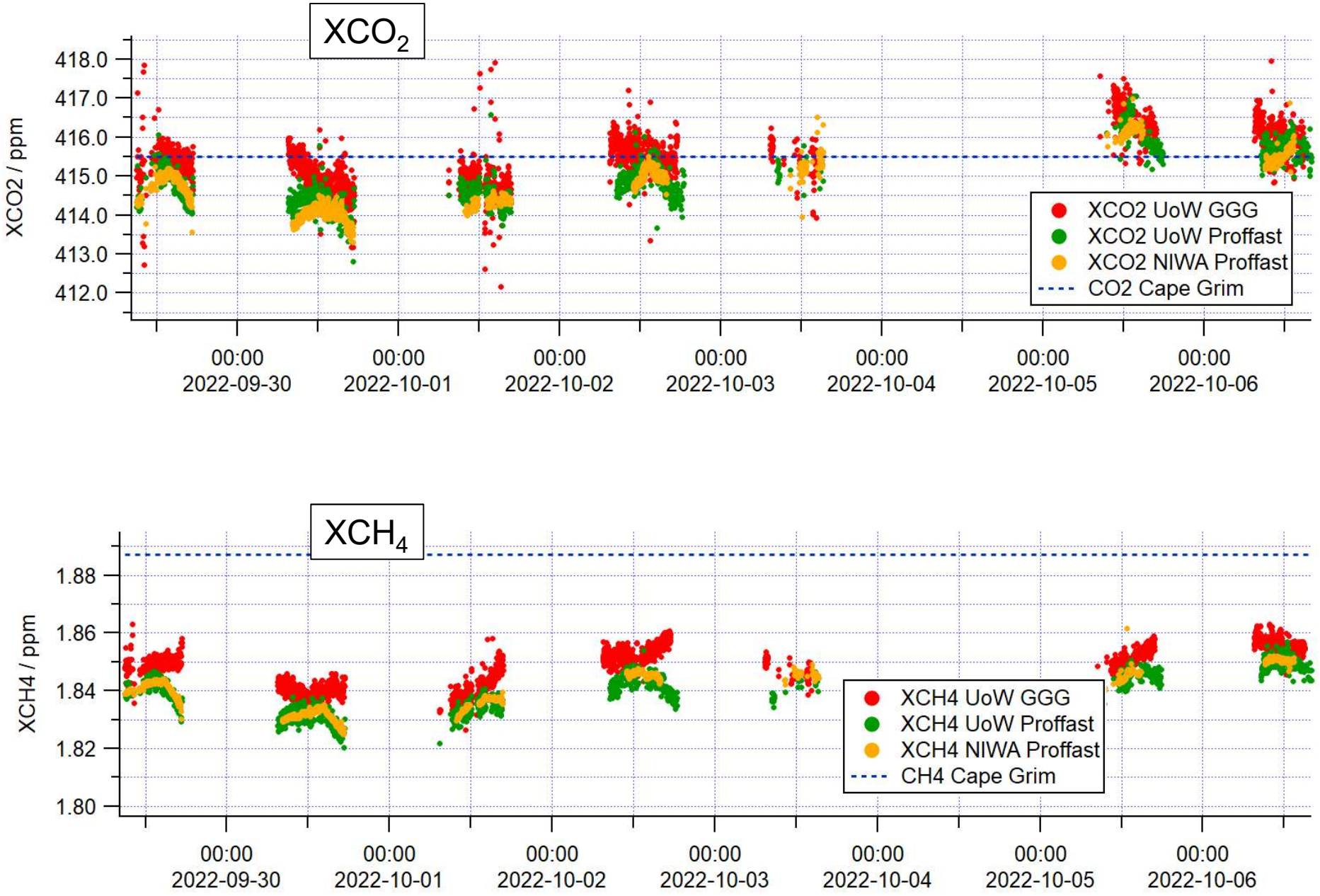


Xgas measurements

EM27-fibre optic, GGG and Proffast

- Two independent retrieval codes
  - GGG (Toon, TCCON), PROFFAST (Hase, COCCON)
- Xgas = column gas / column O_2 x 0.2095
- Xluft (Xair) = pressure / O_2 x 0.2095
  - Reality check: Xluft = 1.00 if O_2 retrieval is perfect




XCO2
XCO2 / ppm
418.0
417.0
416.0
415.0
414.0
413.0
412.0
XCO2 UoW GGG
XCO2 UoW Proffast
XCO2 NIWA Proffast
CO2 Cape Grim
00:00
2022-09-30
00:00
2022-10-01
00:00
2022-10-02
00:00
2022-10-03
00:00
2022-10-04
00:00
2022-10-05
00:00
2022-10-06
XCH4
XCH4 / ppm
1.88
1.86
1.84
1.82
1.80
XCH4 UoW GGG
XCH4 UoW Proffast
XCH4 NIWA Proffast
CH4 Cape Grim
00:00
2022-09-30
00:00
2022-10-01
00:00
2022-10-02
00:00
2022-10-03
00:00
2022-10-04
00:00
2022-10-05
00:00
2022-10-06

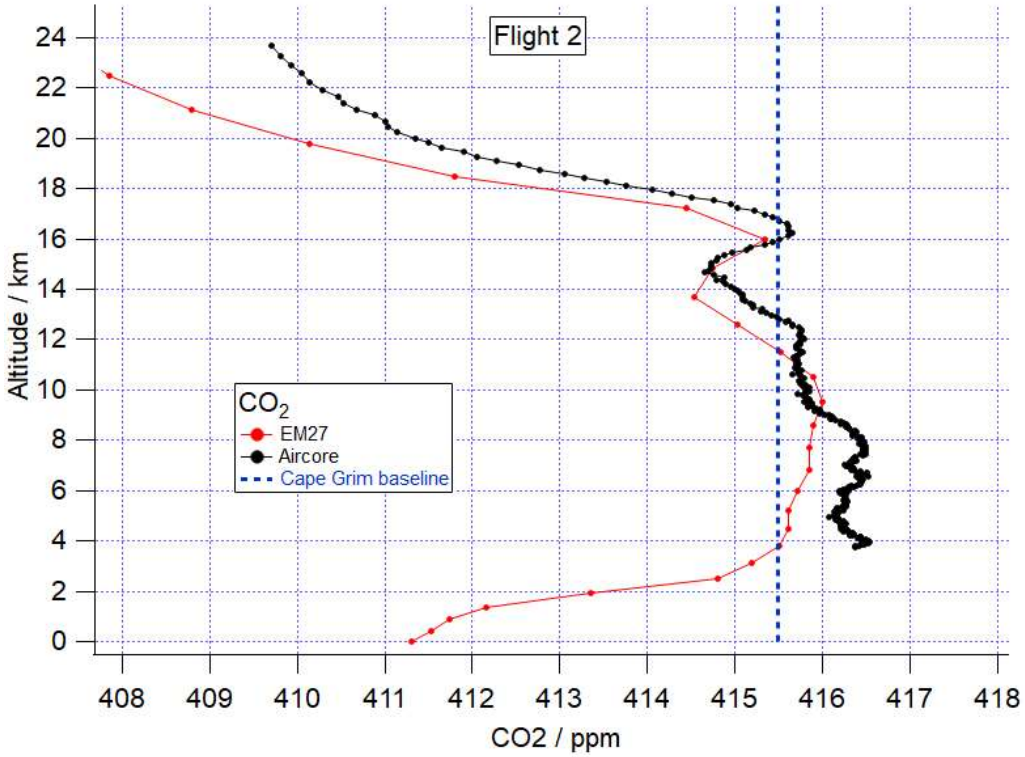
Vertical profiles

- *a priori* profile shape derived from GEOS-FPIT reanalysis 3 hourly
- Profile amplitude scaled to fit measured spectra
- Example: CO_2, flight 2

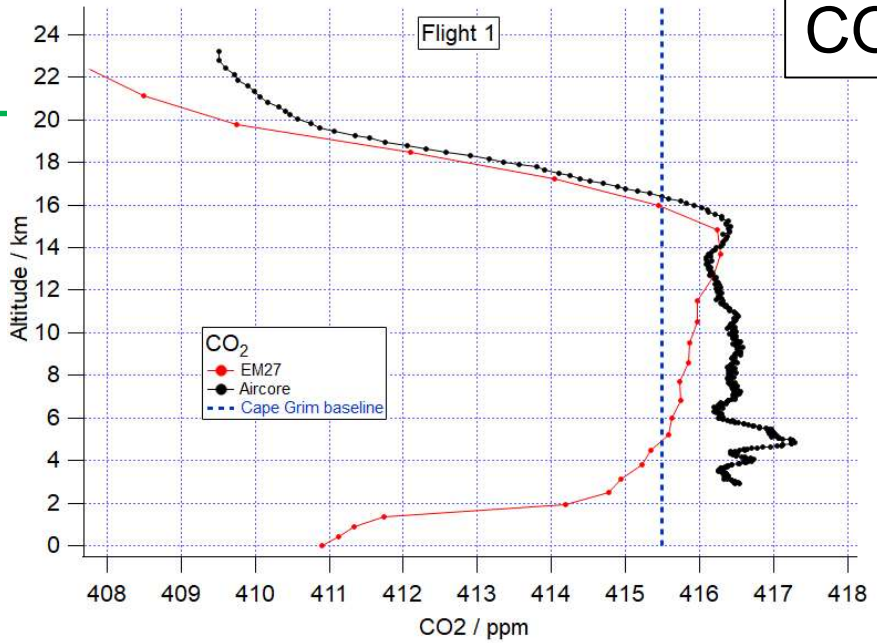
___ scaled EM27 profile

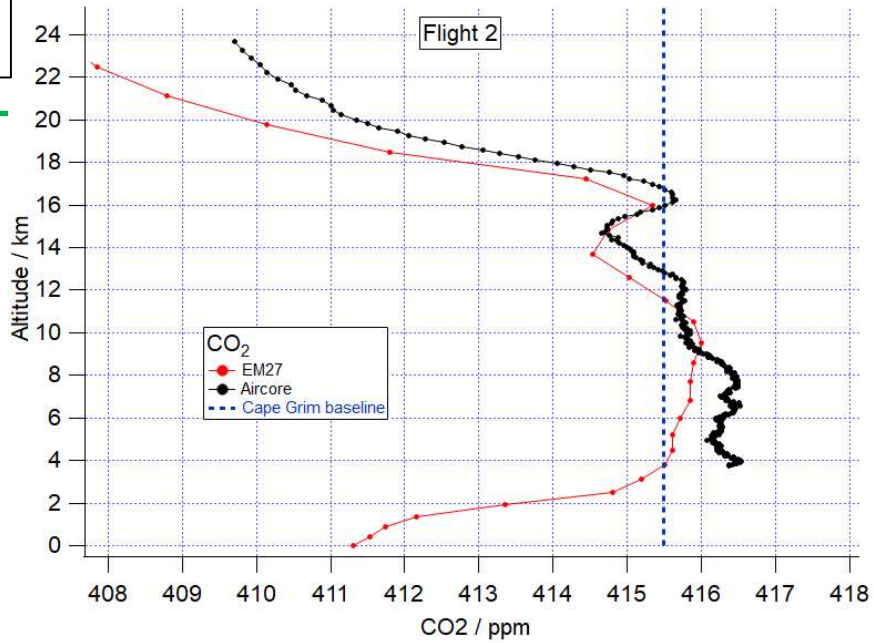
___ Aircore profile

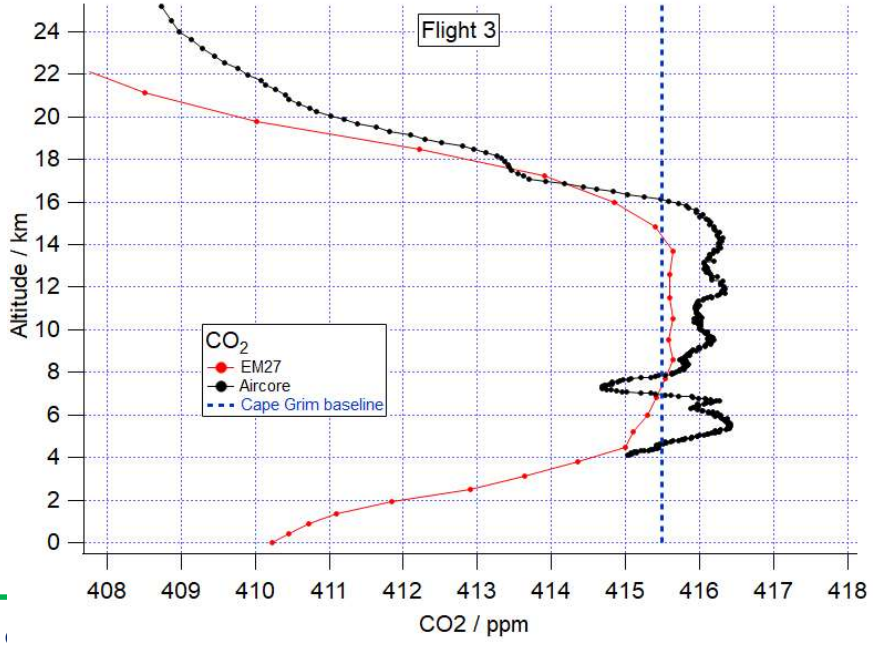
----- Cape Grim Baseline, Sept 2022 (Thanks Paul Krummel)

