FRM4GHG

Fiducial Reference Measurements for Greenhouse Gases

Deliverable D4.2

System intercomparison and characterisation document

Deliverable:	**4.2**
Date:	**25/05/2018**
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Subject:	**ESA-IPL-POE-LG-cl-LE-2015-1129**
Category:	**ESA Express Procurement (EXPRO)**
Our ref.:	**Proposal No. 1129/2015 –** **Proposal from February 16, 2016, comments from May 27, 2016**

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1 Document change record

Issue	Date	Item	Comment
V0	2018-03-27	–	Initial version
V1	2018-04-10	-	Added TCCON / LHR comparison text
V2	2018-04-20		Added contributions from FH, DW, CP, DG and other extensive changes by NJ
V3	2018-05-03		Material reorganised and Allan Variance added
V4	2018-05-23		Final draft for telecon 18-05-24
V5	2018-05-28		Final comments added after telecon

2 Access list

This document is a deliverable "D4.2: System intercomparison and characterisation document (4.2)" 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 document presents the updates of the deliverables for the measurement and retrieval strategy (D2.3, D2.5, and D3.1) as previously submitted to ESA. The updates are provided based on the individual change for each participating instrument.

The deliverable addresses WP Data analysis and Corrective Measures Task T4.2: Perform and document the complete data analysis including the detailed quantitative characterisation of the instrument system differences according to the agreed intercomparison protocol and output D4.2: System intercomparison and characterisation document.

4 Document structure

See Table of Contents

5 Intercomparison and characterisation of instruments

The instruments and their respective retrieval methods are described in deliverable D2.3 and summarised in Table 1. Table 2 summarises activities and interventions for each instrument over the period of measurements, March – October 2017.

Table 1. Summary of instruments and retrieval methods

Instrument	Operator	Hardware setup summary	Resolution cm^{-1} (0.9/OPD)	Measure-ment averaging time (approx., min)	Retrieval method
TCCON	FMI	Standard TCCON HR125 high resolution FTS, reference instrument	0.02	1.3	GFIT 2014, TCCON standard
TCCON-NLC	FMI/KIT	As TCCON, non-linear correction applied in FT to calculate spectra	0.02	1.3	GFIT 2014, TCCON standard
TCCON-LR	FMI	As TCCON, spectra recorded at 0.5 cm^{-1} resolution	0.5	0.5	PROFFIT
EM27/SUN	KIT	Bruker EM27/Sun, integrated tracker, manual daily operation.	0.5	1	PROFFIT
IRcube	UoW	Bruker IRcube, fibre coupled to 50mm telescope on Eko tracker	0.5	1	GFIT 2016
Vertex	Bremen-IUP	Bruker Vertex lab FTS, accepts parallel beam through side-port from BIRA tracker	0.2	2.5	GFIT 2014
LHR	RAL	Laser heterodyne radiometer, pickoff 10 mm diameter beam from BIRA/Vertex tracker	0.02 set by RF filter	0.5	Optimal estimation method, using RFM (Reference Forward Model Provided online, see Results section)

Table 2. Summary of activities and interventions.

Date 2017	TCCON	EM27	IRcube	Vertex	LHR
4 March	Setup week				
6 March		Setup week			
13 March			Setup week		
21 April				Setup week.	
27 April					Setup week.
23 Mar			Fibre broken		
15 May			Fibre replaced, measurements restart		
6 July				20mm aperture stop (variable iris) installed in parallel beam exiting interferometer	
12 Sep				Reduced aperture stop iris to 8-9 mm	
7 Sep					Stop measurements
21 Oct				Stop measurements	
12 Oct					Removal week
22 Oct			Stop measurements		
31 Oct		Stop measurements			
1 Nov	Stop measurements				

This deliverable follows deliverable 3.1, in particular it uses the datasets and strategies in the analysis described in section 3.1.6, working with the final datasets reported in deliverable 4.1 from each participating instrument in the FRM4GHG campaign.

For the purposes of direct numerical comparison of outputs from the participating instruments in this report:

- each dataset was interpolated onto the common TCCON measurement time grid. In general the low resolution (LR) test instrument data are more closely spaced in time than TCCON data. A linear interpolation was used between adjacent LR-instrument points to the TCCON time. The LR measurement points were within 10 minutes of the TCCON measurement times.

- Note this method is slightly different from that in deliverable 3.1, in which both LR and TCCON data were binned into predetermined time intervals of 5 minutes and averaged. The binning method averages a variable number of measurements for each datapoint and provides some averaging, but the averaged datapoints are drawn from distributions with different variances so the statistics are not as well defined. The linear interpolation always provides a weighted average between two points and thus provides less smoothing but the datapoints are drawn from the same statistical distribution. A smoothing spline interpolation or similar could be used (in future) to smooth the higher frequency LR data.

- all differences were calculated and plotted on the TCCON time grid. We used the standard TCCON retrieval without non-linearity correction. By inspection of the plots, means, and standard deviations of differences over the whole dataset are very similar to outputs from deliverable 3.1 but not identical due to the different averaging/interpolation methods.
- Existing comprehensive plots of all instruments referenced to TCCON for CO_2, CH_4, CO, H_2O and Xair are available online, see link in section 8.

6 Results

For systematic comparisons, all instrument data were interpolated onto the TCCON time grid as described above. In this approach, TCCON data are taken as reference, and any changes seen in the difference between TCCON and LR instruments are relative to TCCON. The combined data are provided:

1. As datafiles, one each for X_{CO2}, X_{CH4}, X_{CO} and X_{AIR} containing comparable data for each instrument
2. As a file of mean differences and standard deviations between individual instruments and TCCON over each whole year dataset. The means and standard deviations of the previous comparison of binned data (Deliverable D3.1) are included in the file for comparison.
    a. In addition, a comprehensive set of plots is provided that are an update and extension of those presented as an interim report in deliverable D3.1

Section 8 provides links to the final datasets and plots.

6.1 Comparisons by species

6.1.1 X_{CO2}

Figure 1 shows X_{CO2} data for all instruments over the full year and Figure 2 shows the corresponding differences relative to TCCON for each test instrument.

- All instruments capture the annual summer drawdown in CO_2.
- The EM27 has the lowest mean bias relative to TCCON. The range of biases (excluding LHR) is up to 10 ppm.
- The IRcube has a possible step change in March due replacement of the fibre optic cable.
- The Vertex FTS shows a step change relative to TCCON and other instruments in July 2017 after insertion of the 20mm aperture stop.
- The LHR in its development phase shows larger scatter and larger negative bias than the FTS instruments.

