Towards traceable remote sensing GHG measurements & data products

Before handing over to Benedikt, Annmarie & Elizabeth, a few ideas / comments to start with …

Towards traceable remote sensing GHG measurements

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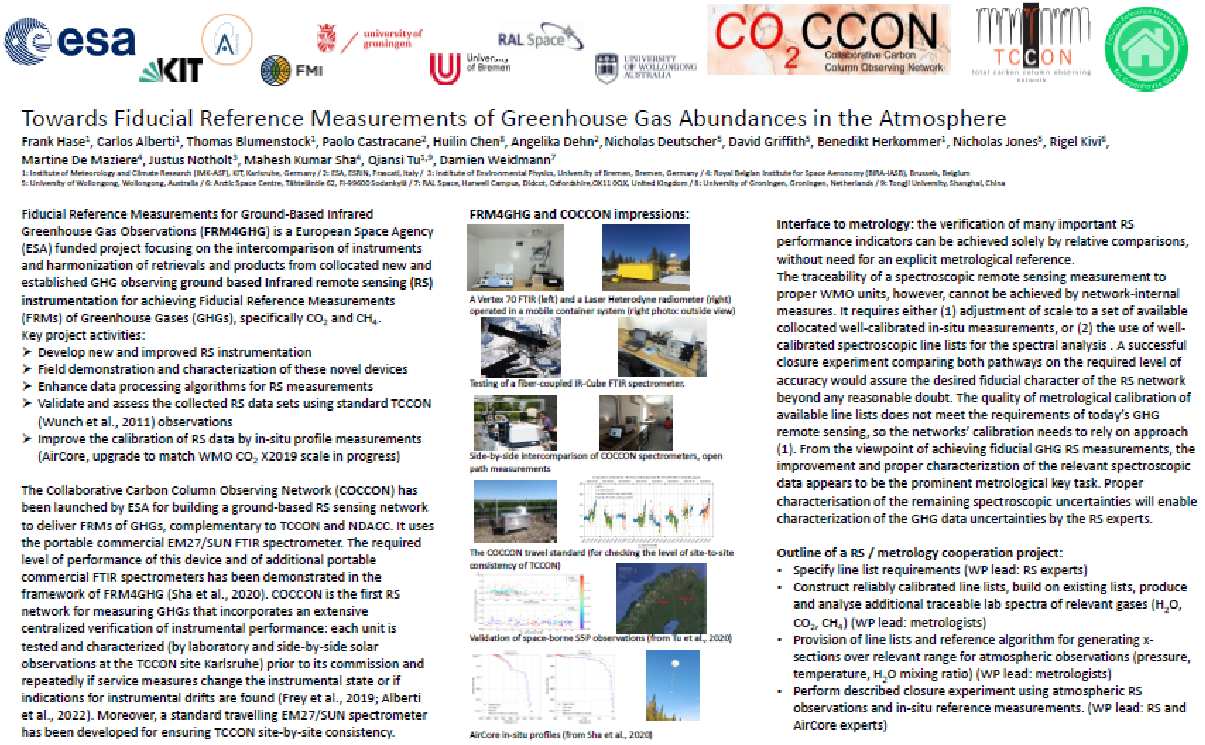
In my feeling, what primarily is required from the metrology agencies for improving the traceability of RS GHG data is pretty clear (my poster for BIPM-WMO meeting in Sept 23 on behalf of FRM4GHG consortium):



Towards Fiducial Reference Measurements of Greenhouse Gas Abundances in the Atmosphere

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Fiducial Reference Measurements for Ground-Based Infrared Greenhouse Gas Observations (**FRM4GHG**) is a European Space Agency (ESA) funded project focusing on the **intercomparison** of instruments and harmonization of retrievals and products from collocated new and established GHG observing **ground based Infrared remote sensing (RS) instrumentation** for achieving Fiducial Reference Measurements (FRMs) of Greenhouse Gases (GHGs), specifically CO_2 and CH_4.