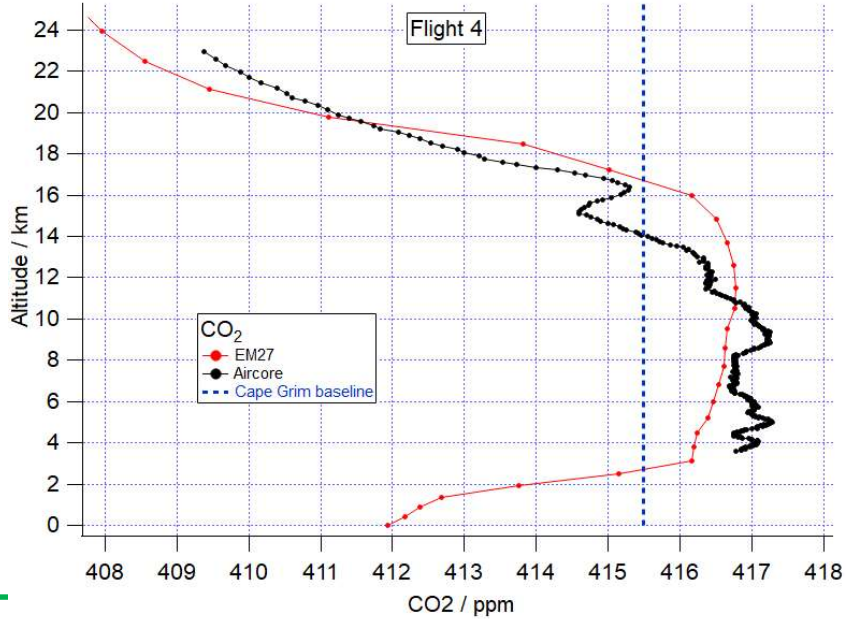


CO_2

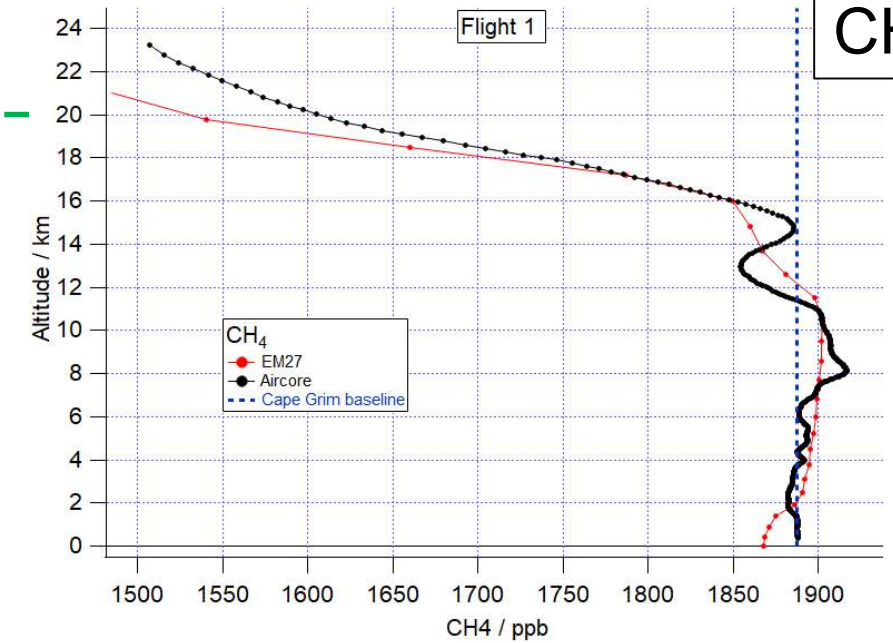

Flight 1
Altitude / km
CO2 / ppm
CO2
EM27
Aircore
Cape Grim baseline

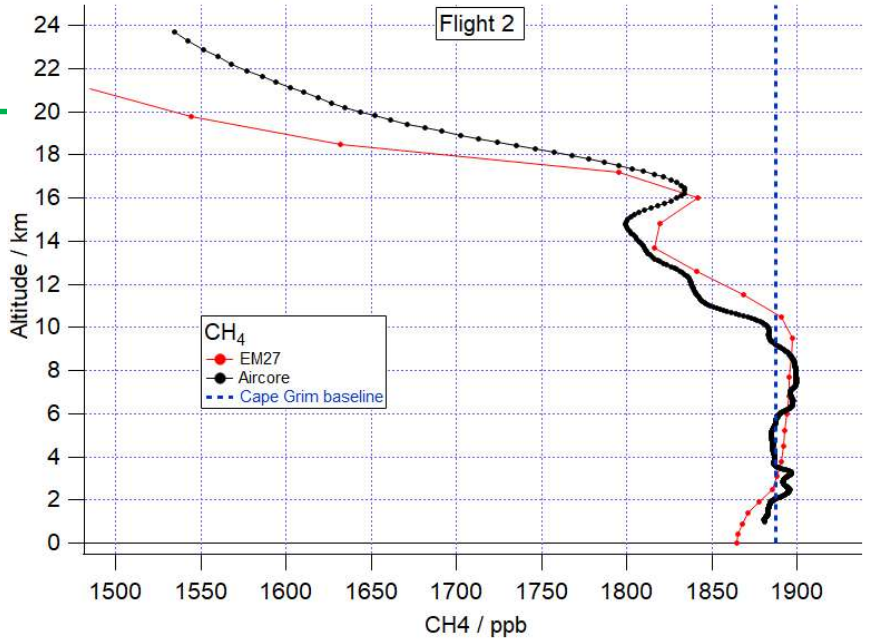

Flight 2
Altitude / km
CO2 / ppm
CO2
EM27
Aircore
Cape Grim baseline

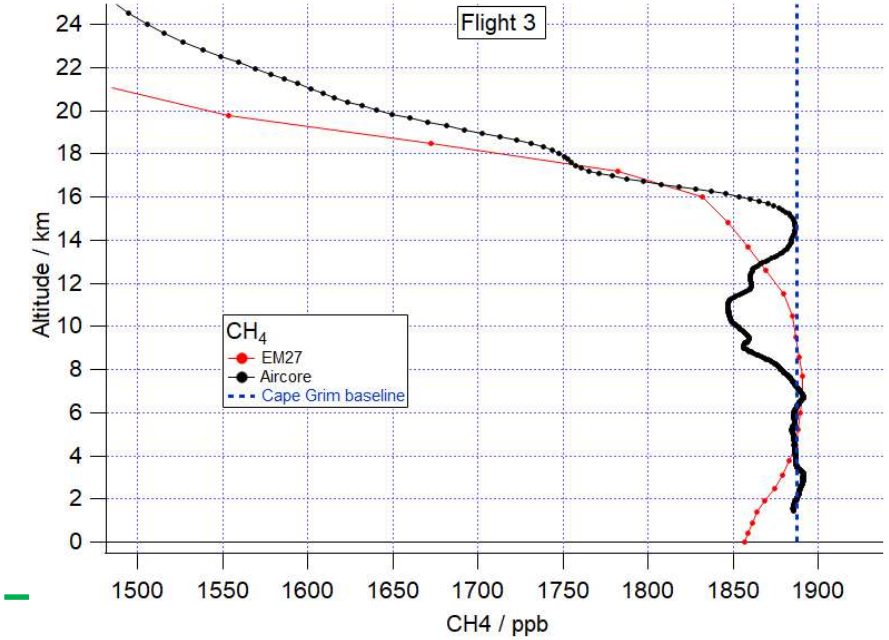

Flight 3
Altitude / km
CO2 / ppm
CO2
EM27
Aircore
Cape Grim baseline

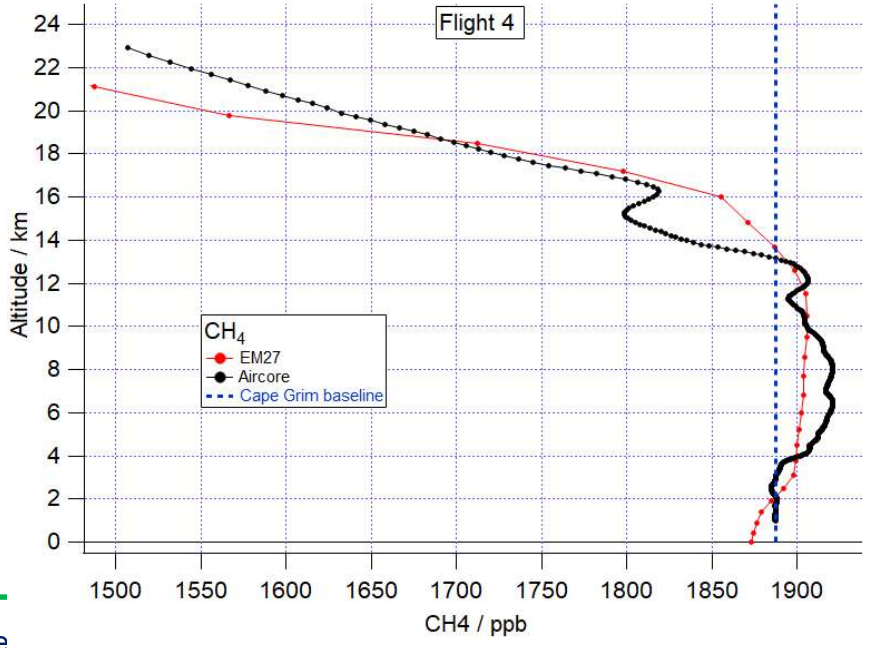

Flight 4
Altitude / km
CO2 / ppm
CO2
EM27
Aircore
Cape Grim baseline

CH_4


Flight 1
Altitude / km
CH4 / ppb
CH4
EM27
Aircore
Cape Grim baseline


Flight 2
Altitude / km
CH4 / ppb
CH4
EM27
Aircore
Cape Grim baseline


Flight 3
Altitude / km
CH4 / ppb
CH4
EM27
Aircore
Cape Grim baseline


Flight 4
Altitude / km
CH4 / ppb
CH4
EM27
Aircore
Cape Grim baseline

nee

Preliminary look only - more to come
Thank you – now back to Nicholas

Report Travel Standard D3.2.1

Benedikt Herkommer*, Frank Hase, Jochen Groß, Isamu Morino, Matthias Frey, Lawson Gillespie, Nasrin Pak, Debra Wunch, Nicholas Deutscher

*benedikt.herkommer@kit.edu

https://frm4ghg.aeronomie.be/

Objectives

Fiducial Reference Measurements for Ground-Based Infrared Greenhouse Gas Observations (FRM4GHG 2.0)

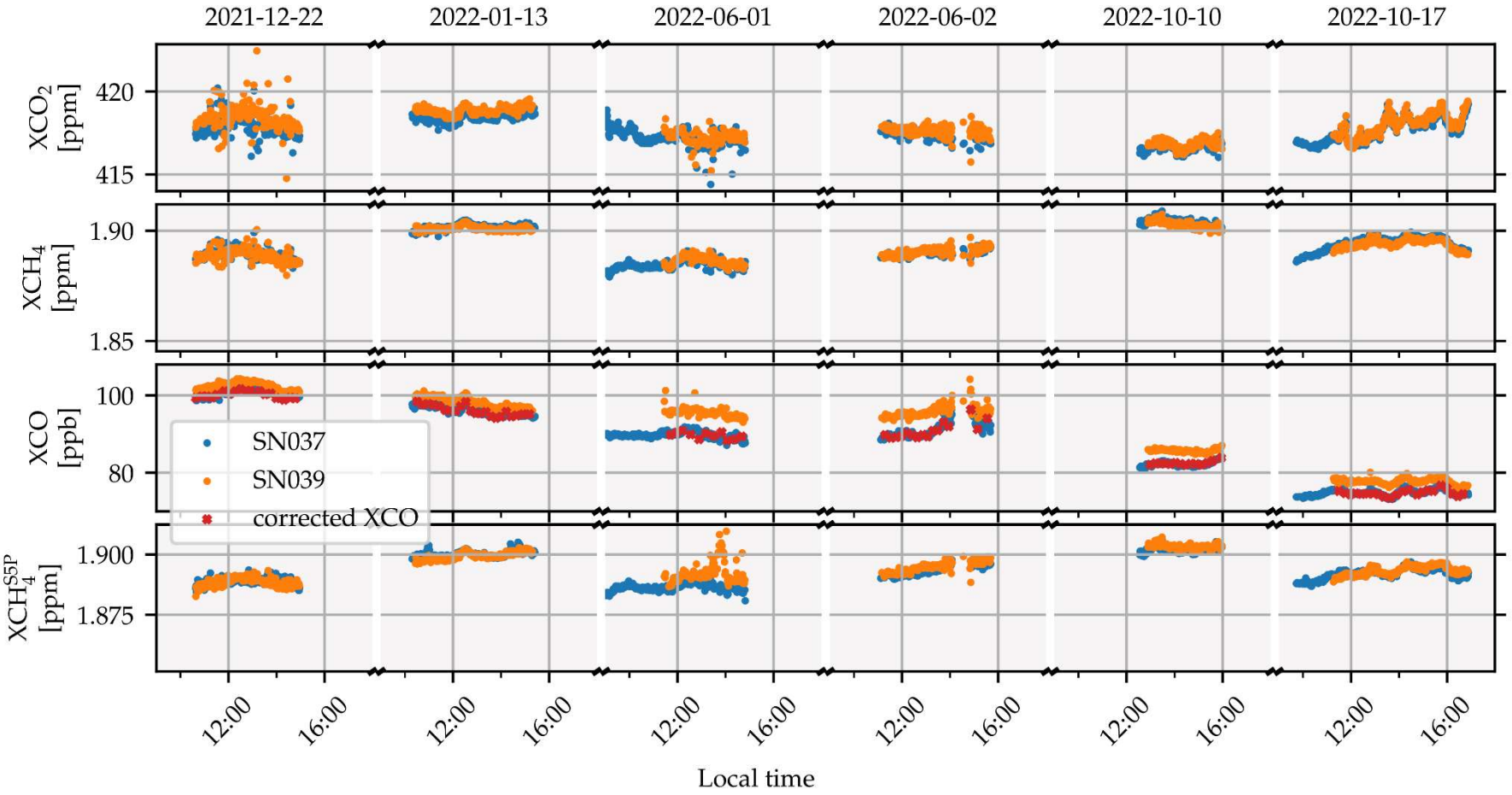
- Status update Travel Standard
- Presentation of calibration procedure

Current Status

Fiducial Reference Measurements for Ground-Based Infrared Greenhouse Gas Observations (FRM4GHG 2.0)

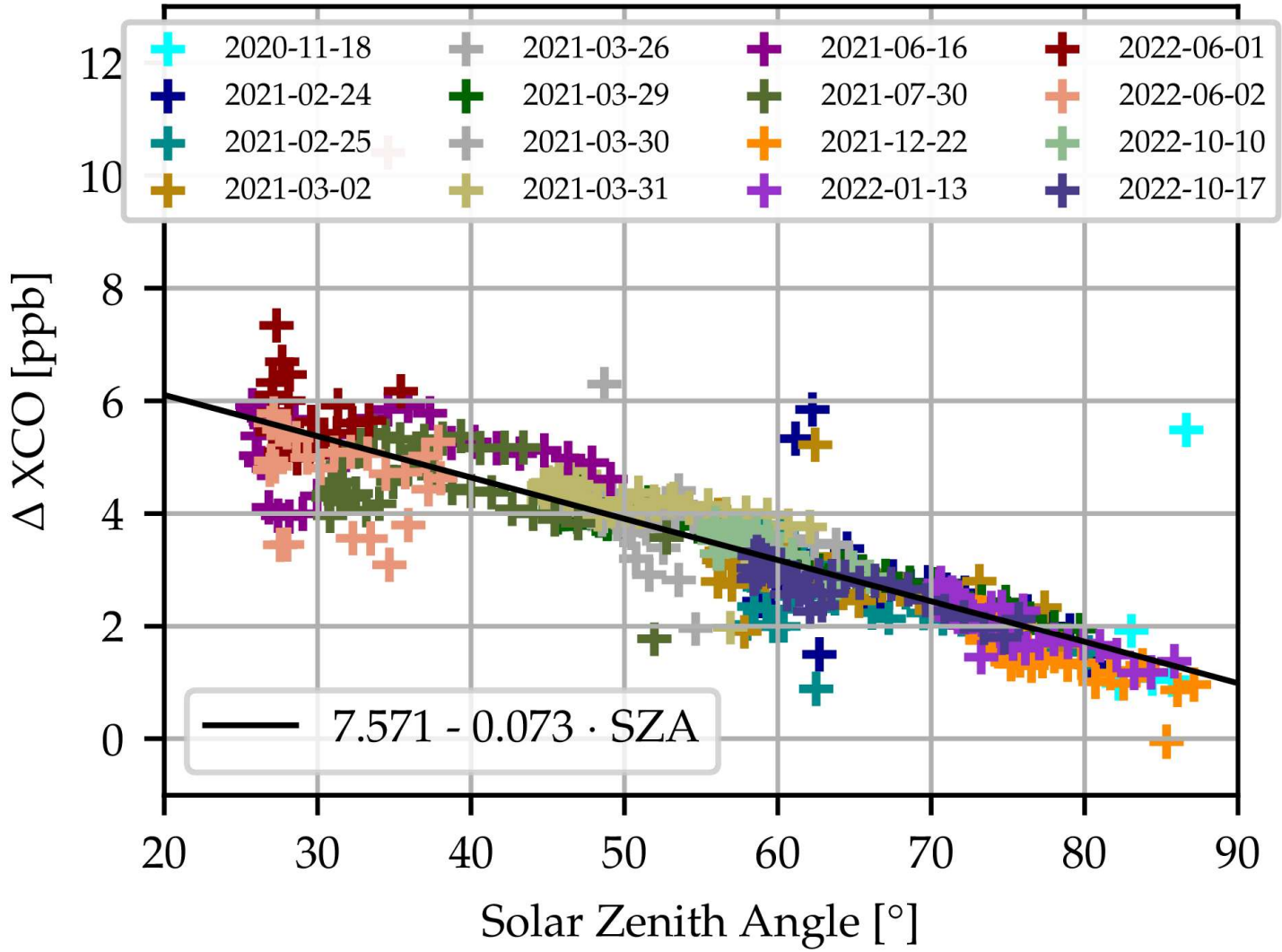
- Visited Tsukuba, ETL, currently in Wollongong
  - Still a lot of problems with the shipment → Delay of the schedule
  - Succesfull campaign in Japan
  - At ETL there was a laser failure → No side-by-side measurements
  - Measurements are going on
- Side-by-side and ILS measurements between each campaign at KIT

Side-by-side measurements in KA

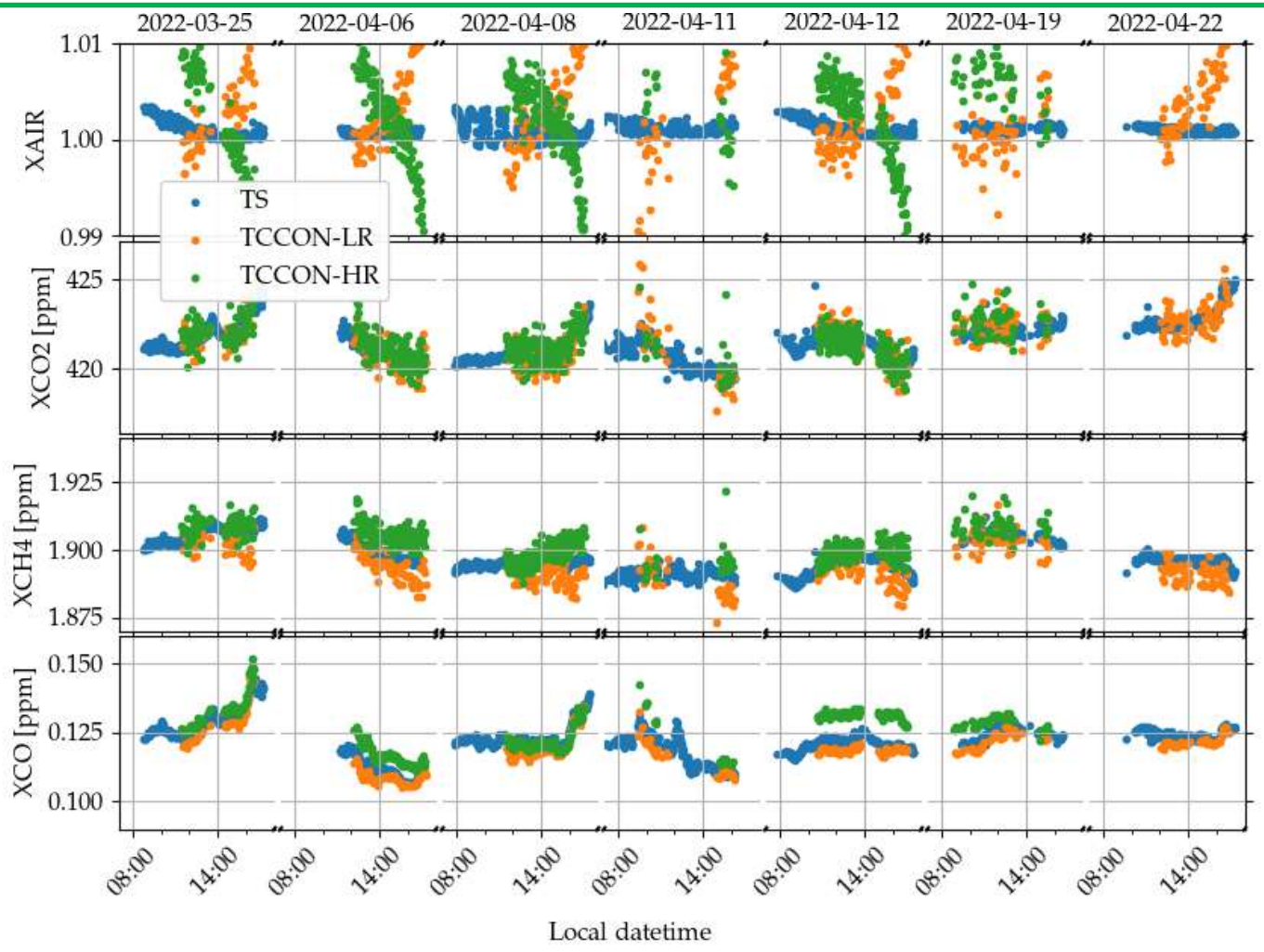


Gives correction factors $c_{TS}^{TCCON\text{-}KA}$ needed later to compare to TCCON-KA

Side-by-side measurements in KA



Results of Tsukuba, Japan



Gives correction factors $c^{TS}_{TCCON\text{-}TS}$

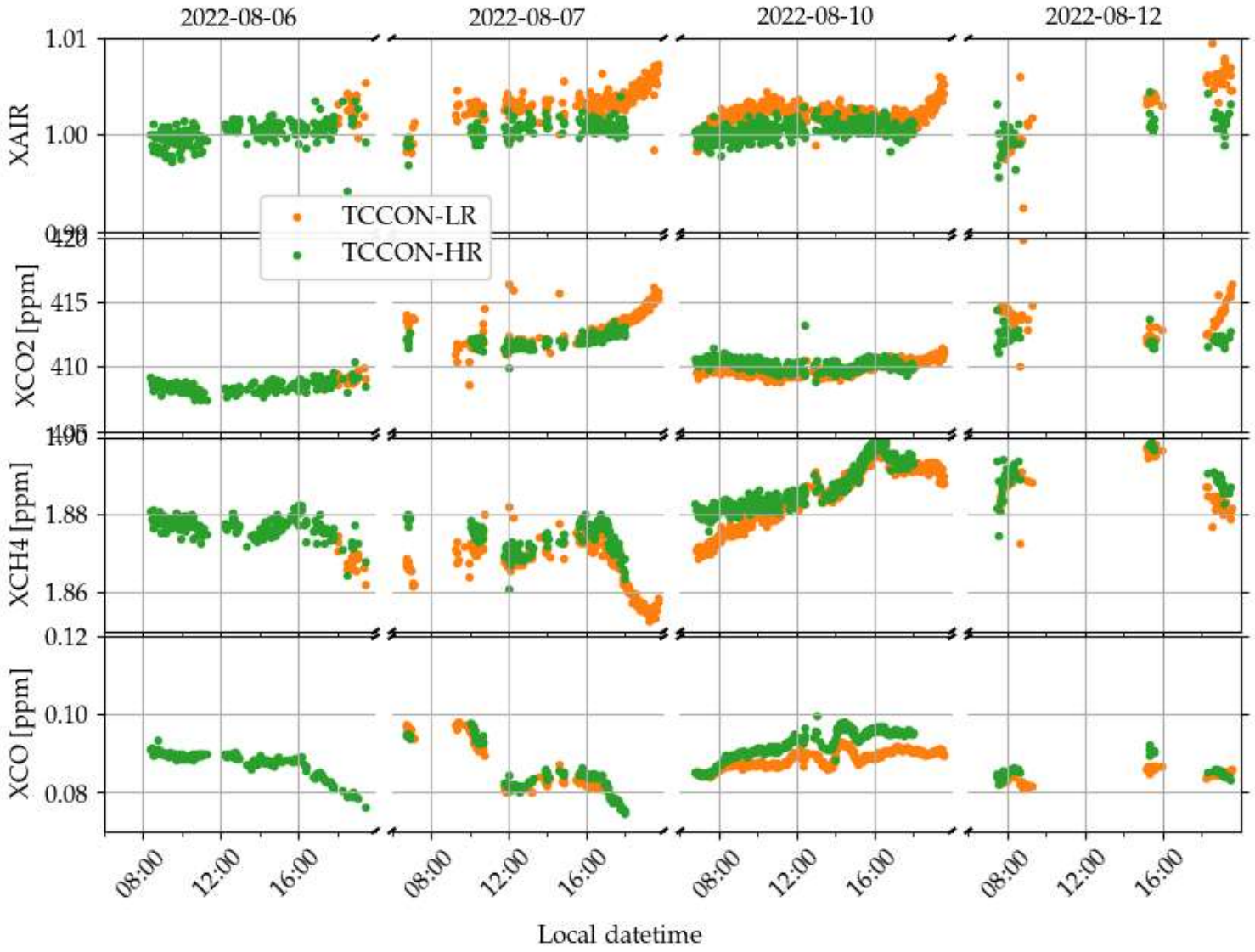
Results of Tsukuba, Japan

- Good agreement for XCO2 and XCH4 for both, high-res and low-res data

- For XCO high-res data, there are some days with less and some days with better agreement
  - This is most probable due to the a-prioris of XCO
  - A known issue in the TCCON community

- High noise in all Tskubua data:
  - Due to a intensity drop in the spectra at the O2 window.
  - This is probably due to the beamsplitter or the detector.