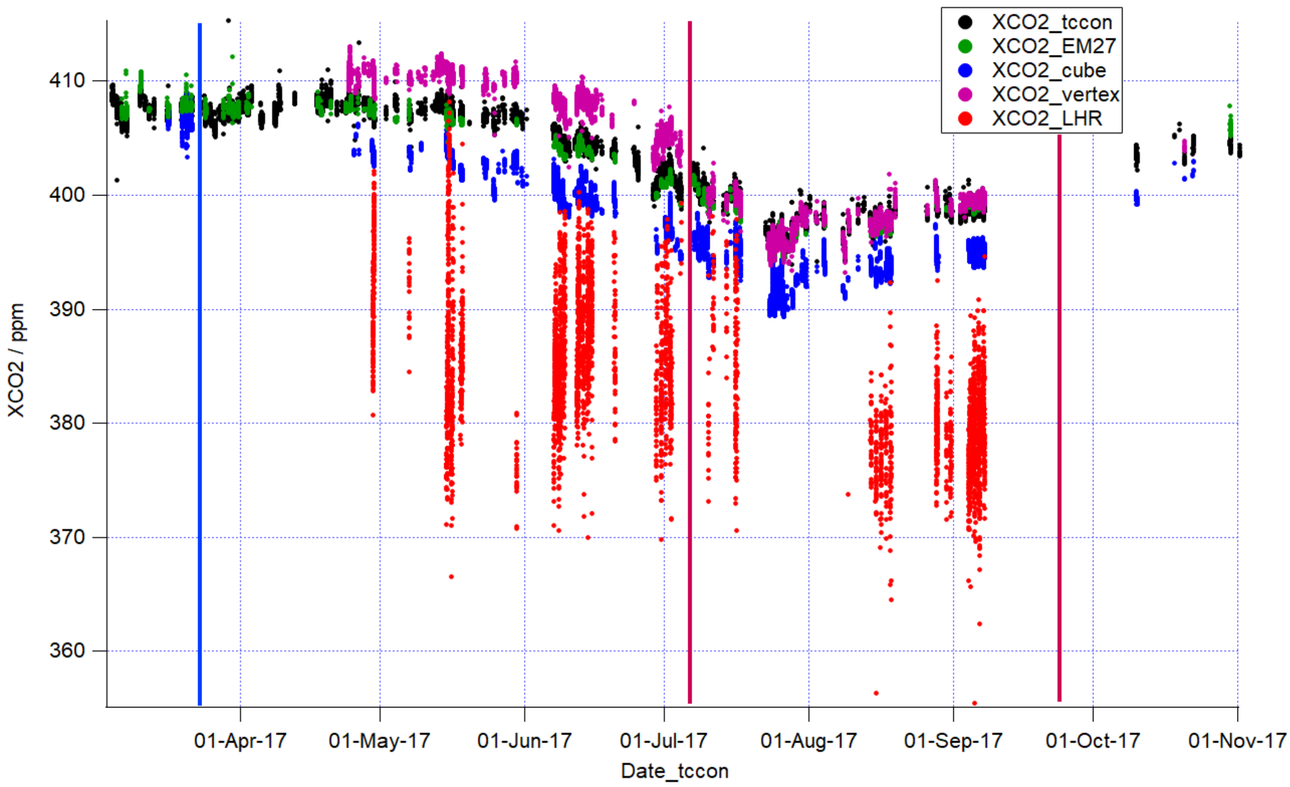

Figure 1. X_{CO2} for each instrument over the full measurement year[1].

[1] **Vertical** lines in all plots indicate instrument changes. Blue = IRcube, broken fibre in March2017. Purple = Vertex, insertion of aperture in July 2017 and reduction of aperture size in Sept 2017.

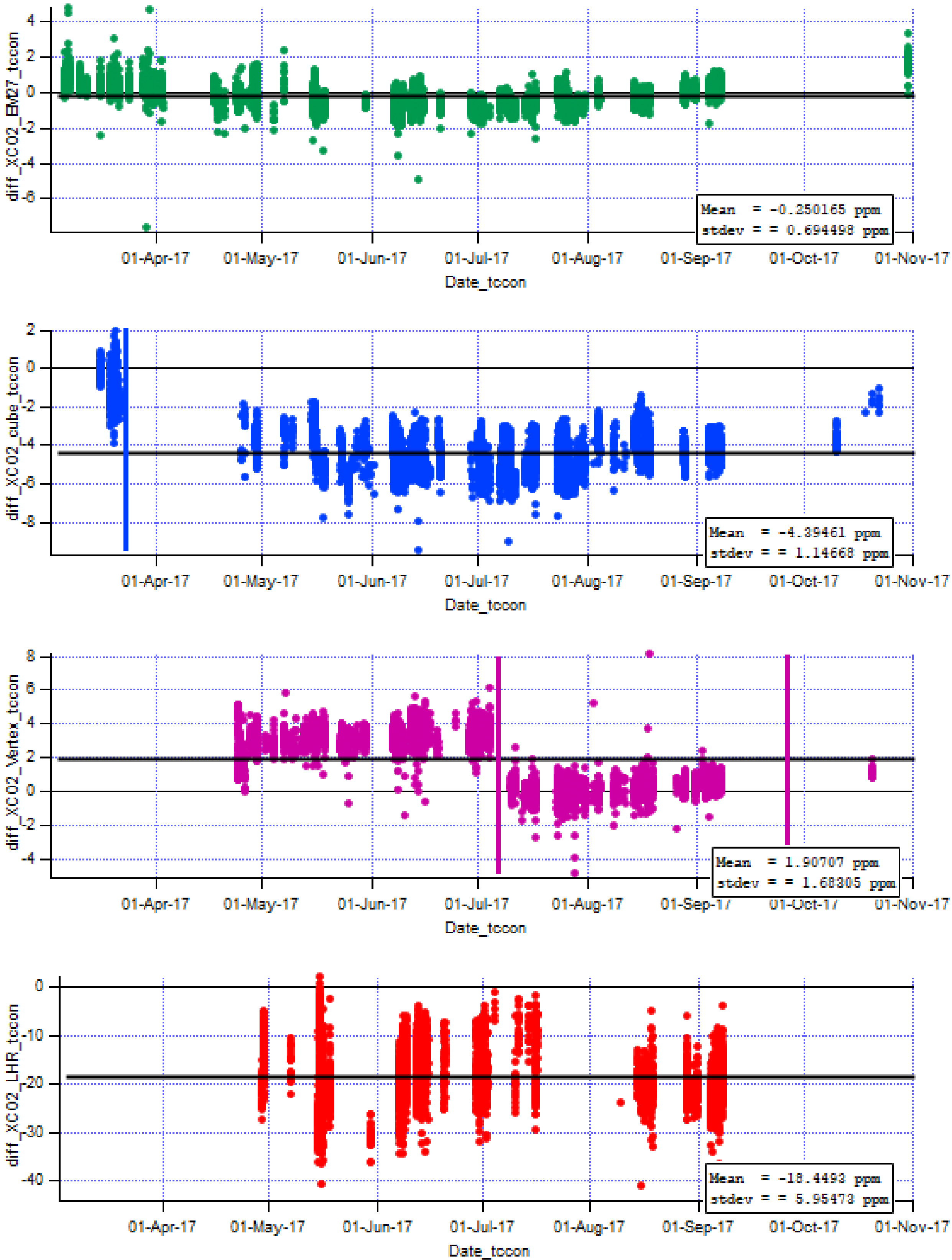

Figure 2. X_{CO2} differences to TCCON for the full year. Top to bottom, EM27, IRcube, Vertex and LHR.

Figure 3 shows X_{CO2} data from Figure 1 for a clear sky day, 6 Sept 2017, and Figure 4 shows data plotted against solar zenith angle for 8 June when the range of solar zenith angles was greatest. Apart from the average biases, different instruments show different time of day or solar zenith angle dependence up to 2 ppm.