Key project activities:

- Develop new and improved RS instrumentation
- Field demonstration and characterization of these novel devices
- Enhance data processing algorithms for RS measurements
- Validate and assess the collected RS data sets using standard TCCON (Wunch et al., 2011) observations
- Improve the calibration of RS data by in-situ profile measurements (AirCore, upgrade to match WMO CO_2 X2019 scale in progress)

The Collaborative Carbon Column Observing Network (COCCON) has been launched by ESA for building a ground-based RS sensing network to deliver FRMs of GHGs, complementary to TCCON and NDACC. It uses the portable commercial EM27/SUN FTIR spectrometer. The required level of performance of this device and of additional portable commercial FTIR spectrometers has been demonstrated in the framework of FRM4GHG (Sha et al., 2020). COCCON is the first RS network for measuring GHGs that incorporates an extensive centralized verification of instrumental performance: each unit is tested and characterized (by laboratory and side-by-side solar observations at the TCCON site Karlsruhe) prior to its commission and repeatedly if service measures change the instrumental state or if indications for instrumental drifts are found (Frey et al., 2019; Alberti et al., 2022). Moreover, a standard travelling EM27/SUN spectrometer has been developed for ensuring TCCON site-by-site consistency.

FRM4GHG and COCCON impressions:

A Vertex 70 FTIR (left) and a Laser Heterodyne radiometer (right) operated in a mobile container system (right photo: outside view)

Testing of a fiber-coupled IR-Cube FTIR spectrometer.

Side-by-side intercomparison of COCCON spectrometers, open path measurements

The COCCON travel standard (for checking the level of site-to-site consistency of TCCON)

Validation of space-borne SSP observations (from Tu et al., 2020)

AirCore in-situ profiles (from Sha et al., 2020)

Interface to metrology: the verification of many important RS performance indicators can be achieved solely by relative comparisons, without need for an explicit metrological reference.
The traceability of a spectroscopic remote sensing measurement to proper WMO units, however, cannot be achieved by network-internal measures. It requires either (1) adjustment of scale to a set of available collocated well-calibrated in-situ measurements, or (2) the use of well-calibrated spectroscopic line lists for the spectral analysis . A successful closure experiment comparing both pathways on the required level of accuracy would assure the desired fiducial character of the RS network beyond any reasonable doubt. The quality of metrological calibration of available line lists does not meet the requirements of today's GHG remote sensing, so the networks' calibration needs to rely on approach (1). From the viewpoint of achieving fiducial GHG RS measurements, the improvement and proper characterization of the relevant spectroscopic data appears to be the prominent metrological key task. Proper characterisation of the remaining spectroscopic uncertainties will enable characterization of the GHG data uncertainties by the RS experts.

Outline of a RS / metrology cooperation project:

- Specify line list requirements (WP lead: RS experts)
- Construct reliably calibrated line lists, build on existing lists, produce and analyse additional traceable lab spectra of relevant gases (H_2O, CO_2, CH_4) (WP lead: metrologists)
- Provision of line lists and reference algorithm for generating x-sections over relevant range for atmospheric observations (pressure, temperature, H_2O mixing ratio) (WP lead: metrologists)
- Perform described closure experiment using atmospheric RS observations and in-situ reference measurements. (WP lead: RS and AirCore experts)

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What‘s about traceability of the processing chain?

Overshooting schemes (imho) were proposed by European metrologists a while ago:

- Generation of any fiducial GHG data products requires a processing chain certified by a metrology angency.
- The certified processing setup needs to be coded, tested, and distributed by a metrology agency.

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I believe the proposed scheme was neither sensible nor practicable:

- A reference code does not become a reference by claiming it to be a reference (example: KOPRA versus “Hogwarts“ reference code).

F. Hase & M. Höpfner: Atmospheric ray path modeling for radiative transfer algorithms – technical note, AO, 1999

- A reference code would be unfit for operational processing.
- If the strict certification scheme is taken seriously, it would encompass software + hardware (e.g. Pentium processor bug).

The correct value of the calculation is:

$$\frac{4{,}195{,}835}{3{,}145{,}727} = 1.333820449136241002$$

When converted to the hexadecimal value used by the processor, 4,195,835 = 0x4005FB and 3,145,727 = 0x2FFFFF. The "5" in 0x4005FB triggers the access to the "empty" array cells. As a result, the value returned by a flawed Pentium processor is incorrect at or beyond four digits:[8]

$$\frac{4{,}195{,}835}{3{,}145{,}727} = 1.333739068902037589$$

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In contrast, it is highly sensible to compare and cross-evaluate results generated by different networks and codes! -> Thanks to Elizabeth and Annmarie for their efforts!

There is a further approach to demonstrate that our processing schemes are „reliable“ (a sensible re-interpretation of the overstretched ideas mentioned on slide 4): run the codes on a given data set on various platforms, show that the level of agreement is within the expected numerical precision (will discover improper algorithmic approaches, near singularity inversion schemes, could reveal that a source code is buggy, …). -> Benedikt