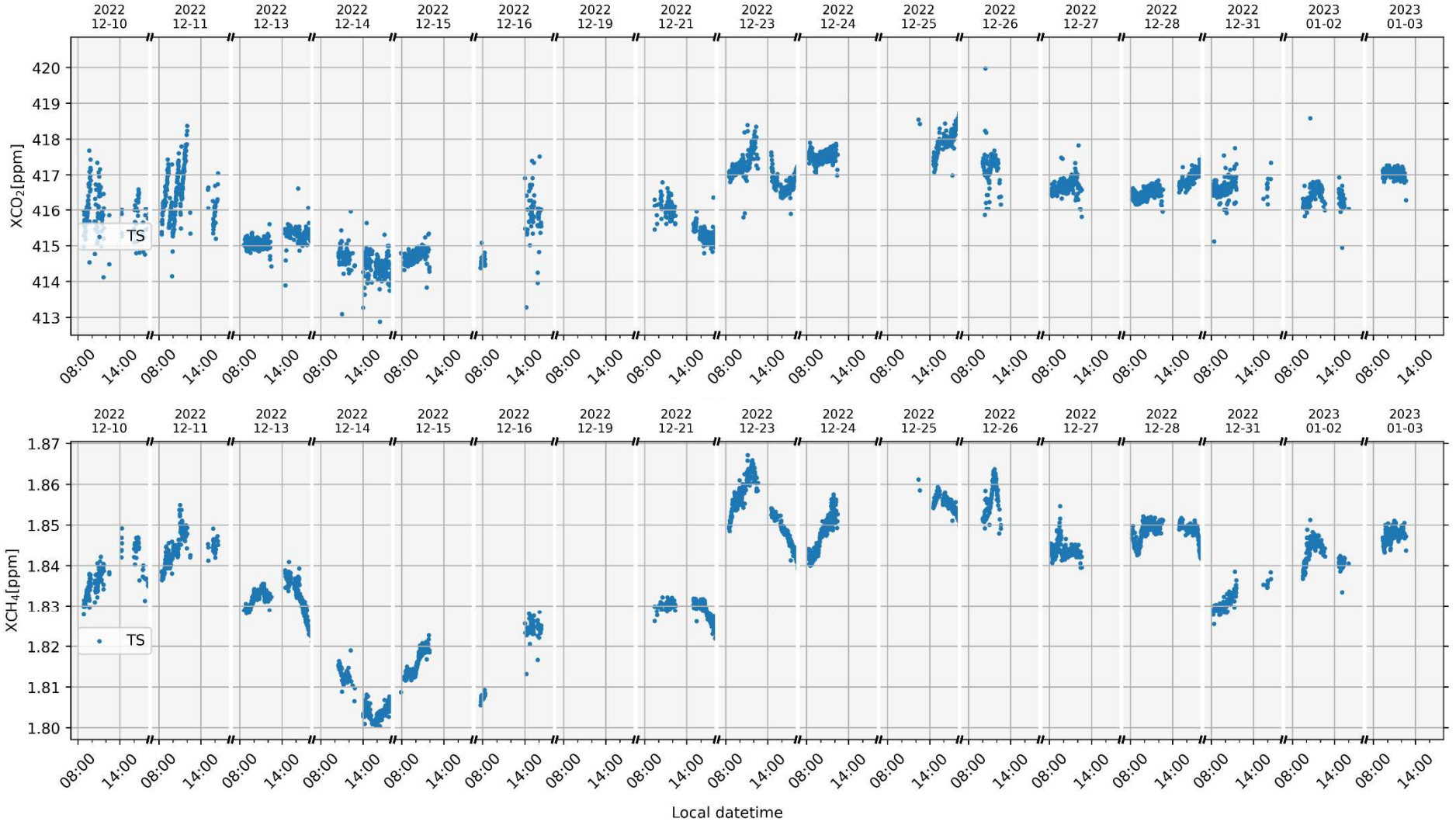
Results of ETL, Canada



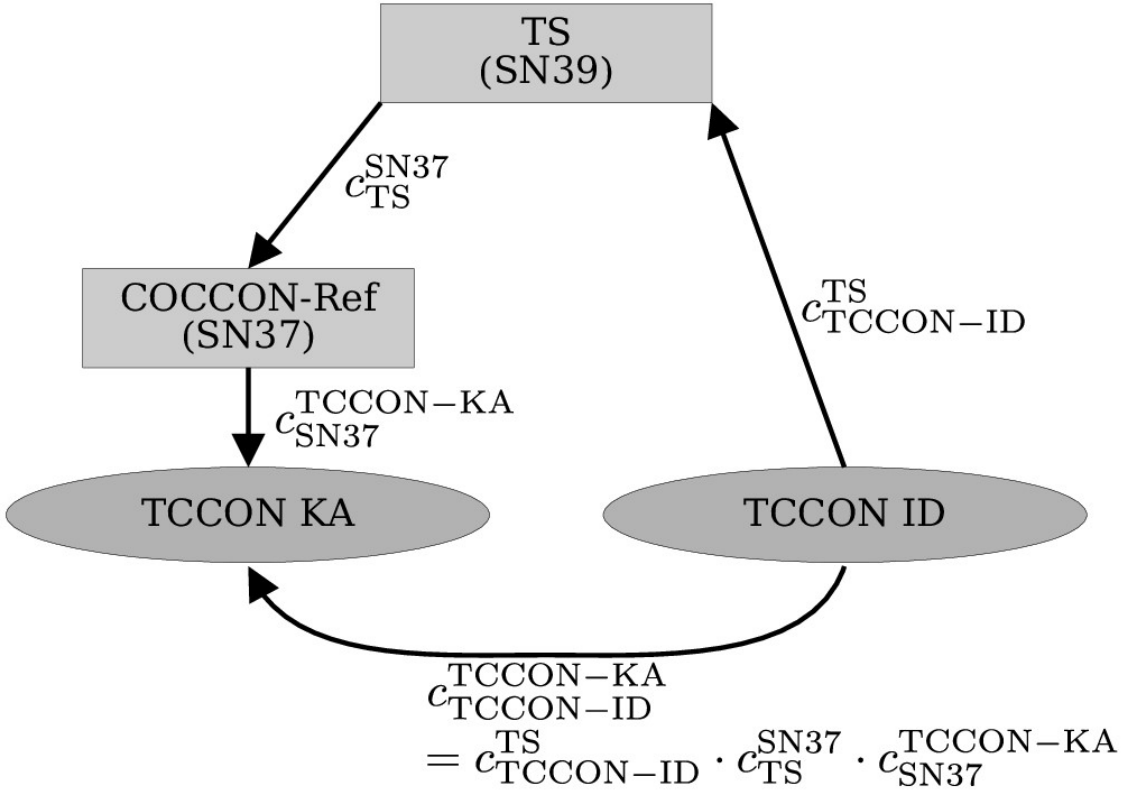
Results of ETL, Canada

- Due to LASER failure no side-by-side measurements.
- No problem with the noise level detected.
- Maybe possible to use CAMS data for extrapolation.

First results of measurements in WG



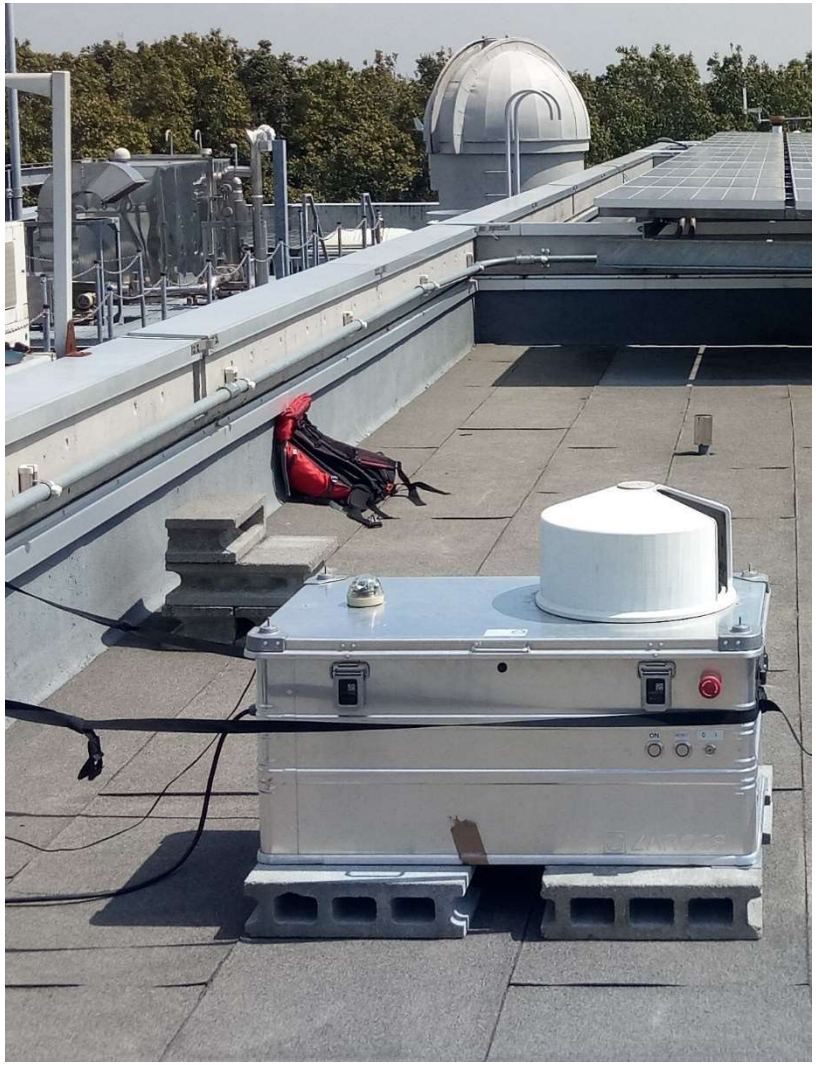
Correction factor scheme



Deviations to Karlsruhe

Species	$\Delta^{\mathbf{SN37}}_{\mathbf{TK-LR}}$ [%]	$\Delta^{\mathbf{SN37}}_{\mathbf{TK-HR}}$ [%]
XCO2	$0.14417 \pm 0.08254 - 0.05414\%$	$0.10812 \pm 0.09331 - 0.05412\%$
XCH4	$0.18642 \pm 0.08277 + 0.07111\%$	$-0.24248 \pm 0.09318 + 0.07080\%$
XCO	$7.07261 \pm 0.40896 - 0.00748\%$	$1.19027 \pm 0.41081 - 0.00707\%$

Thank you for your attention



PREPROCESS for all

Presenter: Frank Hase*

*frank.hase@kit.edu

https://frm4ghg.aeronomie.be/

PREPROCESS for all

Fiducial Reference Measurements for Ground-Based Infrared Greenhouse Gas Observations (FRM4GHG 2.0)

Introduction: One task of FRM4GHGII is to enable a processing compatible with COCCON requirements for a wider range of spectrometers. The COCCON processing chain has three steps:

- The pre-processing or L1-processing (performed by PREPROCESS): from raw OPUS interferograms to spectra. The resulting spectra are used for the quantitative trace gas analysis.
- The daily calculation of lookup tables with x-sections of gases for given atmospheric conditions (performed by PCXS)
- The trace gas retrievals (performed by INVERS)

In order to enable processing of observations with different spectrometers (Vertex70, Invenio, IRCube, IFS125HR in addition to EM27/SUN), mainly extensions of PREPROCESS are required (and some adaptions in INVERS + calculation of vertical sensitivities). This talk describes the extended version of PREPROCESS coded for this purpose.

PREPROCESS for all

Contents:

- **Raw data / interferograms used for this work**
- **Required technical adaptions**
- **Single-sided interferograms and phase correction**
- **Analytical phase calculation**
- **Analytical phase calculation with blending option**
- **Conclusions on analytical phase approach, instrumental issues**
- **Call for beta testers**

PREPROCESS for all

Raw data / interferograms (all in Bruker's OPUS format):

- EM27/SUN (Sodankyla, Karlsruhe)
- IFS125HR (Karlsruhe, Izana): Ka: NIR split in two subregions, Izana: broadband

Kindly provided by FRM4GHG partners:

- IRCube (Wollongong)
- Vertex70 (Sodankyla)
- Invenio (Uccle)

Issues noted on closer inspection of raw interferograms:

IRCube: Two channels stored in file – AC+DC from same detector? Uneven number of scans?
Invenio: DC quite variable - problems with tracker? (Poor weather?)
Vertex70 + Invenio: IFG centerbursts are nearly point symmetric around ZPD (instead of the expected axial symmetry)??

PREPROCESS for all

Required technical adaptions:

So far, interferograms to be processed were all of the same kind:

- The EM27/SUN collects data from two detector channels: SN + SM
- Two IFGs in OPUS file: first IFG block: SN, second IFG block: SM)
- All EM27/SUNs have the same FOV
- All EM27/SUNs record double-sided IFGs with RES = 0.5 cm-1

So we need

- Wideband detector used: derive SN+SM from one broadband channel
- The channels might be swapped (IFS125HR Ka) or the broadband channel to be used might be associated with the second IFG block.
- User specification of semiFOV in PREPROCESS input file required (reported in *.bin file header)
- Enable different choices for spectral resolution (user-selectable, support clipping of IFGs)
- Support processing of SS IFG recording

PREPROCESS for all

Required technical adaptions: New extended input file (1)

Generate ASCII output for testing
mpowFFT (17 for EM27/SUN and IR Cube: 1.8 cm MPD, 181/182: 2.5 cm /3.0 cm MPD, 19 for VERTEX / INVENIO: 4.5 cm MPD, 20 for 125HR: 16.2 cm MPD)
DCmin
DCvar
$
.false. ←For operational work, please select F – otherwise, your HDD will be filled up with
17
0.05
0.10

ILS parameter: apo + phase error
primary channel
secondary channel
semiFOV [rad]
$
0.9825 -0.001
0.9825 -0.001
2.36e-3

…

PREPROCESS for all

Required technical adaptions: New extended input file (2)

…

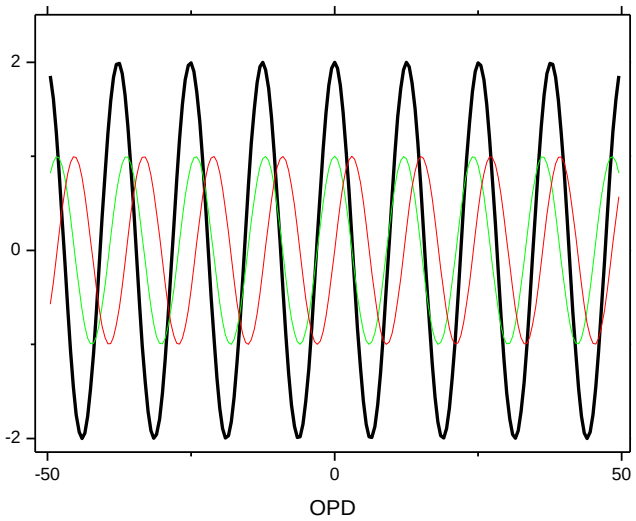
Quiet execution (no user requests)
Output path diagnosis
Output path bin spectra
Dual IFG recording (T/F)
Swap channels (applies for dual IFG recording: 1st channel SN, second channel SM - otherwise choose swap = true)
use analytical phase (T/F)
band selection (0: only generate SN from first channel, 1: generate SN from first and SM from second channel, 2: generate SN + SM from first channel)
$
.true.
standard
standard
.true.
.false.
.false.
1

PREPROCESS for all

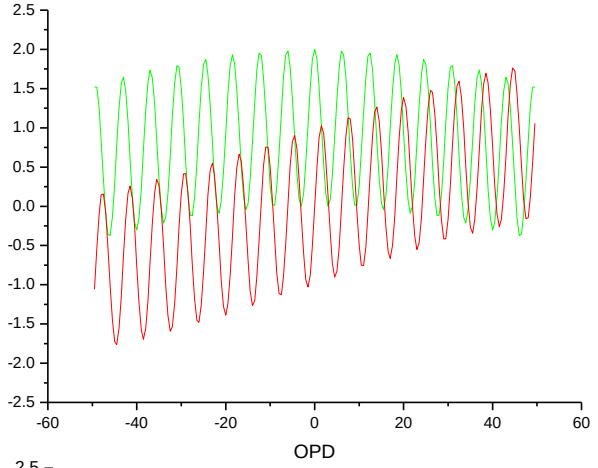
Single-sided interferograms and phase correction