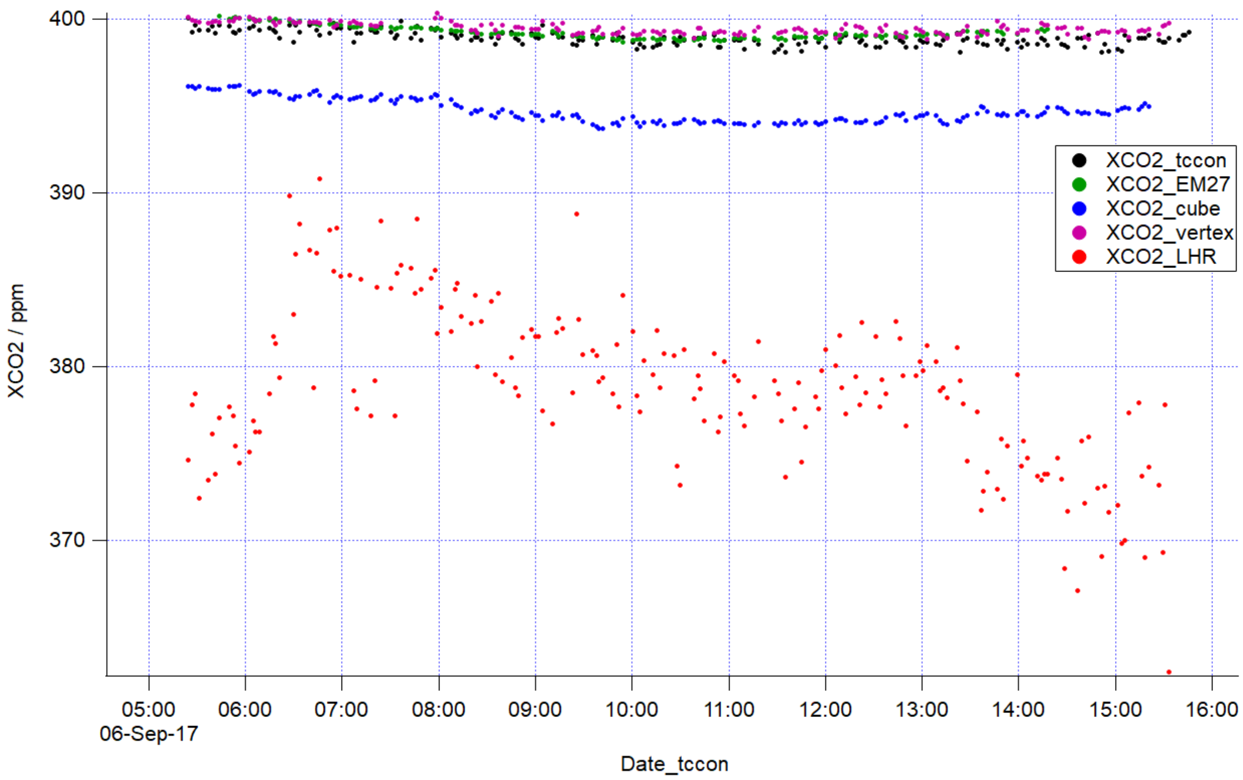

Figure 3. X_{CO2} for all instruments on 6 Sept 2017.

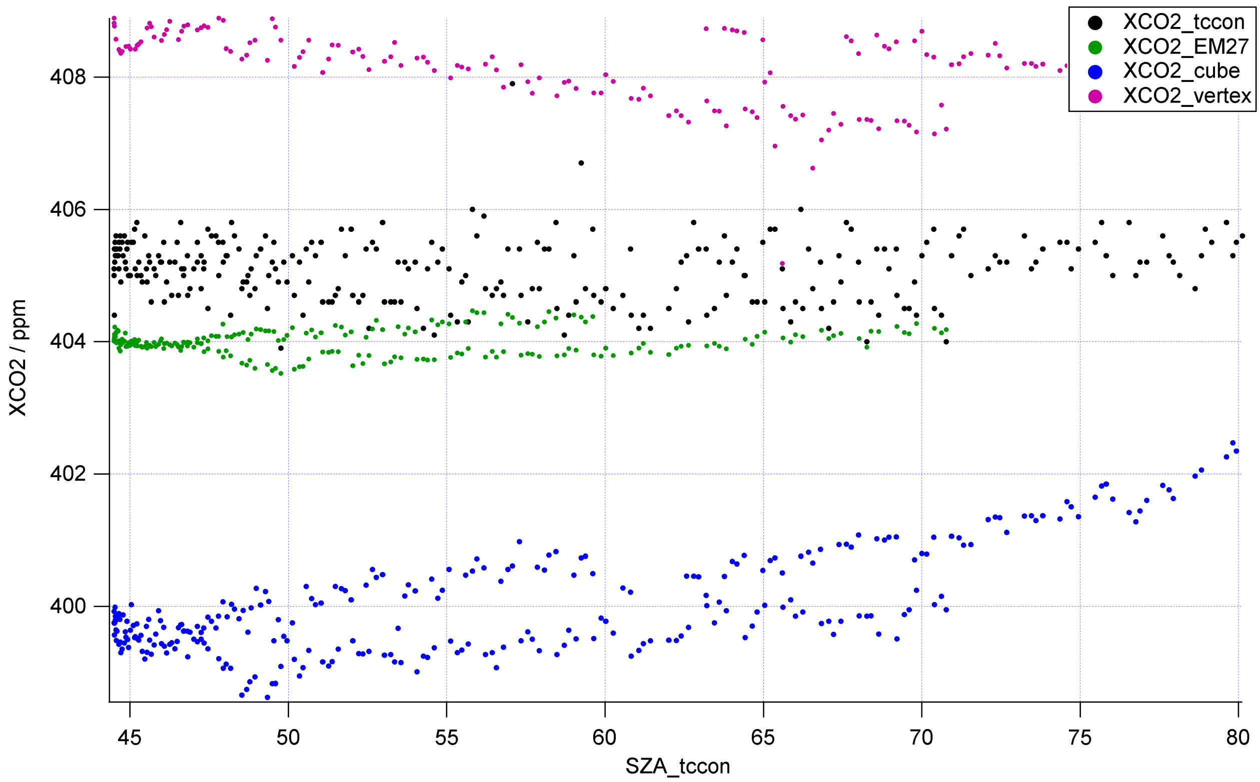

Figure 4. X_{CO2} data for 8 June 2017 plotted against solar zenith angle.

6.1.2 X_{CH4}

Figure 5 shows X_{CH4} data for all instruments over the full year and Figure 6 shows the corresponding differences relative to TCCON for each test instrument. Figure 7 shows all instrument data for the clear sky day 6 Sept 2017.

- The annual cycle is consistent for TCCON EM27 and IRCube.
- Both EM27 and IRCube show a change in bias (0.01 ppm) of the data with respect to TCCON between the early March-April-May time period.
- Vertex has a step change (-0.02 ppm) in July consistent with the change noted in X_{CO2} following the introduction of an aperture stop. The positive bias remains with respect to TCCON before and after the step change. The annual cycle appears to be also captured with respect to TCCON if the bias is qualitatively taken into account.