DS IFG recording is superior when high photometric accuracy is required:

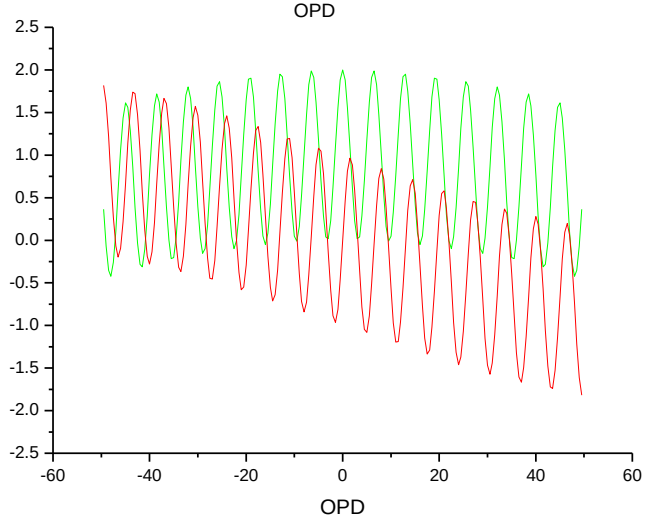
Imagine a monochromatic, pure cosine IFG:



$f_{test} > f_{sig}$



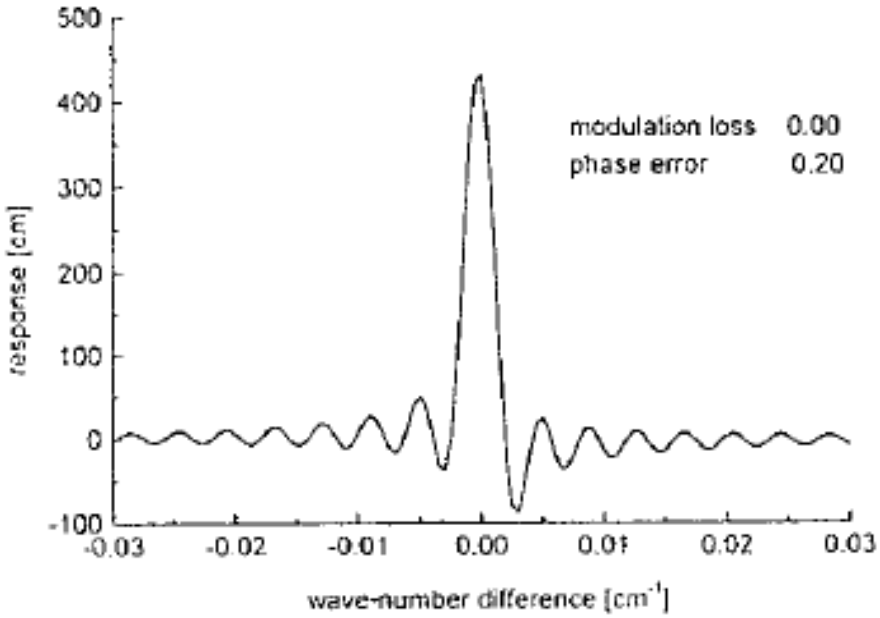
$f_{test} < f_{sig}$



In a DS IFG, the integral over the red curve is zero
In a SS IFG, this integral gives birth to a pulse asymmetric around f_{sig}, a cosinc function.

PREPROCESS for all

Single-sided interferograms and phase correction



PREPROCESS for all

Single-sided interferograms and phase correction

Therefore, the calculation of the phase spectrum is important especially in case of SS ifgs!

We expect that the phase spectrum is rather smooth, it is shaped by:

- Signal propagation delays (mismatch between laser and IR signal propagation delay, IR delay expected to depend on frequency)
- Optical effects: the BS is not fully symmetric when viewed from either interferometer arm (thickness mismatch of BS substrate + compensating plates, BS is a multilayer system with asymmetric refractive boundaries)

Standard approach: Construct the phase from a shorter DS-IFG (this needs careful numerical apodization!)

Residual problem: the phase spectrum might be still smoother than the phase resolution. But a further reduction of phase resolution will end up in an unreliable interpolative performance (spectral sections with high signal just will dominate sections with low signal & the resulting phase spectrum is built on just a few IFG point in the direct vicinity of ZP).

PREPROCESS for all

Single-sided interferograms and phase correction

Preferable would be a method which constructs a smooth analytical phase from a medium-resolution phase spectrum. In the fit procedure, each phase point is ascribed a weight according to the length of the spectral pointer, in addition, a lower threshold for taking points into account for determining the fit can be set.

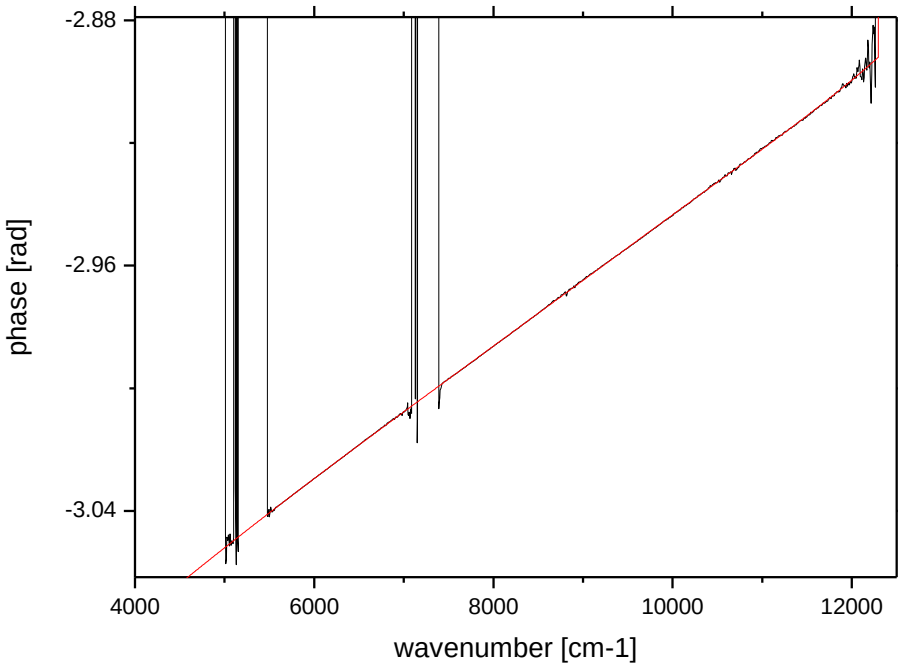
The new PREPROCESS offers an "analytical phase" option in addition to the standard approach. Procedure:

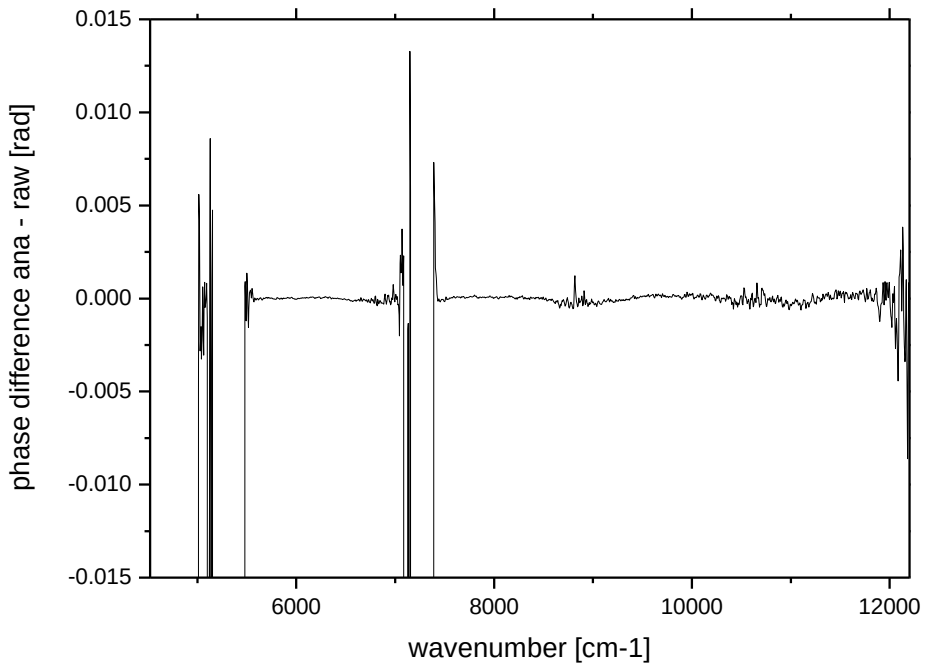
- The phase spectrum is developed out of the complex spectrum (as derived from the low-res DS IFG)
- The phase set by the orientation of the complex pointer at the spectral position with biggest complex amplitude acts as pivotal point for calculating the phase spectrum
- From this reference position, the phase is constructed towards higher and towards lower frequencies, using the cross product of two normalized complex vectors to determine the phase changes.
- A smooth curve (polynomial, 14 parms) is fitted to this phase spectrum, taking into account weights and clipping weights below a threshold (5% of max complex amplitude).
- Note when using this option: the analytical fit is restricted to the 3500 – 12300 cm-1 range!

PREPROCESS for all

Single-sided interferograms and phase correction

Results for the EM27/SUN analytical phase:

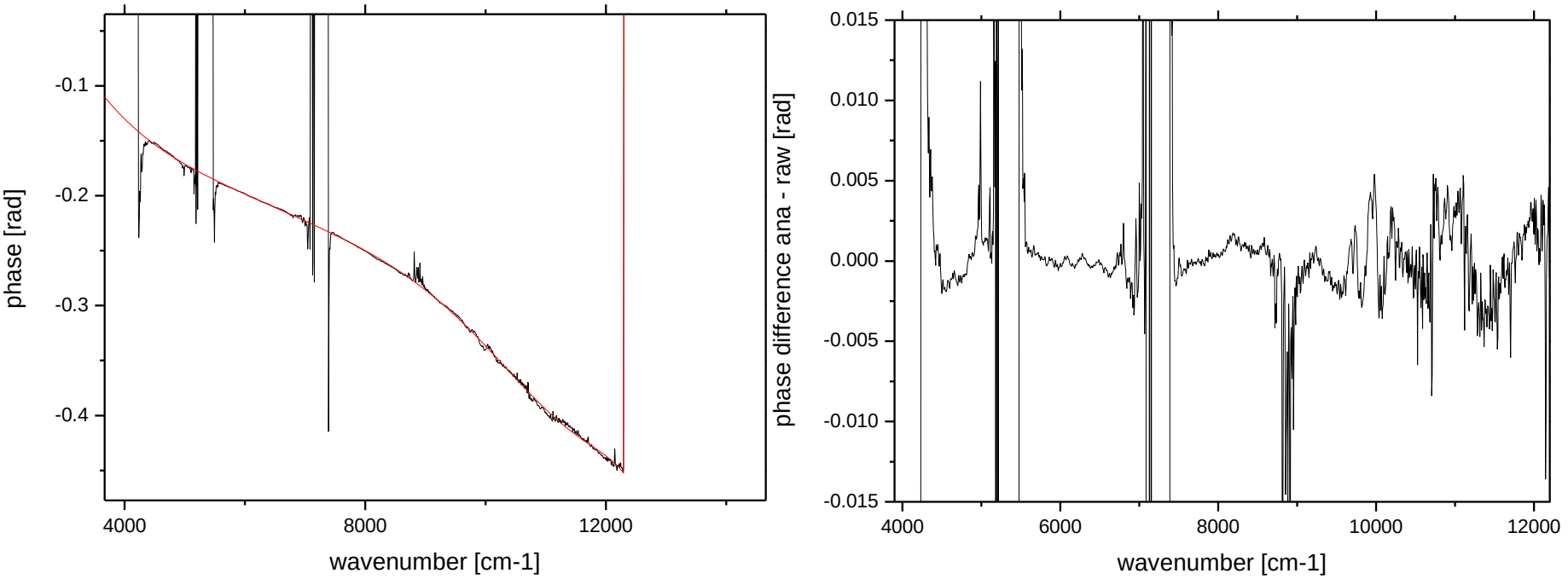




PREPROCESS for all

Single-sided interferograms and phase correction

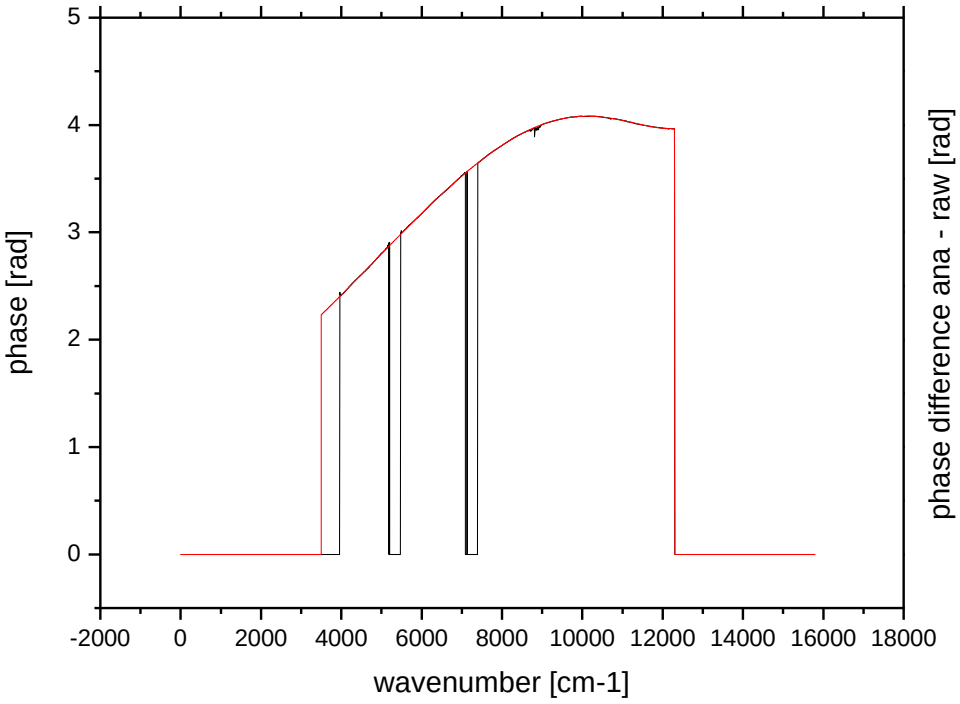
Results for the IR Cube analytical phase:

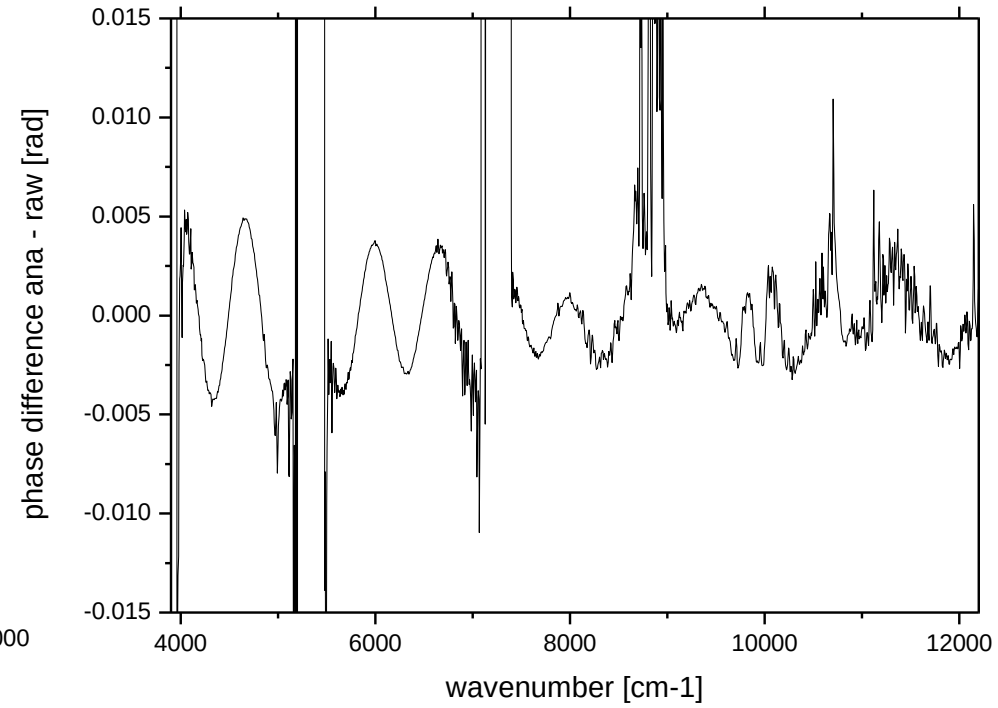


PREPROCESS for all

Single-sided interferograms and phase correction

Results for the Vertex70 analytical phase (the Invenio looks surprisingly similar, both contain a strange phase oscillation, ~ 400 … 500 cm-1 period):