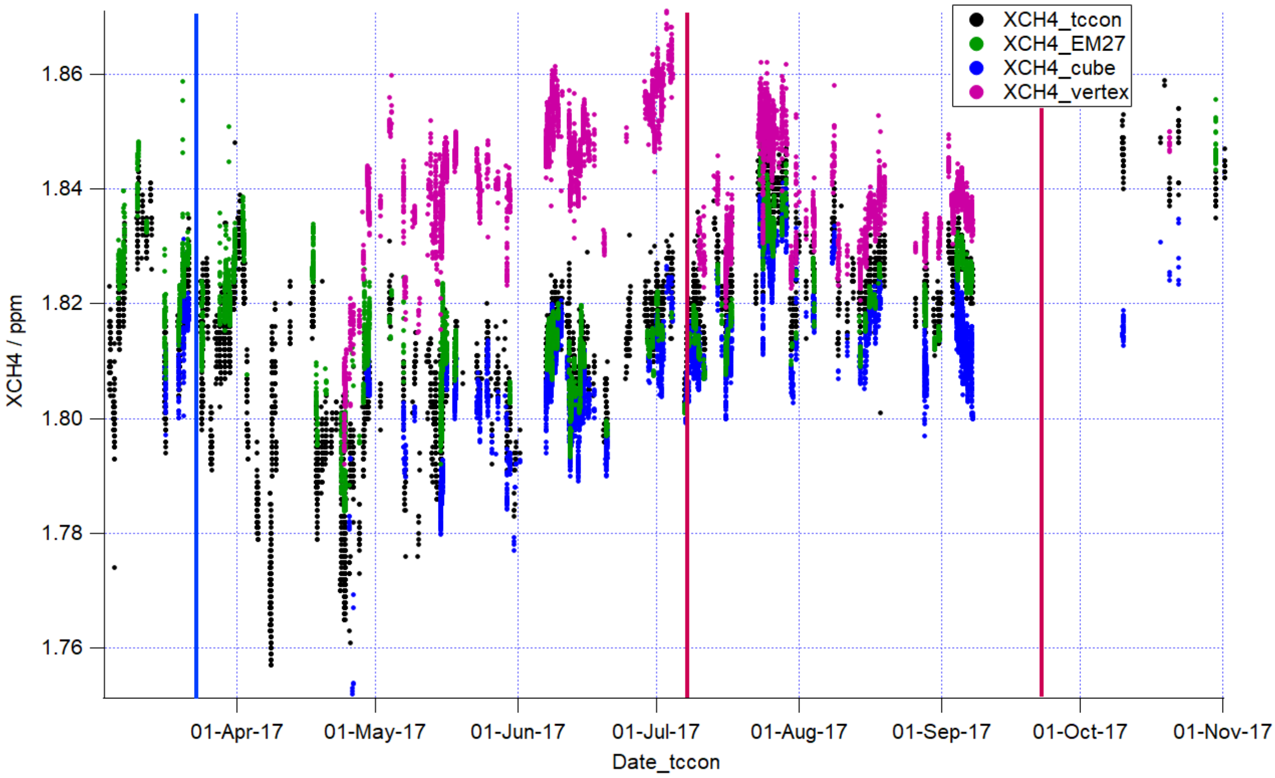

Figure 5. X_{CH4} for each instrument over the full measurement year.

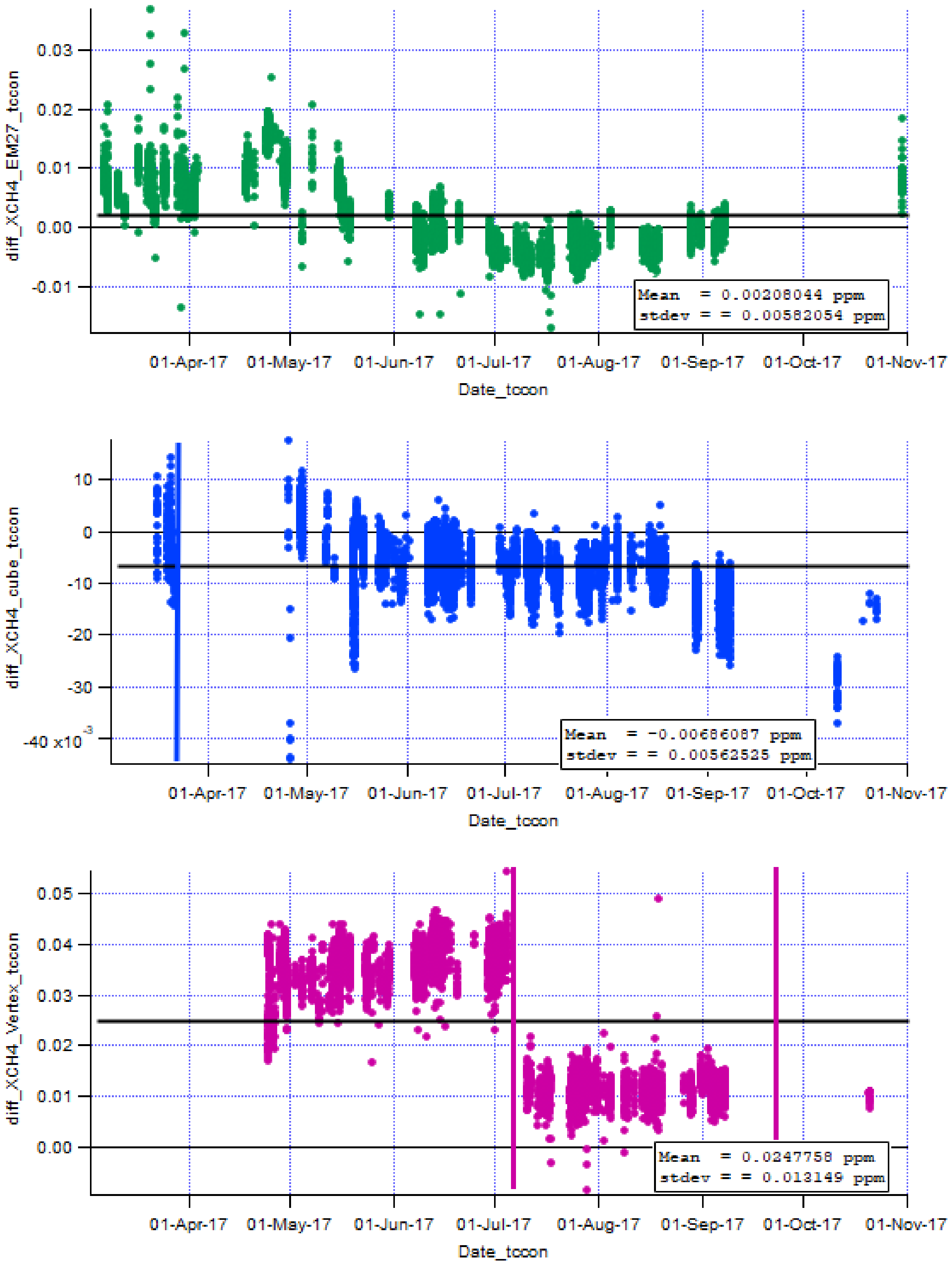

Figure 6. X_{CH4} differences to TCCON for the full year. Top to bottom, EM27, IRcube, Vertex.

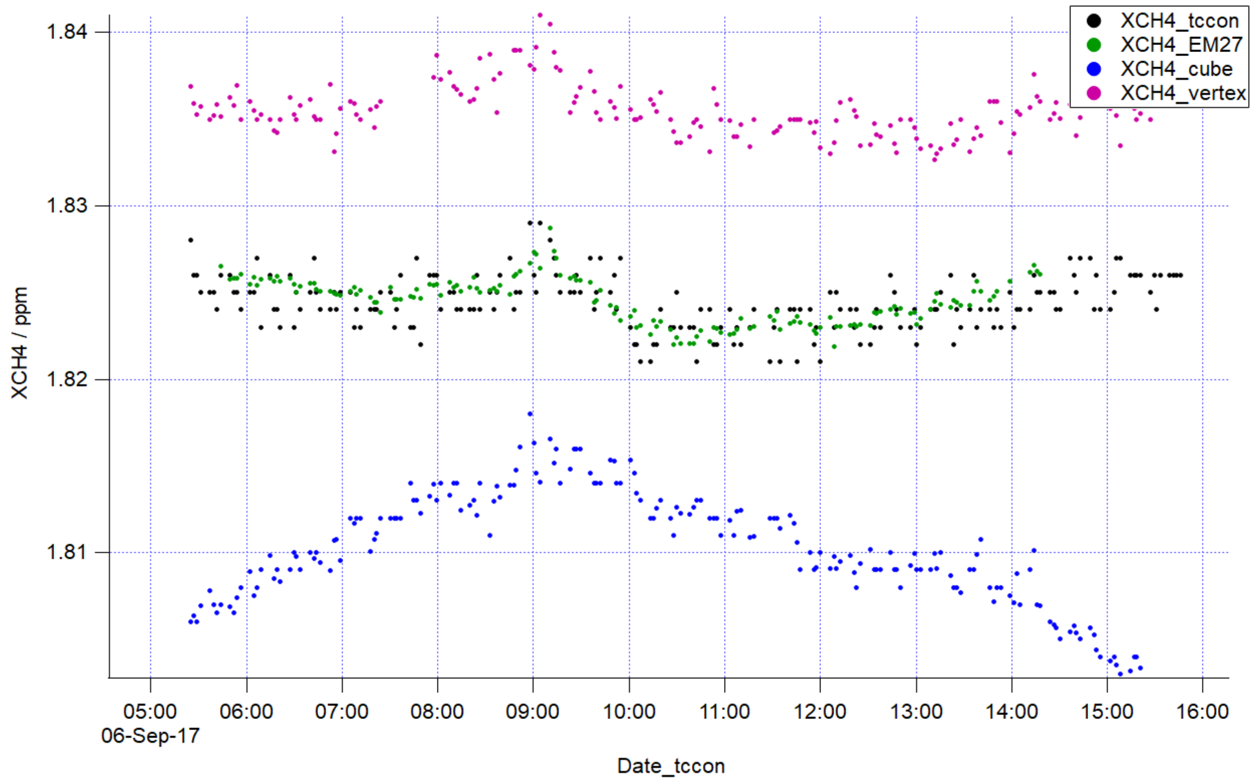

Figure 7. X_{CH4} for all instruments on 6 Sept 2017.

Figure 7 shows X_{CH4} data from Figure 5 for a clear sky day, 6 Sept 2017.

- The EM27 and Vertex capture the TCCON X_{CH4} variation over the day from 6am to 3pm, with a clear bias of ~10 ppb for the Vertex .
- The IRCube has a more pronounced SZA dependence.

6.1.3 X_{CO}

Figure 8 shows X_{CO} data for the EM27/SUN and Vertex70 instruments over the full year and Figure 9 shows the corresponding differences relative to TCCON for each test instrument. Figure 10 shows the EM27 and Vertex X_{CO} data for the clear sky day 6 Sept 2017.

- All instruments capture the seasonal cycle of X_{CO} with summer minimum.

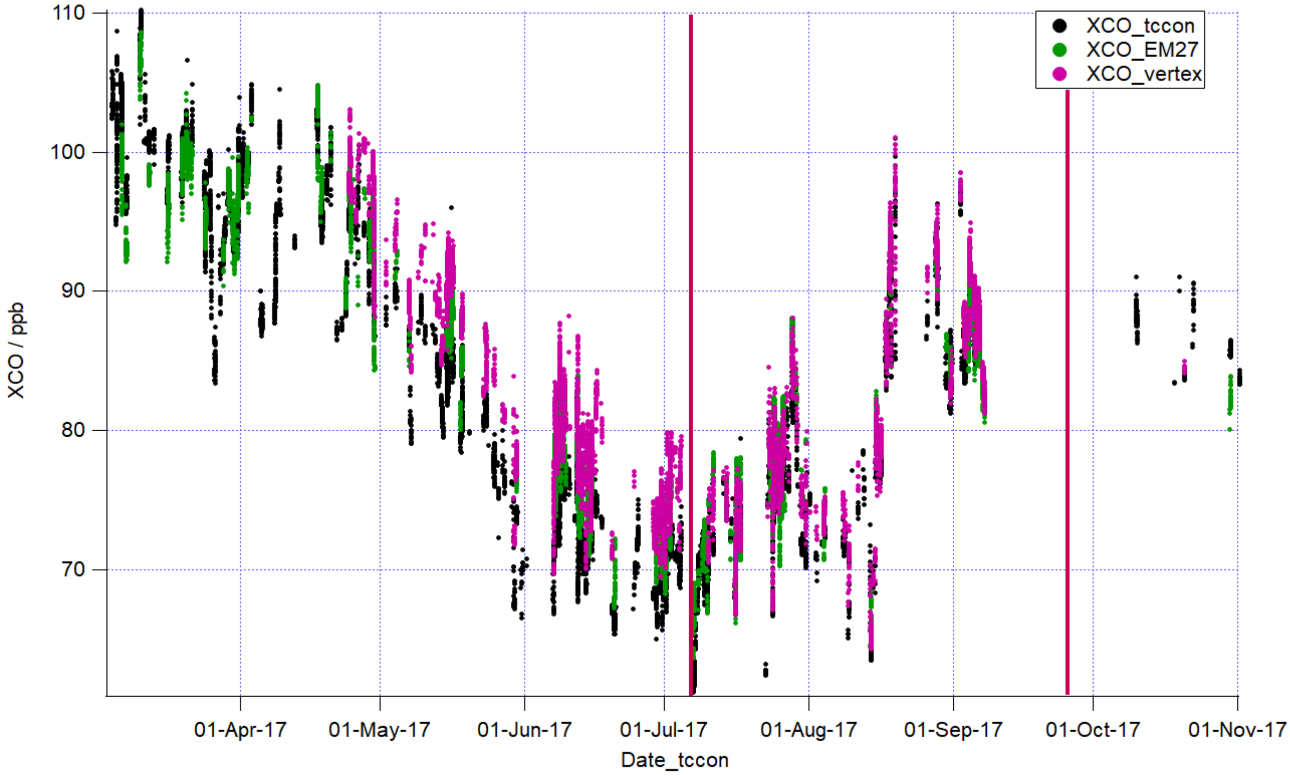

Figure 8. X_{CO} for each instrument over the full measurement year.