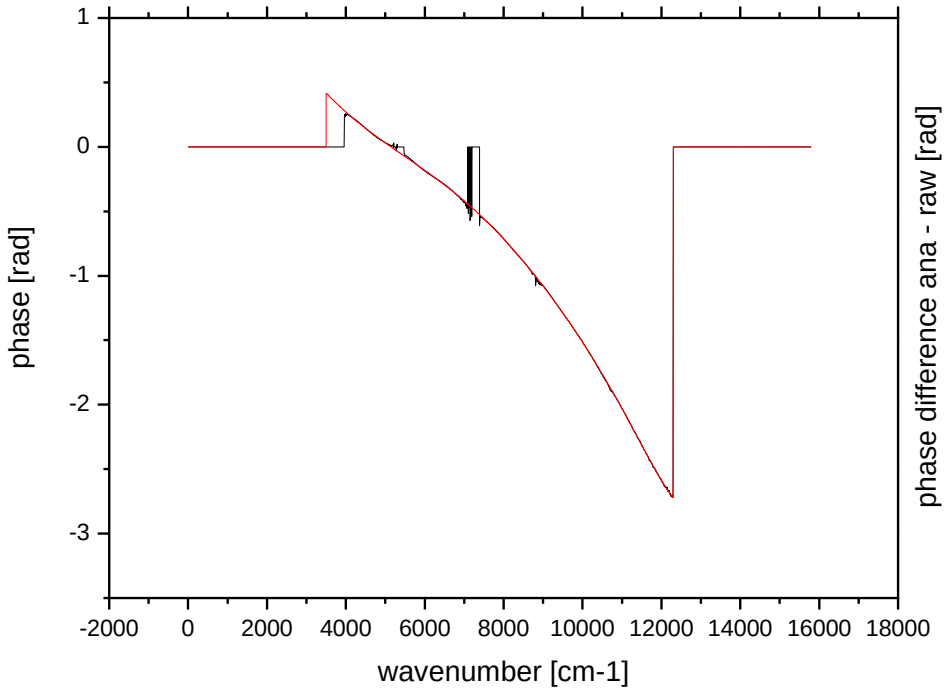


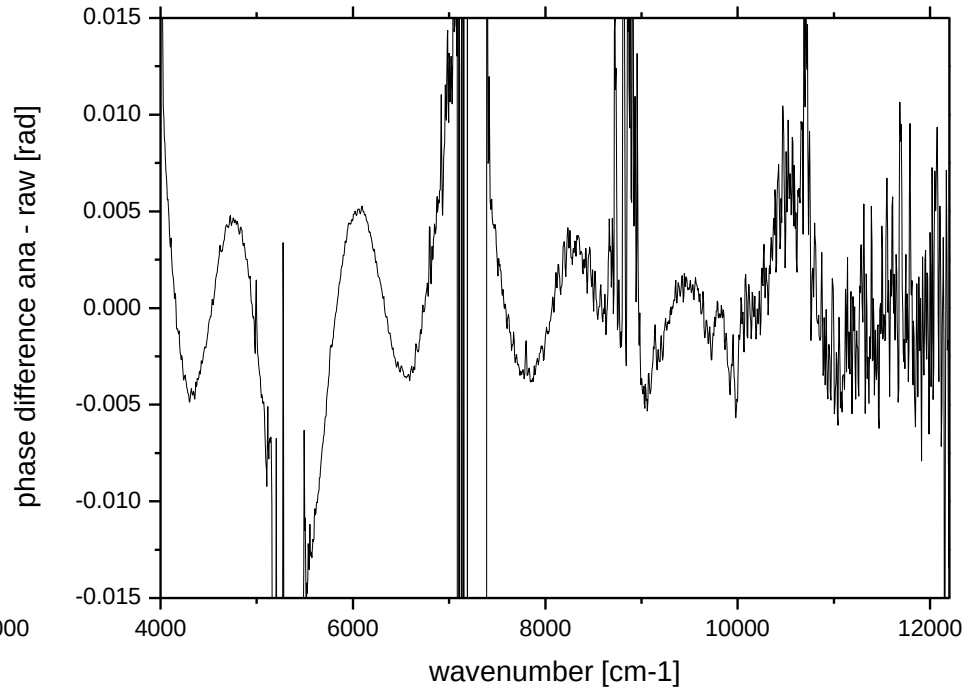


PREPROCESS for all

Single-sided interferograms and phase correction

Results for the Invenio analytical phase (similar oscillatory pattern as seen for Vertex70):

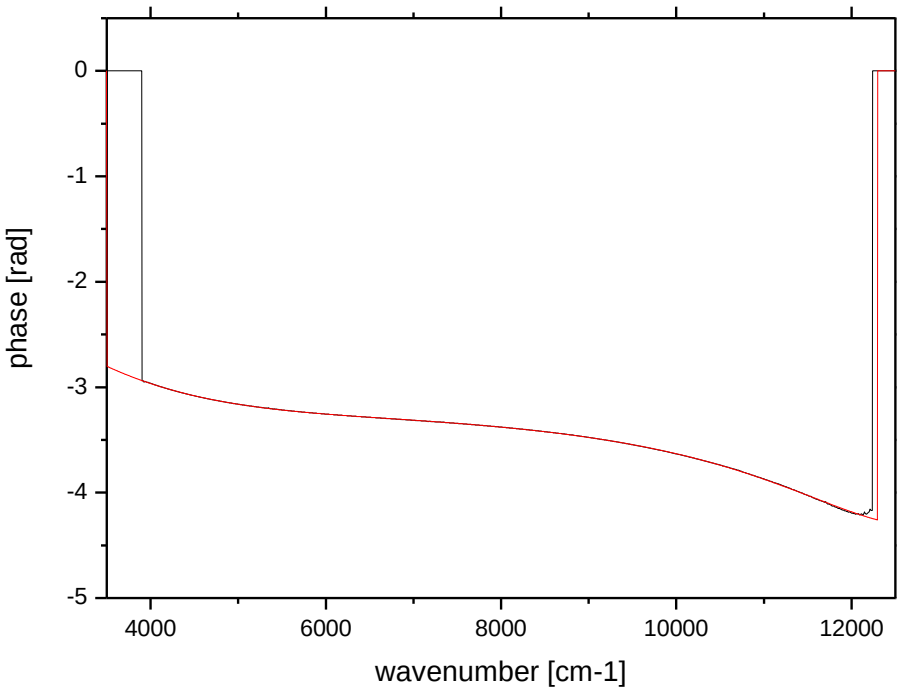


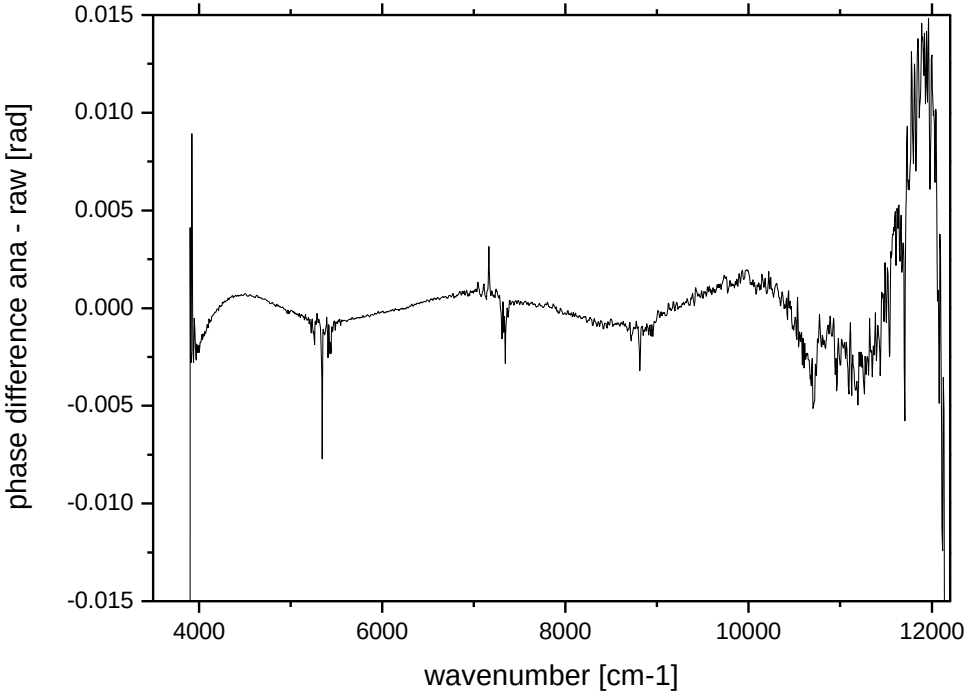


PREPROCESS for all

Single-sided interferograms and phase correction

TCCON example (125HR Izana, 2019):

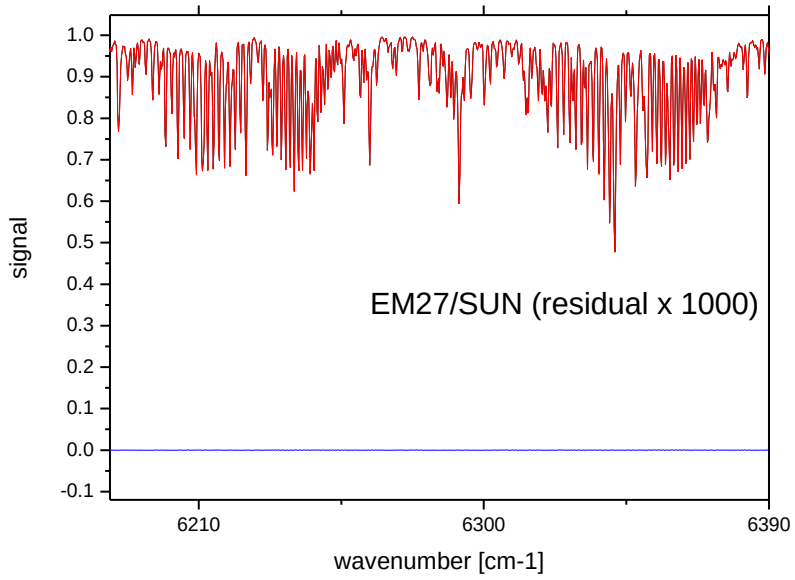


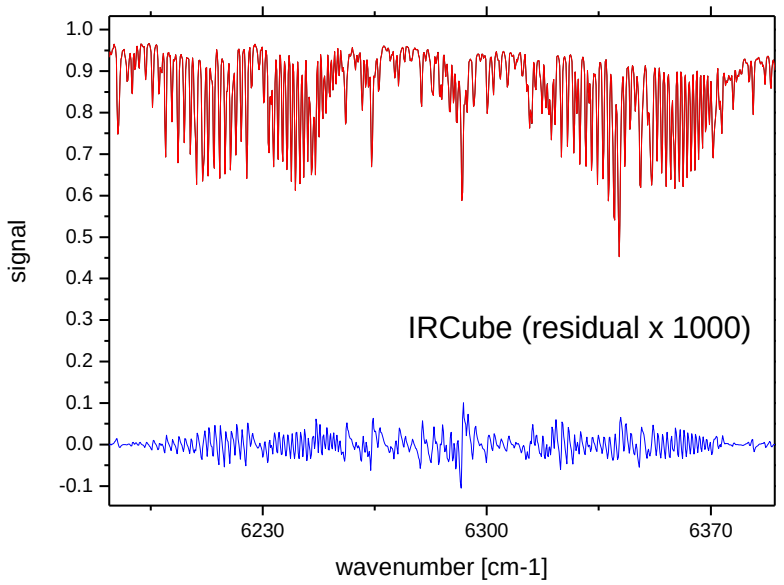


PREPROCESS for all

Single-sided interferograms and phase correction: intercomparison SS versus DS

These plots demonstrate the error propagation of phase errors into the spectrum for the SS and DS case (comparing spectra generated with the standard and analytical phase calculation schemes)



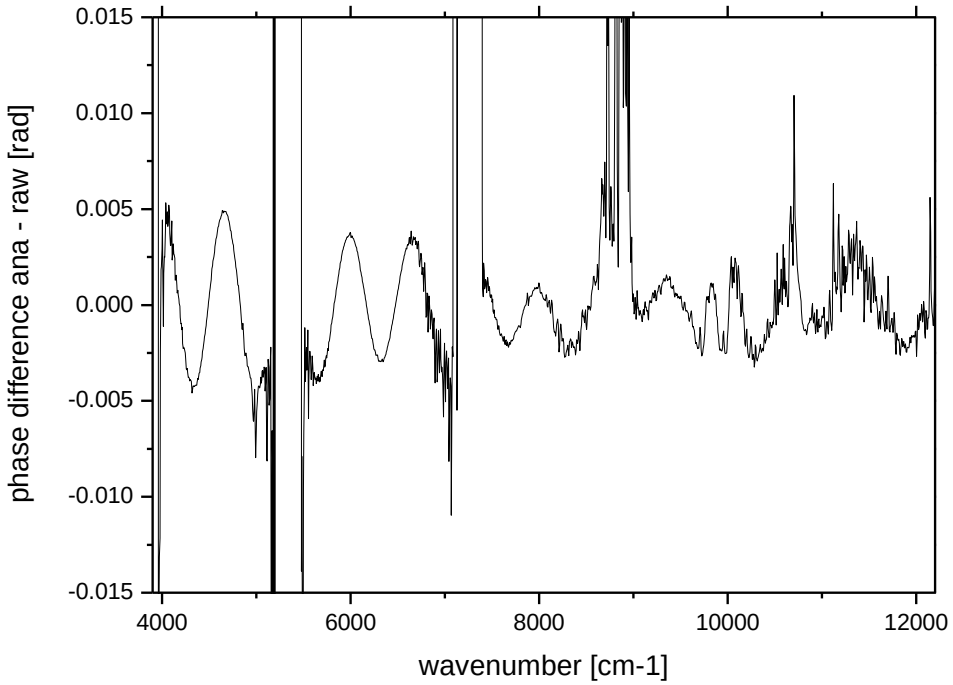


PREPROCESS for all

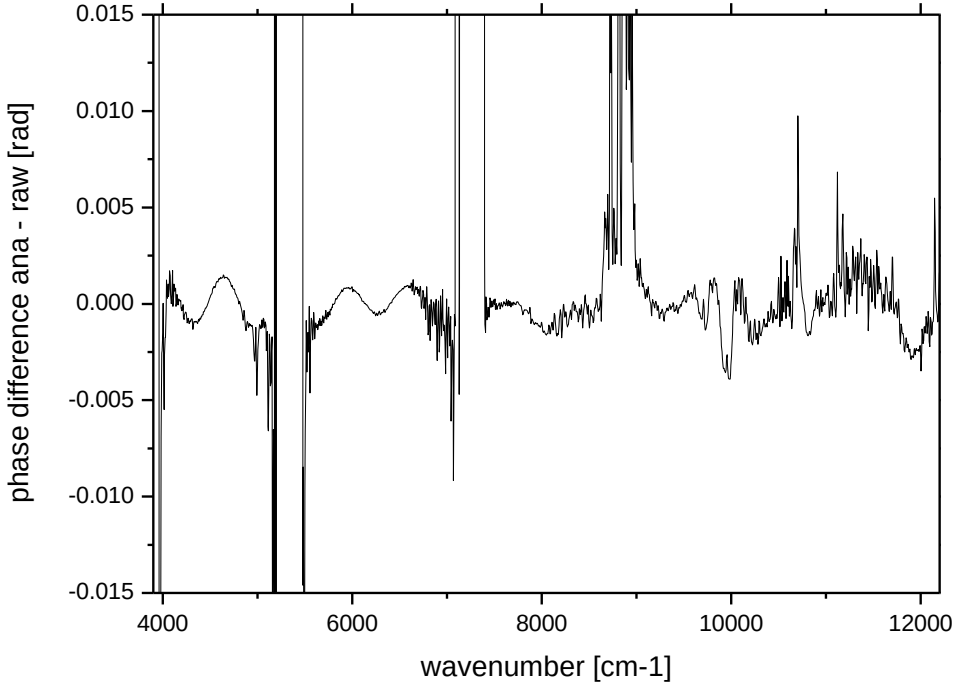
Single-sided interferograms and phase correction – phase blending option

Idea: feed in additional information on permanent phase structures too narrow to be resolved by the smooth analytical phase – ideally from additional, e.g. lamp measurements. (The blending option is activated by adding a table named "refphase.inp".)

No blending



use blending



PREPROCESS for all

Single-sided interferograms and phase correction

Conclusions on analytical phase method:

- The analytical phase fitting seems to work well, with blending option approaching an optimal reconstruction of the actual phase spectrum.
- The EM27/SUN ironically has outstanding phase quality - note: nearly linear, no dispersion! (Exactly here, it's of lesser importance…)
- The IR-Cube phase looks ok, insertion of a long pass filter for limiting the signal below ~ 12000 cm-1 might be recommendable (significant signal level at HFL!)
- The Vertex70 / Invenio phase is very unusual (oscillating phase, amplitude ~ 10 mrad pp) – instrumental issue?
- The tested TCCON Izana spectrum looks reasonable, but also some detectable variations superimposed on smooth phase (pp variation < 5 mrad), larger variations beyond > 10 000 cm-1.

For the moment, I would recommend to use the standard method for operational work, the analytical phase approach seems useful for instrumental investigation. (Note that in presence of an underlying disturbing spectral signal which disturbs the phase spectrum especially in regions of lower flux, even the use of superior phase information can only reject the orthogonal component of the interfering signal.)

PREPROCESS for all

Call for beta testers

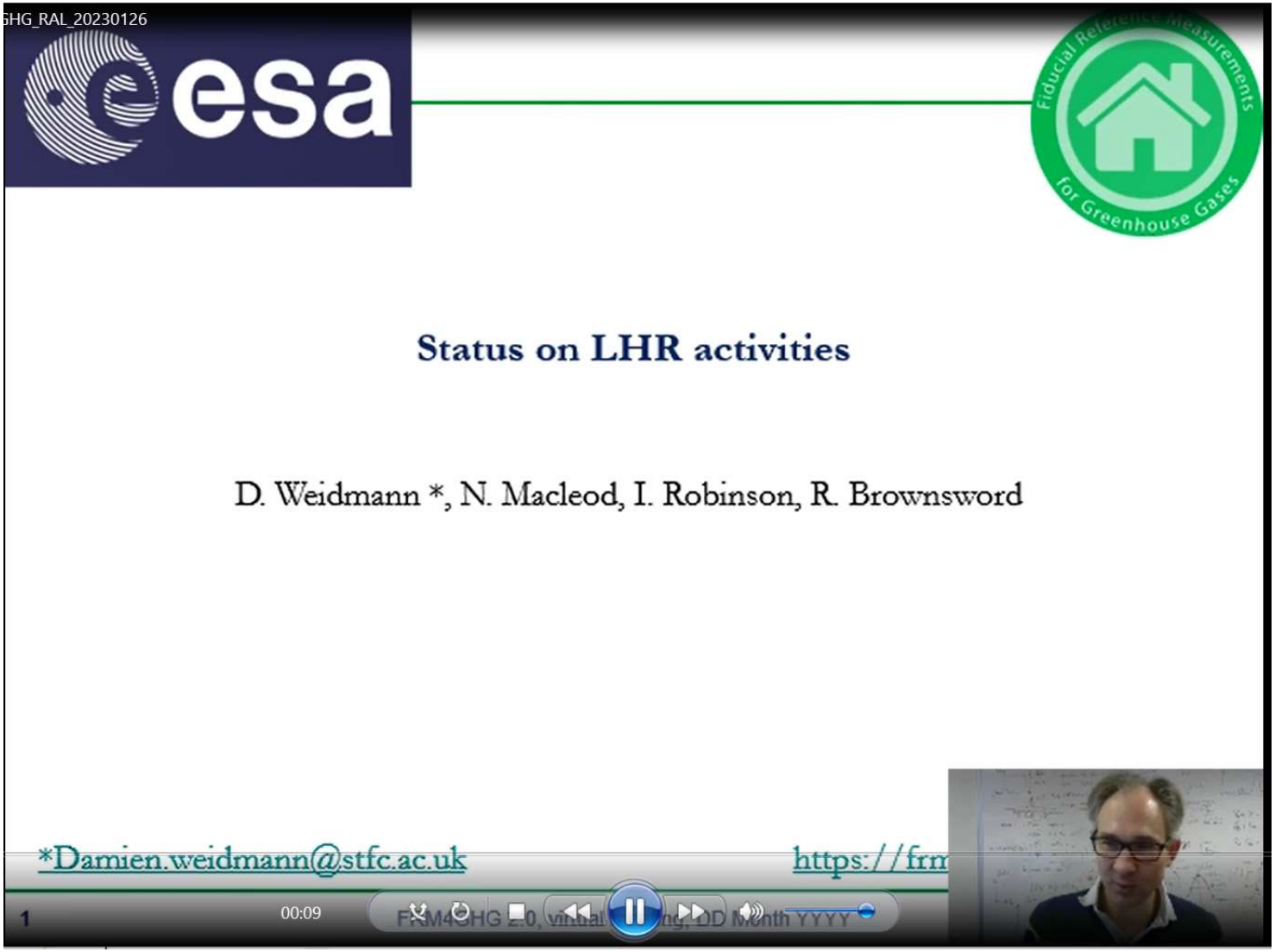
We will upload the code, the samples and the demo input files and would like to ask you to do further testing / evaluation of results.

- I have worked through all example OPUS files you provided and I tested the plausibility of results, however, please do not regard my demo input files for different cases as a reference (e.g. coordinates, time offset on time reported by OPUS, etc).
- For single files or small sets, the diagnostic ASCII files are worth to inspect (they show all the intermediate results along the processing chain…).
- Please check the contents of the *.bin header. Are the reported numbers what you would expect?

Technical hints, please note:

- Please switch off the generation of diagnostic ASCII files when working on larger number of spectra.
- When using the PREPROCESS code manually (without the Pylot), you need to manually create a folder "cal" in the directory containing the OPUS files.
- PREPROCESS is checking the spectral calibration of the generated spectra (SN + SM) versus reference spectra. The pair of reference spectra ("refspec.dat","refspec2.dat") need to reside in the folder of the executable. For the Invenio / Vertex70, these need to be replaced with dedicated higher res reference spectra (unless you clip the result to the EM27/SUN standard resolution).

The presentation by Damien Weidmann was given as a pre-recorded movie.
Questions have been asked during the meeting on February 9, 2023

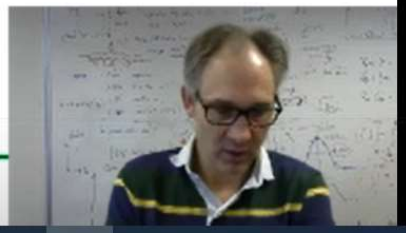


Damien-FRM4GHG_RAL_20230126

Objectives

- Overall objectives:
  - Update and upgrade the ground-based LHR based on conclusion from FRM4GHG 1
  - Do so by running a side by side measurement campaign of the updated LHR with TCCON Harwell

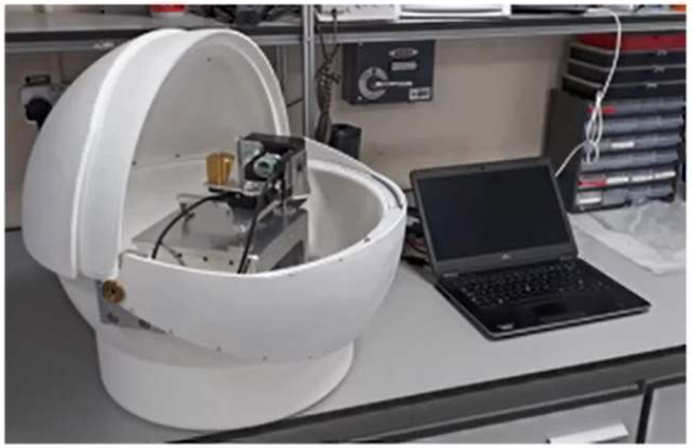
- Specific system elements we are working on:
  - Sun tracker – Hardware and software updates
  - LHR instrument updates
  - Data Processor updates
  - TCCON / LHR integration



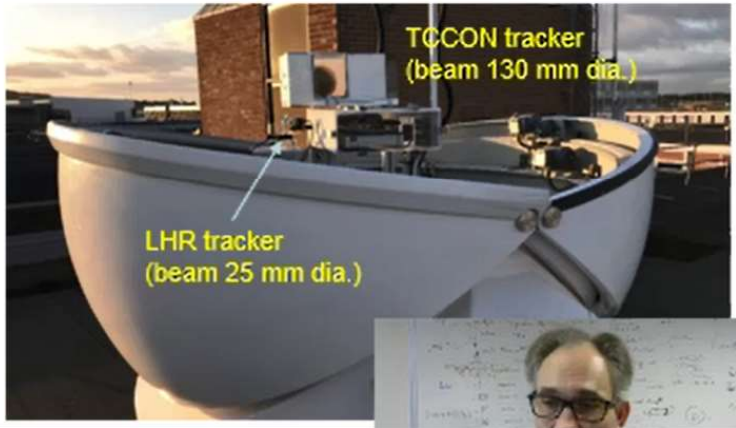
Damien-FRM4GHG_RAL_20230126

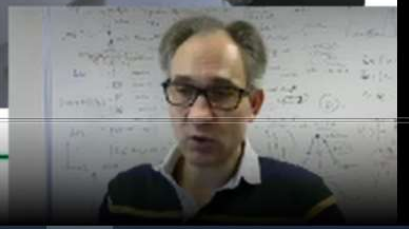
LHR sun tracker

- Refer to April 2022 presentation for details
- Tracker taken off the "small dome" for installation in the "large dome"



TCCON dome installed on RAL roof





3

02:02

FRM4GHG 2.5, virtual meeting, DD Month YYYY

Suchen

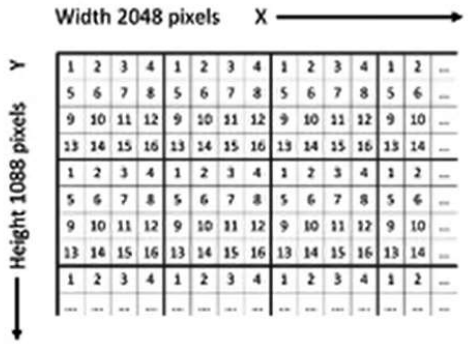
Luft:...

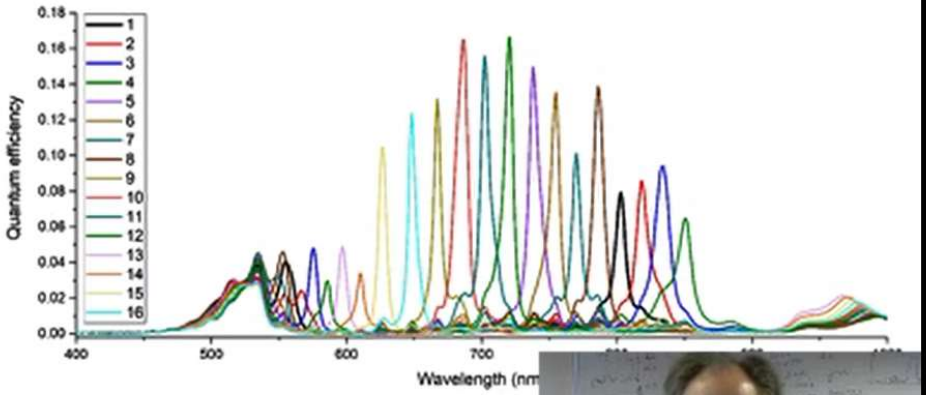
11:35
08.03.2023

Damien-FRM4GHG_RAL_20230126

Sun tracker camera upgrade

- Replaced CMOS camera with hyperspectral camera
  - Following the concept developed for CubeMAP [1]
  - 16 channels ~16 nm wide
  - 580 – 870 nm range
  - Info on O_2 (A, B, X bands), H_2O, possibly aerosols





1- doi: 10.1117/12.2573727

04:14

FRM4GHG 2.0, virtual meeting, DD Month YYYY

Suchen

2°C

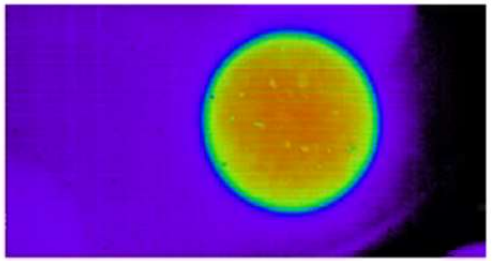
11:37
08.03.2023

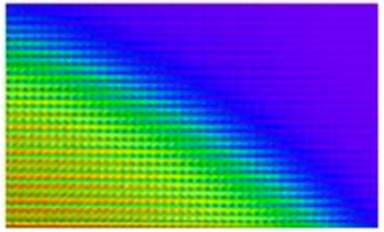
Damien-FRM4GHG_RAL_20230126

Demonstration of cam-tracking

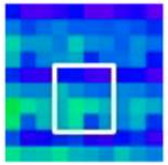
- Integration of camera hardware into the LHR
- Update of control software
- Demonstration of hyperspectral cam-tracking over few hours (~240 urad)

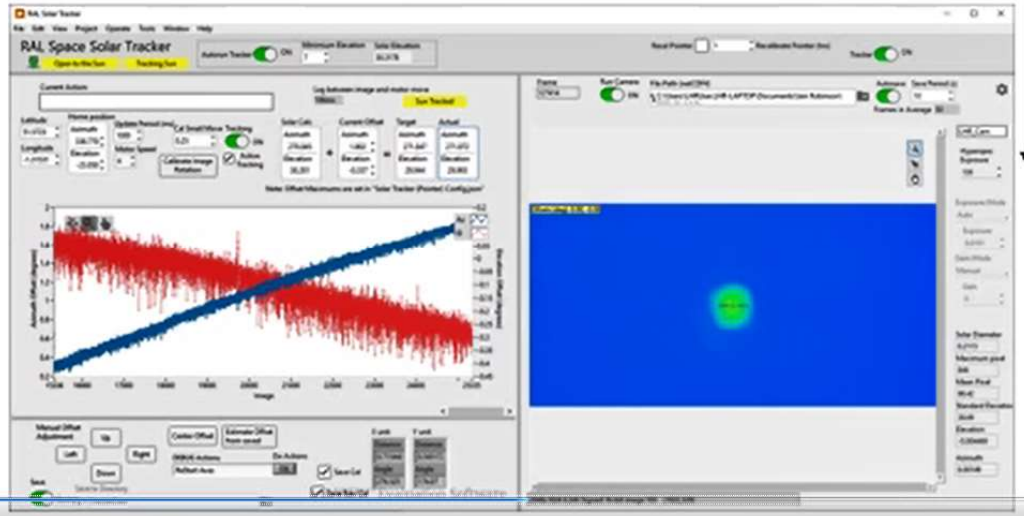
Full resolution
2048 x 1088





Mosaic level





5

06:33

FRM4GHG 2.0, virtual meeting, DD Month YYYY

Suchen

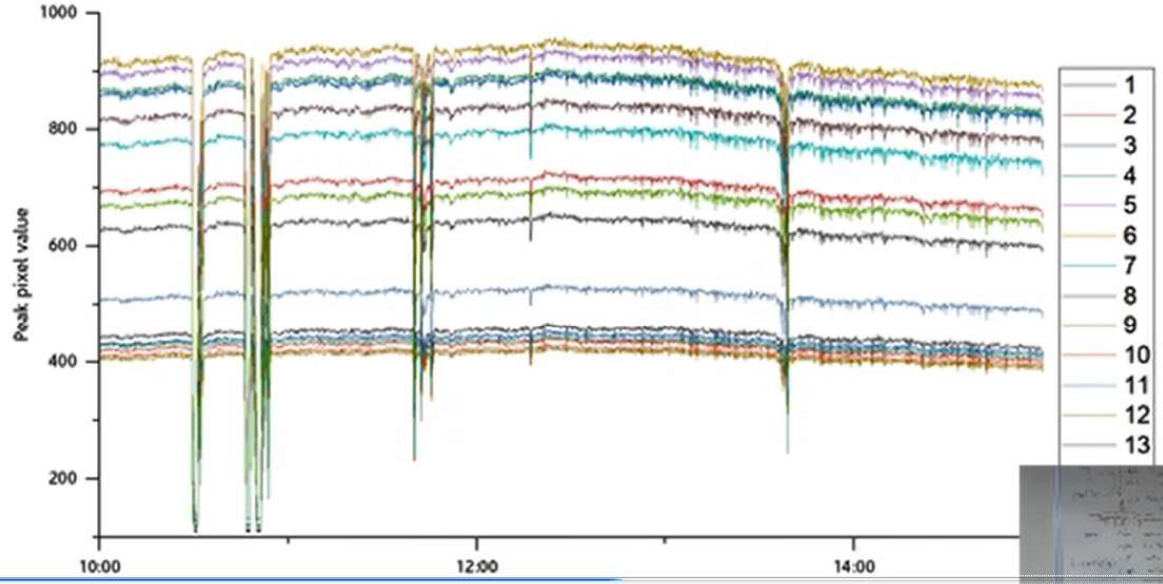
2°C

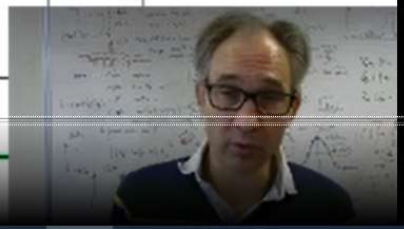
11:38
08.03.2023

Damien-FRM4GHG_RAL_20230126

Time evolution

- Very raw data of hyperspectral signals during tracking
  - Sanity check on band centre coincidence with water and O_2 bands
  - Much more processing needed…





6 08:39

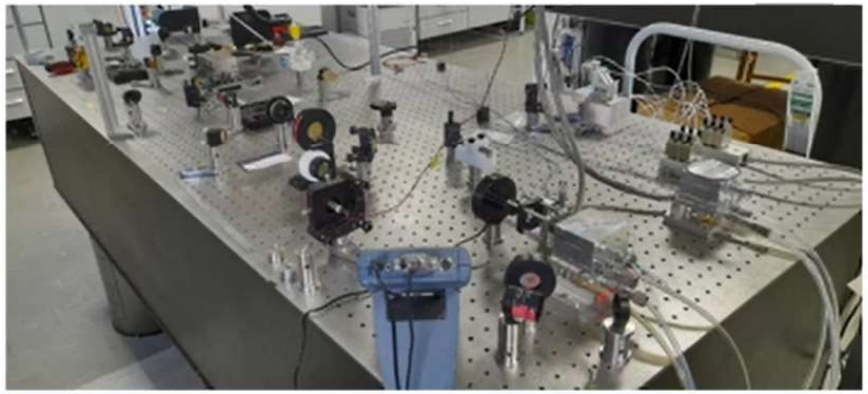
Suchen

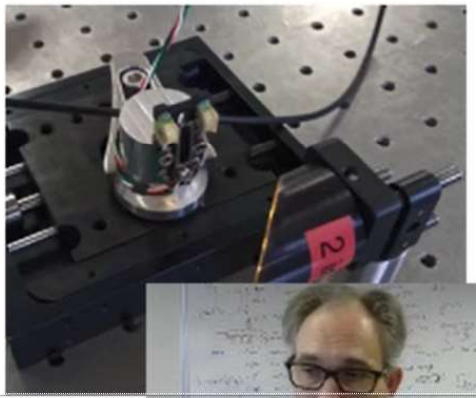
2°C 11:38 08.03.2023

Damien-FRM4GHG_RAL_20230126

LHR instrument updates

- Procurement of some equipment
  - Narrow-band optical bandpass filters
  - Motorised opto-mechanics for automation
  - Solid state chiller
- Possible upgrades tested on separate bench
  - Impact of filter bandwidth on heterodyne background signal validated (<20x reduction)
  - Demonstration of a resonant tuning fork chopper (@3 kHz)





7 09:42

Suchen

2°C 11:38 08.03.2023

Damien-FRM4GHG_RAL_20230126

Processor updates

- Improvement of instrument forward model ongoing
  - Physical model for background signal
  - Physical model for non-linearity
  - Test bench being used for validation

- Option to use the CubeMAP L2 prototype processor ?
  - Needs to be adapted from limb to ground-based SO

8 12:31

Suchen

2°C 11:39 08.03.2023

Damien-FRM4GHG_RAL_20230126

TCCON LHR integration

- Plan for TCCON/LHR joint measurement this summer
  - Should add an EM27 to the suite
  - Currently running late on instrument upgrades

9 14:34

Suchen

2°C 11:39 08.03.2023

Damien-FRM4GHG_RAL_20230126

Next steps

- Move the LHR back into lab for recommissioning
  - Integration of new optical components
  - Full realignment
  - Re-characterization
- Upgrade the processor (including hyperspectral information)
- Execute the joint campaign with Harwell TCCON

16:29

Suchen

2°C

11:39

08.03.2023

RUG progress in WP 1 – 3 during April – December 2022

Huilin Chen, Steven van Heuven, Alessandro Zanchetta, Xin Tong, University of Groningen

Rigel Kivi, Pauli Heikkinen, Finnish Meteorological Institute

Huilin.Chen@rug.nl https://frm4ghg.aeronomie.be/

RUG Leading/Participating Tasks

- **WP1 T4 (RUG, FMI) Develop AirCore for retrieving OCS and N_2O in addition to $CO_2/CH_4/CO$**

- **WP2 T5 (FMI, RUG): Improving AirCore retrievals and historical AirCore dataset**

RUG Leading/Participating Task I

WP1 T4 (RUG, FMI) Develop AirCore for retrieving OCS and N_2O in addition to $CO_2/CH_4/CO$

- Progress on the analyses of AirCore OCS and N_2O profiles in Kiruna during the HEMERA campain **(August 2021)**

- Progress on the analyses of AirCore OCS flights in Rotterdam during the Ruisdael campaign **(September 2022)**

- Planning the Sodankylä campaing **(31 July – 14 August 2023)**

WP1 T4 (RUG, FMI) AirCore for OCS and N_2O: AirCore Development

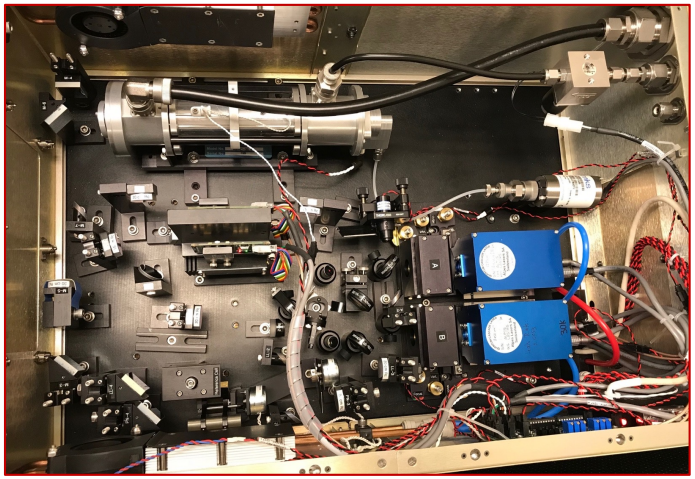
➢ RUG participating in HEMERA, a large balloon flight in Kiruna, August 2021