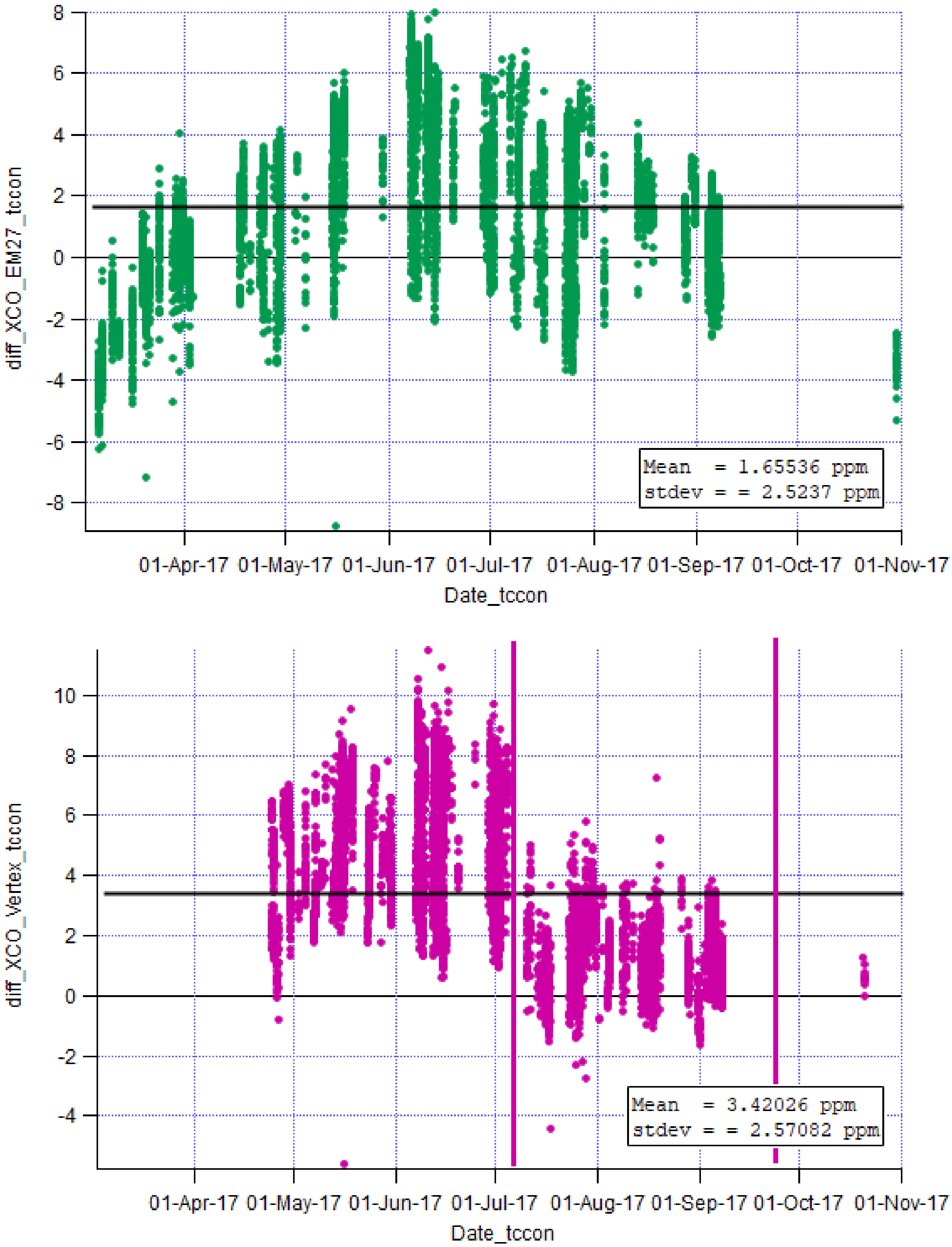

Figure 9. X_{CO} differences to TCCON for the full year. Top to bottom, EM27, Vertex.

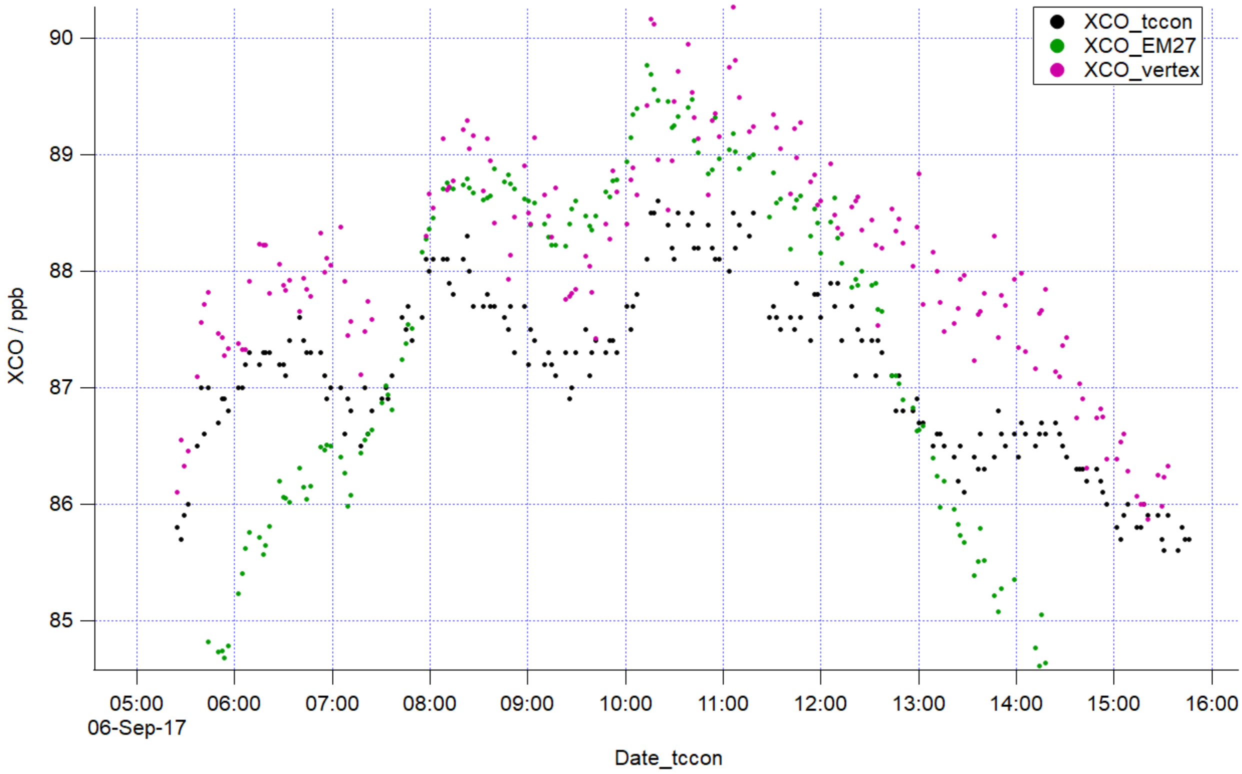

Figure 10. X_{CO} for all instruments on 6 Sept 2017.

6.1.4 X_{air}

Figure 11 - Figure 14 show equivalent data for X_{air}, which is proportional to the ratio of the surface pressure to the total retrieved O_2 column and should be 1.00 in the ideal case. X_{air} is a measure of both instrument and analysis code performance.

- The IRcube and Vertex airmass dependence follows TCCON (decrease with increasing SZA)
- The EM27/SUN shows the smallest airmass dependence.
- The two "branches" of the Vertex data are due to the addition of the aperture stop in July – the higher branch with $X_{air} > 0.99$ are all from the earlier period without the aperture stop.
- there is a known inconsistency in the EM27/SUN X_{air} determination as the 20% spectroscopic offset of our retrieved H_2O for the calculation of X_{air} has not been included, but the H2O dependence is still relatively low as it is for the IRCube and Vertex, see document FRM4GHG_2017_TCCON_LHR_Vertex70_IRcube_EM27SUN.pdf, page 45.