Balloon and auxiliary balloon being filled. Source: hemera-h2020.eu

- *Cryogenic samples*
- *AirCores*
- *bigLISA*
- *Spectrometers*

RUG AirCore + bigLISA

➢ RUG measurements of $OCS/N_2O/CO_2/CH_4/CO$ during HEMERA



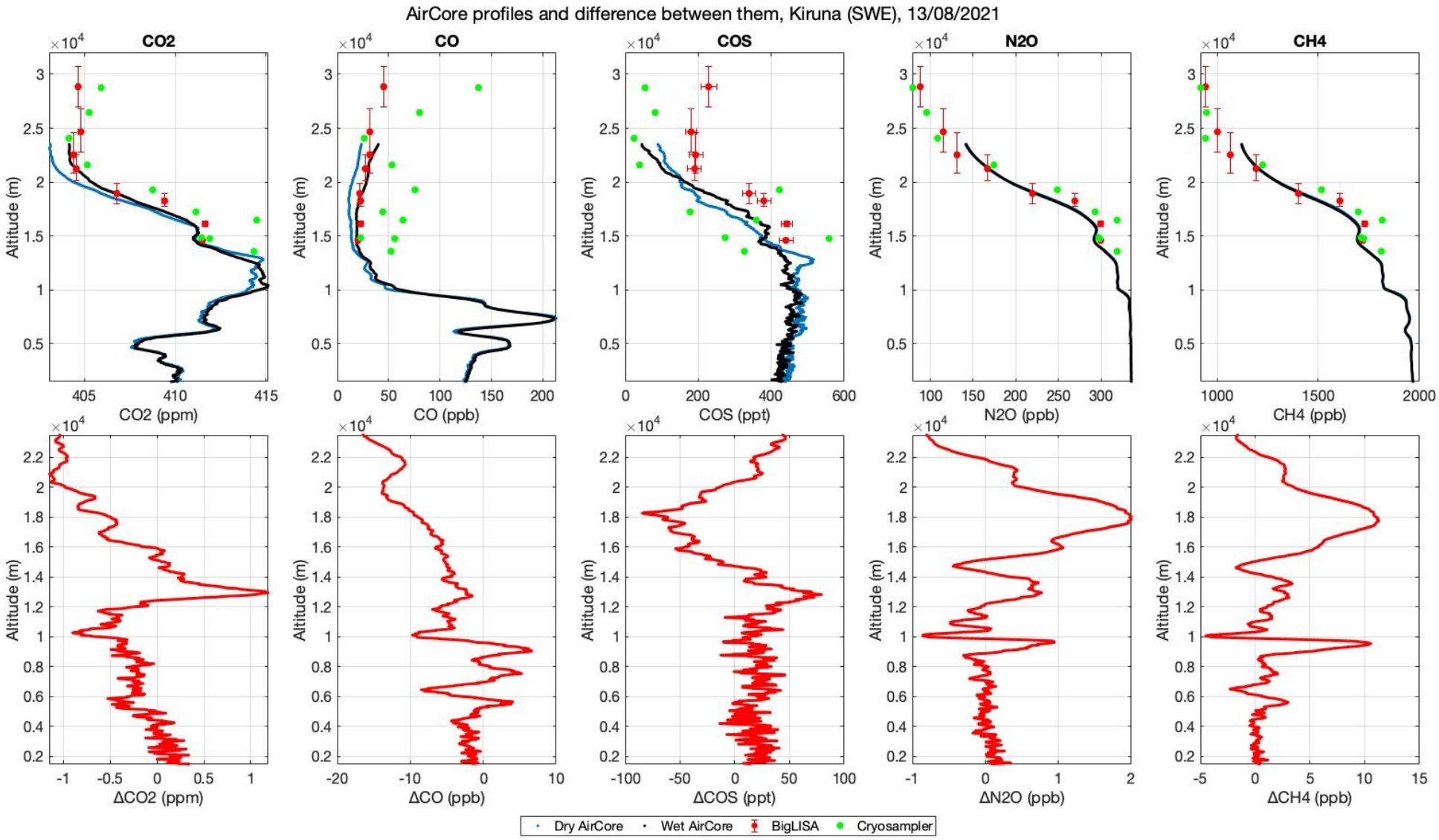
Aerodyne Research Inc.

Cell volume	150 mL
Optical Path length	36 m
Pressure	40 – 60 Torr

Effective Cell Volume at 50 Torr: ~ 10 mL

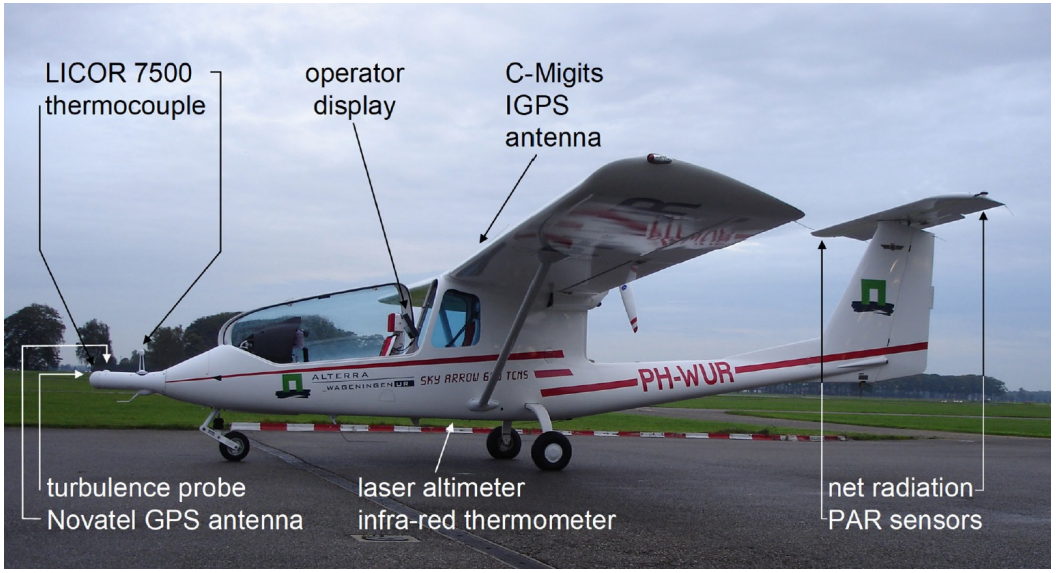
Species	COS (ppt)	N_2O (ppb)	CO_2 (ppm)	CH_4 (ppb)	CO (ppb)	H_2O (ppm)
1-sigma	~ 12	0.1	0.08	0.45	0.65	7.2

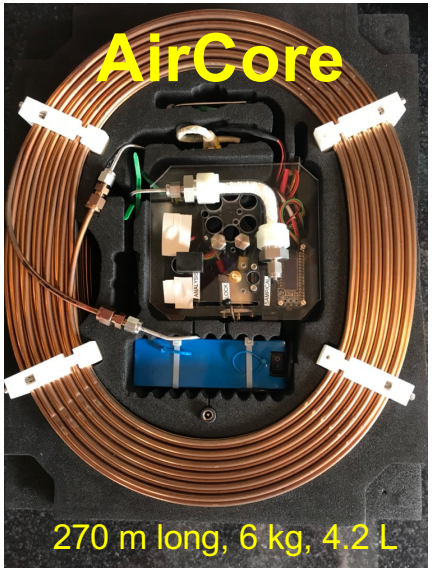
WP1 T4 (RUG, FMI) AirCore for OCS and N2O: AirCore Development



WP1 T4 (RUG, FMI) AirCore for OCS and N_2O: AirCore Development

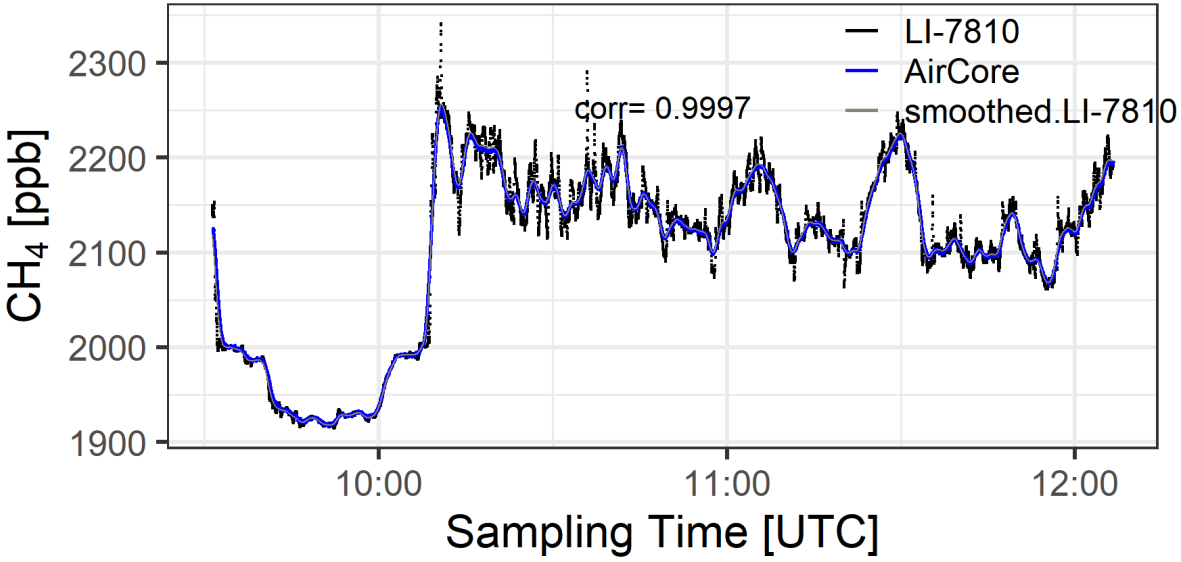
➢ **RUG participating in Ruisdael, an urban campaign in Rotterdam, September 2022**

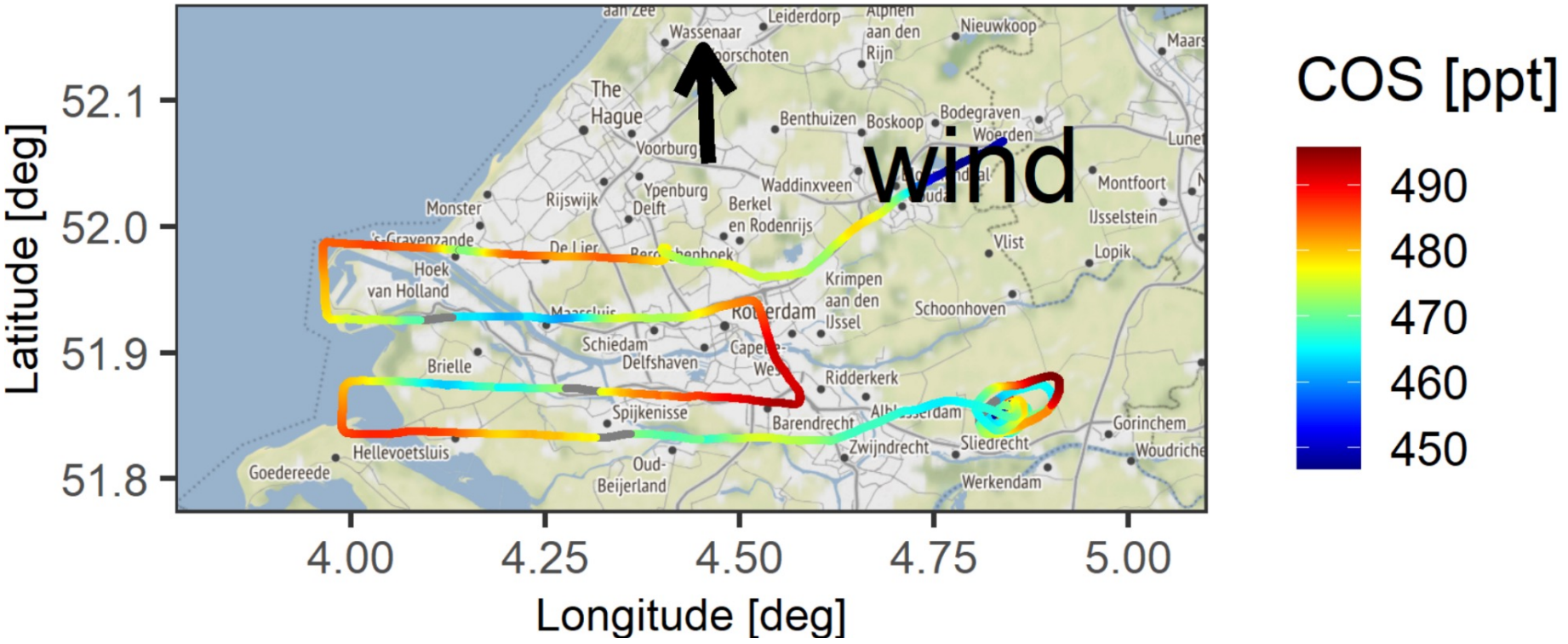




AirCore mounted in "SkyArrow"

- Sampling actively (upstream pump, dryer)
- Logging gps data, T, p, sampled V
- Analyzed on Aerodyne QCLS
  - CO_2, CO, CH_4, COS, N_2O
- Compared with in-situ LI-COR





September 5th, 2022
Southerly winds

WP1 T4 (RUG, FMI) AirCore for OCS and N_2O: AirCore Development

- RUG planning the Sodankylä campaing **(31 July – 14 August 2023)**

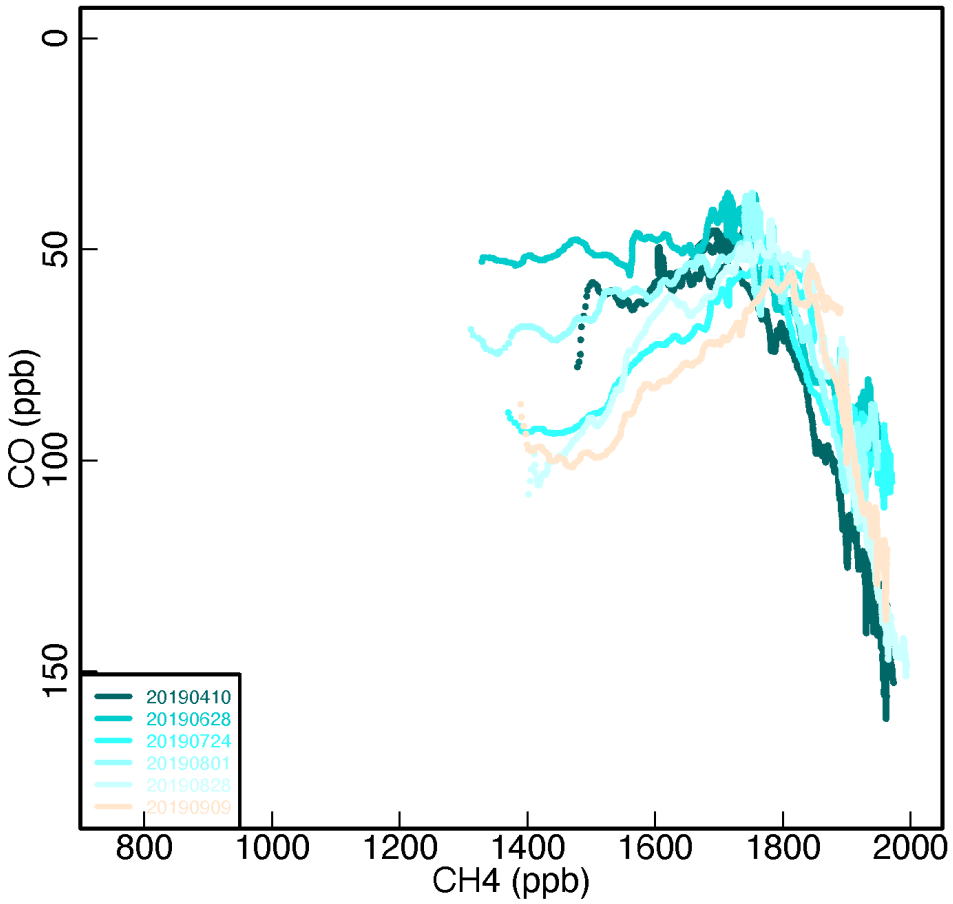
  - AirCore&LISA OCS and N_2O observations
  - AirCores with and without an ozone scrubber
  - Dual AirCore and LISA launches at Sodankylä (WP2 T5 with FMI)

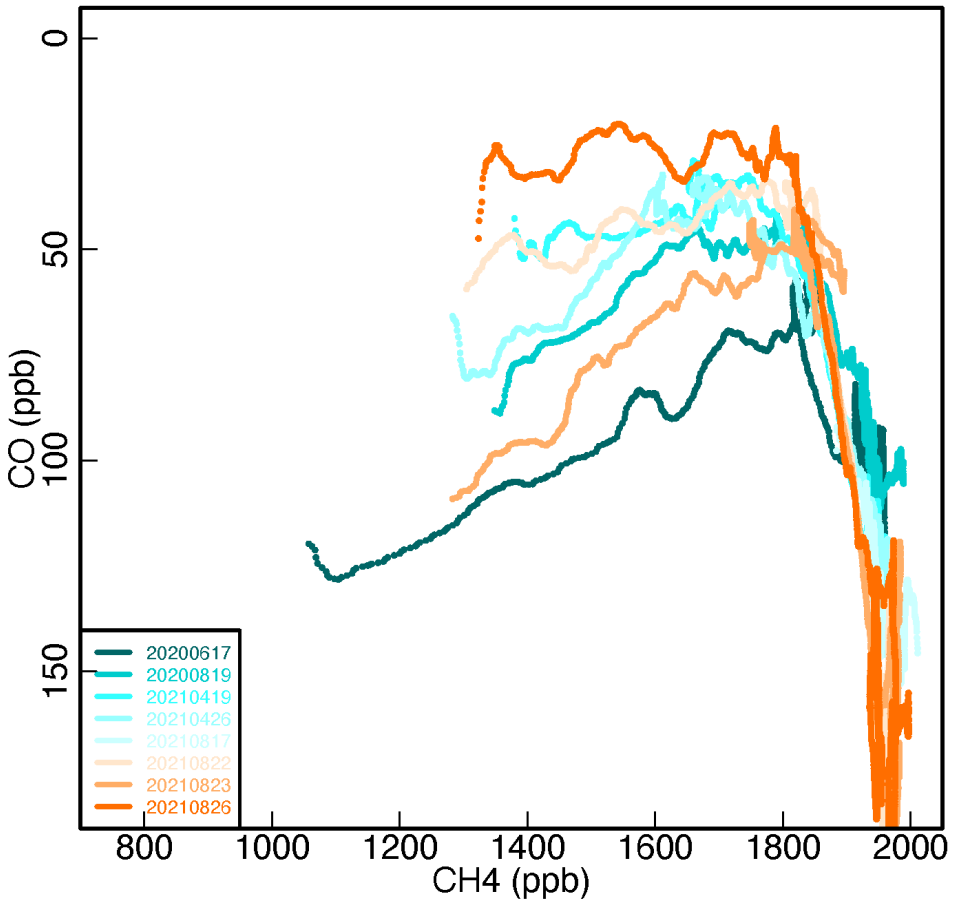
RUG Leading/Participating Task II

WP2 T5 (FMI, RUG): Improving AirCore retrievals and historical AirCore dataset

- Perform additional AirCore launches during the 4 years of the project to have enough statistical coverage (**5 AirCore launches 2022**)
- Improve retrieval of CO and CH4 profiles in the stratosphere from AirCore measurements based on
  - ✓ Dual AirCore launches (**First flight done in August 2022**)
  - ✓ Dual AirCore and LISA launches at Sodankylä **(31 July – 14 August 2023)**
- Reprocess all 2017-2019 AirCore data at Sodankylä **(Wait until the dual launches are analyzed)**

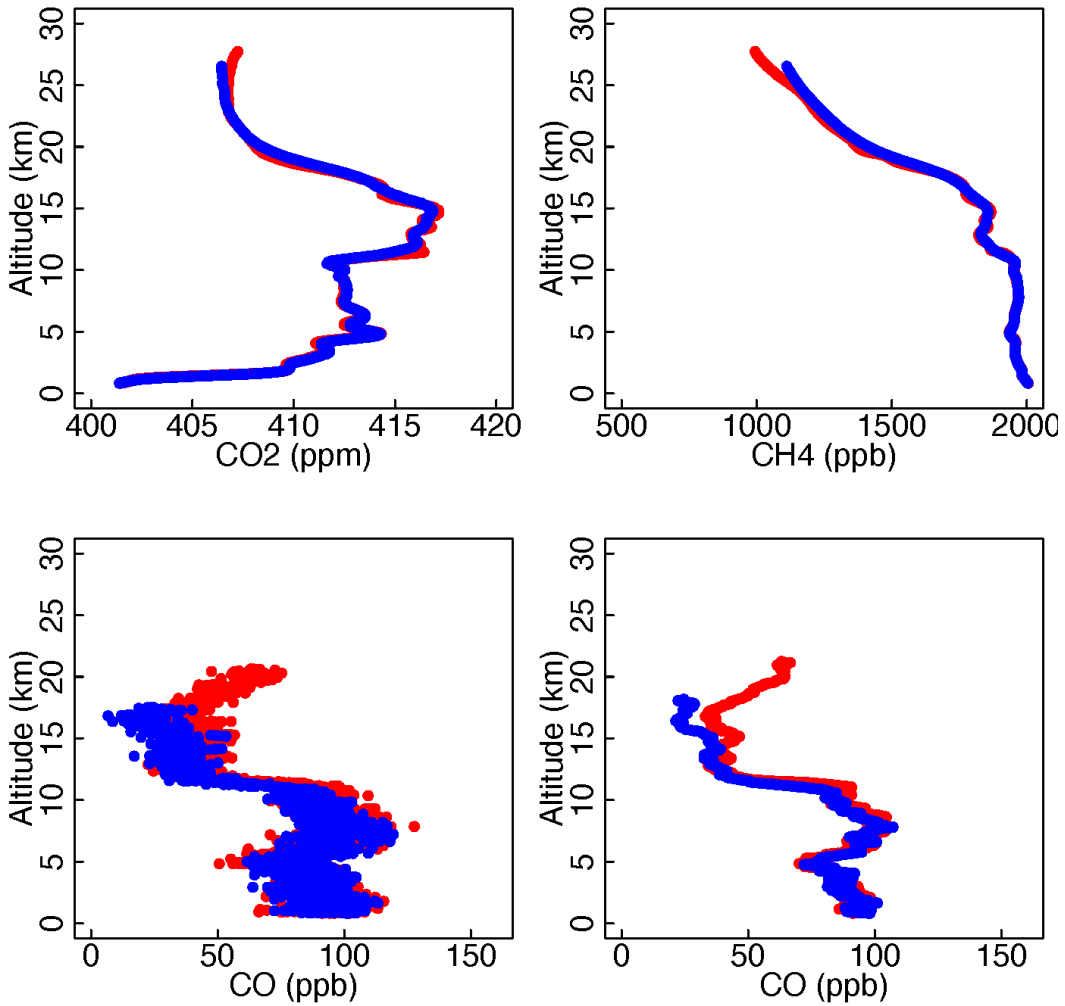
WP2 T5 (FMI, RUG): Improving AirCore retrievals and historical AirCore dataset





- Hypothesis: surface coating issue? Yes, quite likely
  - Dual AirCore flights
  - Recoating the surface

WP2 T5 (FMI, RUG): Improving AirCore retrievals and historical AirCore dataset



- Agreement very good for CO_2 and CH_4, but clear difference for CO

  (**confirmation of previous suspect, not sure issues with surface coating**)

Summary and Outlook

- AirCores tested for sampling COS and N_2O in Kiruna and Rotterdam
- First dual AirCore launch confirmed the suspected CO bias, and the performance of the new AirCore for CO_2 and CH_4
- Update the CO product of historical FRM4GHG
  - Version 1: remove unrealiable stratospheric part
  - Version 2: possible correction or composite product with LISA?
- Upcoming Sodankylä campaign August 2023
  - With and without an ozone scrubber
  - Dual AirCore launches
  - AirCore and LISA launches

Thank you for your attention

FMI progress in WP 1 – 3 during March 2022 – January 2023

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https://frm4ghg.aeronomie.be/

Objectives

Fiducial Reference Measurements for Ground-Based Infrared Greenhouse Gas Observations (FRM4GHG 2.0)

FMI objectives:

- AirCore development
- Simultaneous NIR and MIR spectra recording with TCCON instrument at Sodankylä
- Perform additional AirCore launches
- Update FRM4GHG dataset based on latest version of PROFFAST and GGG
- Project management (contributor)
- Outreach (contributor)

Measurements

Fiducial Reference Measurements for Ground-Based Infrared Greenhouse Gas Observations (FRM4GHG 2.0)

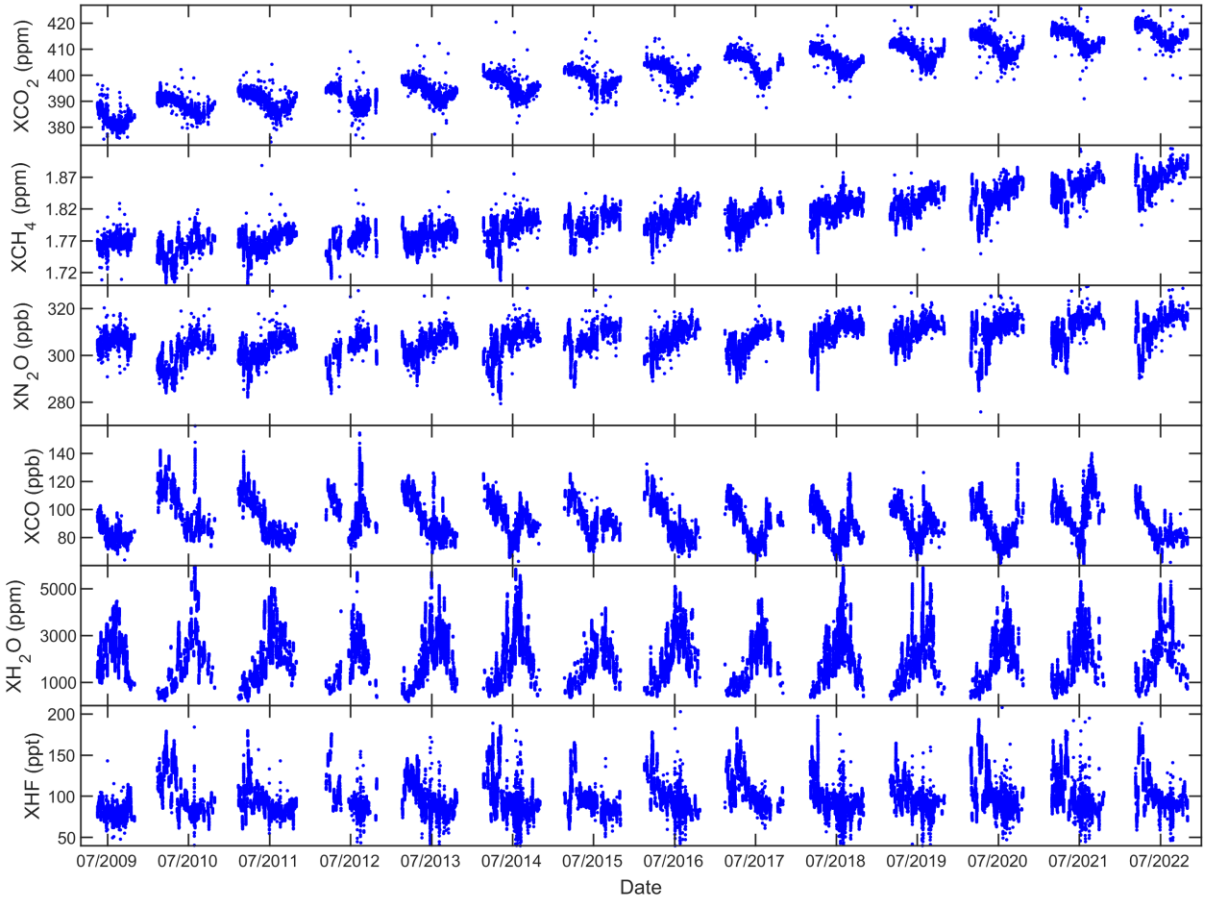
FMI:
FRM4GHG 2.0 measurements were made at Sodankylä: TCCON, AirCores, etc.
Possibility to host visiting instruments and field campaigns.

Measurements

Bruker *IFS 125HR* with *A547N* solar tracker.
Detectors:
RT-InGaAs: *12800 - 4000 cm^{-1}*
RT-Si: *25000 - 9000 cm^{-1}*
LN-InSb: *10000 - 1850 cm^{-1}*

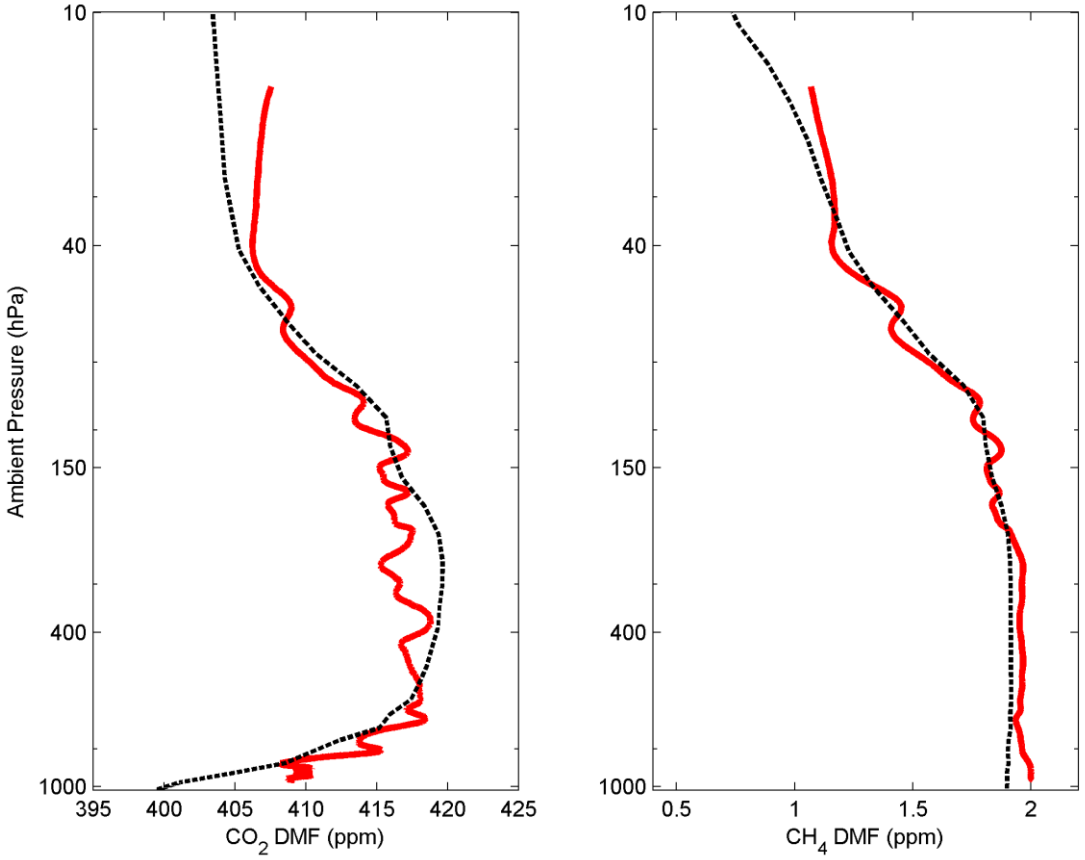
In operation since FEB-2009

Map of the TCCON sites



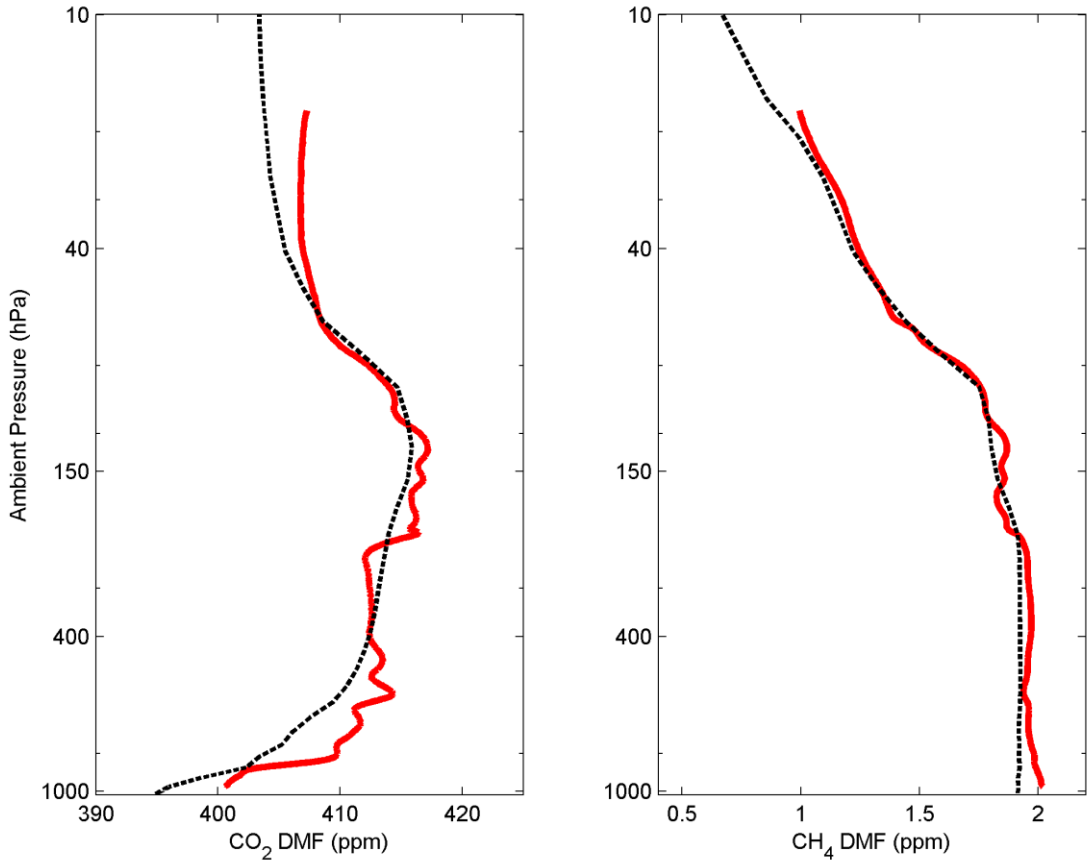
Column-averaged dry air mole fractions at Sodankylä since 2009. Updated from Kivi and Heikkinen (2016), using GGG2020.

AirCores



AirCore profiles (red) and TCCON GGG2020 a priori (dashed line).
Sodankylä 29 June 2022 08:09 UTC.

AirCores



AirCore profiles (red) and TCCON GGG2020 a priori (dashed line).
Sodankylä 25 August 2022 08:02 UTC.

Summary and outlook

Summary:

- AirCore development work is ongoing. N2O analyser was calibrated. First N_2O measurements were performed. Also dual soundings were made having two AirCore instruments in one payload.
- Comparison with GGG2020 prior profiles was made for the AirCore flights performed in 2022. We found improved agreement with TCCON priors, compared to the previous version of GGG software.
- TCCON retrievals using the latest GGG version were made. Historical data sets since 2009 were postprocessed using GGG2020.
- TCCON instrument has been operational. We updated software to operate the FTIR. Replaced solar tracker controller and solar tracker hatch motor. Installed new sensors for FTIR hatch operation. We also ordered a new filter wheel from Bruker. The delivery was delayed, the equipment should arrive in February 2023.
- Installed a new Vaisala weather station for the FRM4GHG container.
- Both HR and LR measurements have been made.
- We have readiness to host visiting instruments and campaigns.

Summary and outlook

Outlook:

- More AirCore flights are planned for the upcoming 6 month period.
- NIR and MIR spectra recordings.
- Update the FRM4GHG dataset: AirCores and TCCON.
- Host visiting instruments.

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Zhou, M., Langerock, B., Sha, M. K., Hermans, C., Kumps, N., Kivi, R., Heikkinen, P., Petri, C., Notholt, J., Chen, H., and De Mazière, M.: Atmospheric N_2O and CH_4 total columns retrieved from low-resolution FTIR spectra (Bruker Vertex 70) in the mid-infrared region, Atmos. Meas. Tech. Discuss. [preprint], https://doi.org/10.5194/amt-2022-17, in review, 2022.

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Thank you for your attention

Photo: Sodankylä site in April 2022.