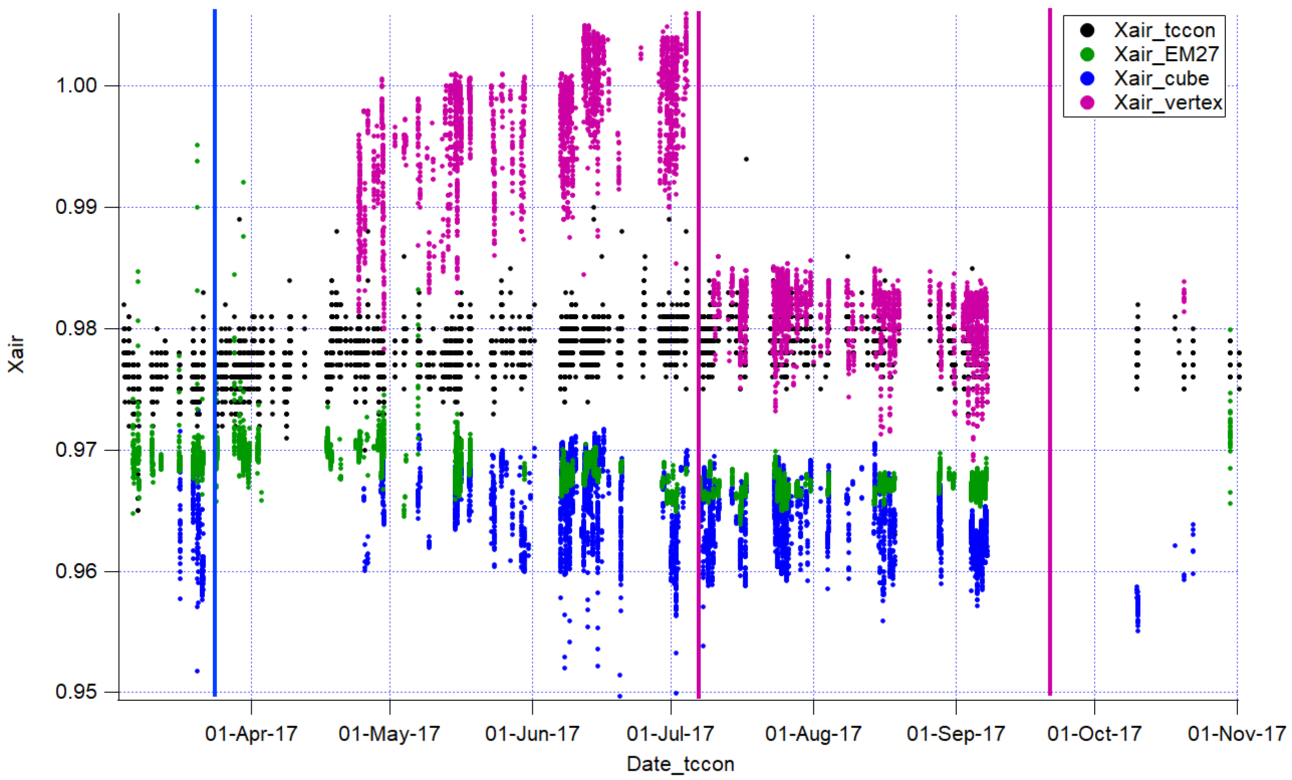

Figure 11. X_{air} for each instrument over the full measurement year.

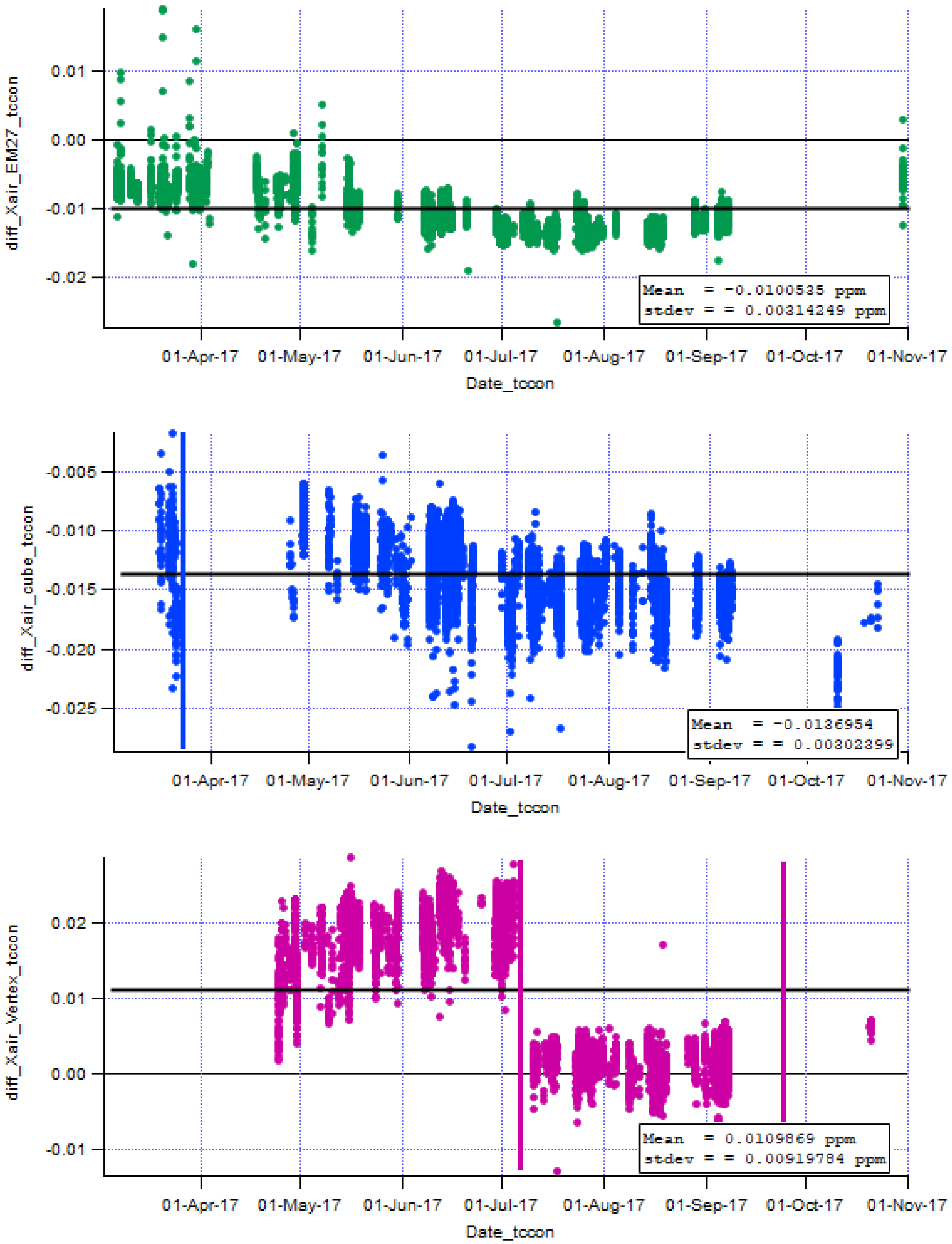

Figure 12. X_{air} differences to TCCON for the full year. Top to bottom, EM27, IRcube, Vertex.

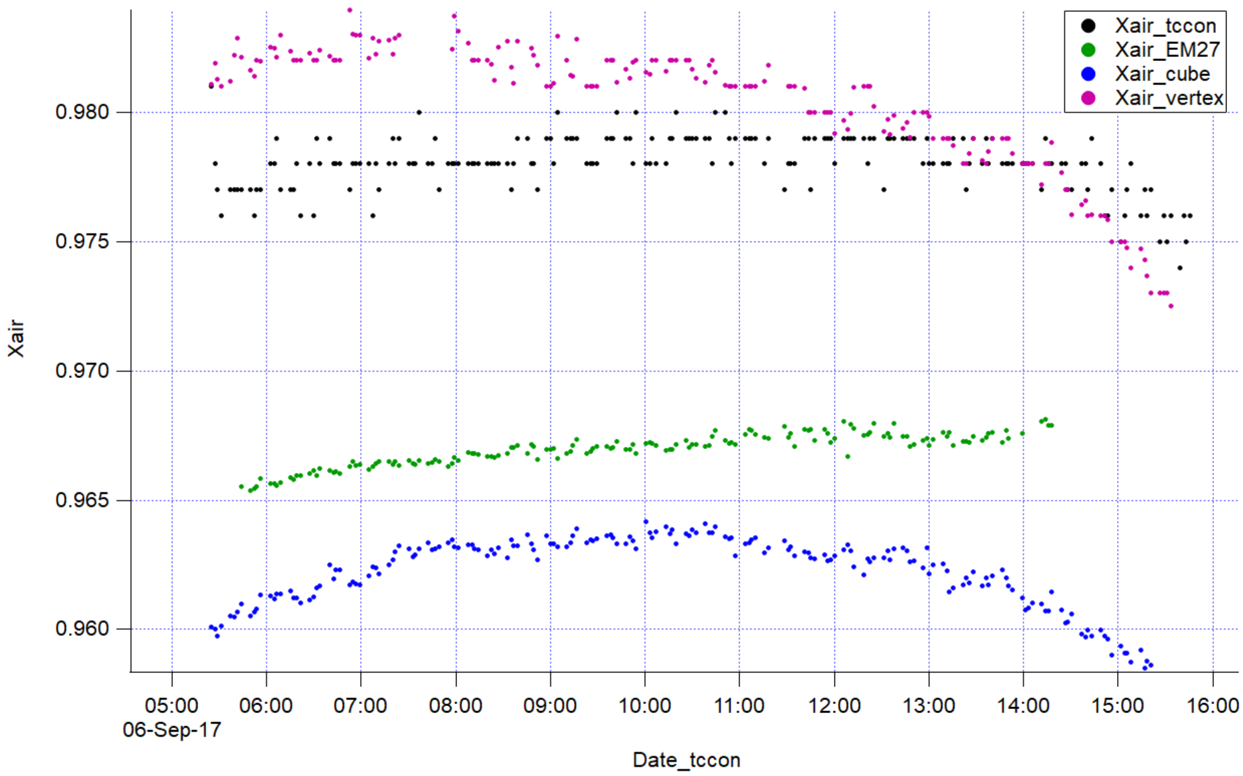

Figure 13. X_{air} **for all instruments on 6 Sept 2017.**

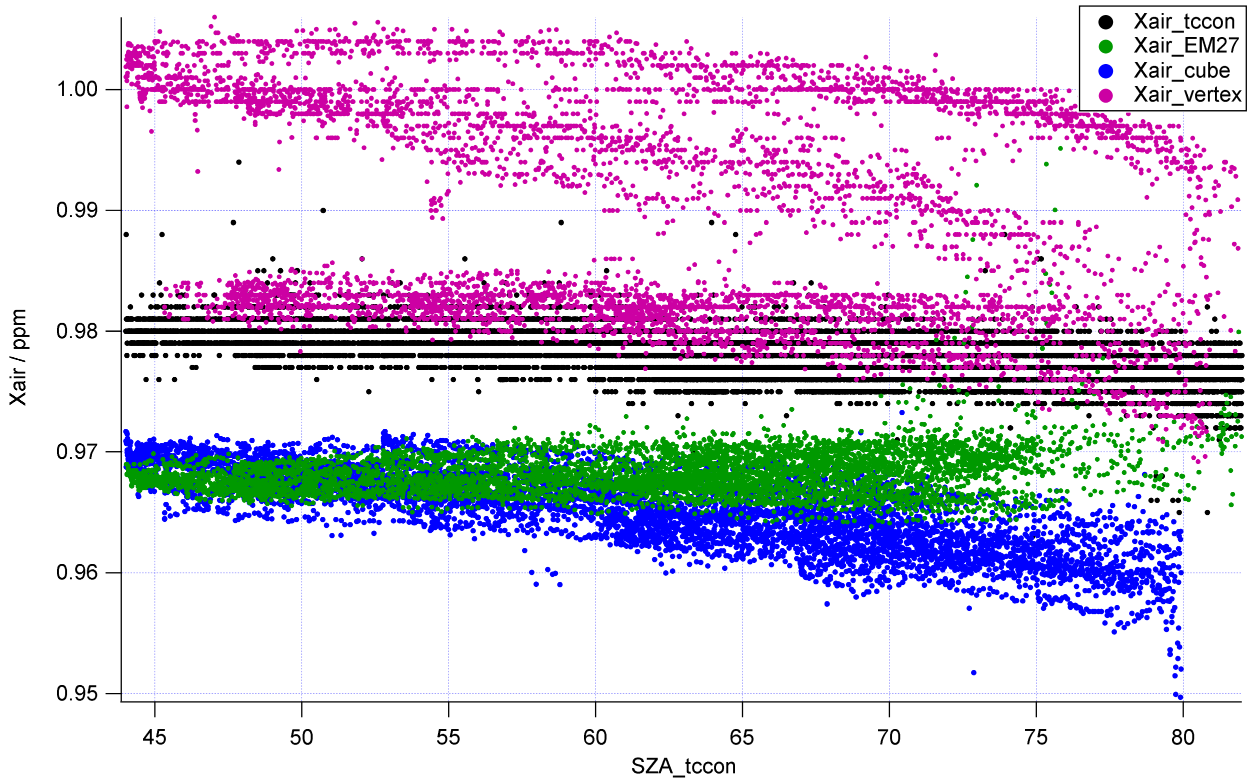

Figure 14. X_{air} **vs solar zenith angle for all instruments**

6.2 Annual mean measurement biases

The data of the preceding section contain real day-to-day and seasonal variability and step changes due to operator interventions and other instrument configuration changes. It is therefore inappropriate to compare specific figures of merit between instruments for the full datasets. Table 3 summarises the annual mean differences or biases relative to TCCON as an indicative measured of comparability only.

Table 3. Mean bias relative to TCCON for the entire data set. The top section is calculated from the linearly interpolated values on the TCCON time grid; the lower section from deliverable 3.1 is calculated from the low resolution data binned and averaged for both TCCON and test instruments around fixed comparison times. The Vertex mean includes data both before and after the instrument change on 6 July.

	cube	EM27	vertex	LHR
Mean bias D4.2				
XCO2 / ppm	-4.39	-0.250	1.91	-18.4
XCH4 / ppm	-0.007	0.002	0.024	
XCO / ppb		1.656	3.42	
Xair	-0.013	-0.010	0.011	
Mean Bias D3.1				
XCO2 / ppm	-4.29	-0.258	1.379	-18.4
XCH4 / ppm	-0.005	0.002	0.021	
XCO / ppb		1.685	2.75	
Xair	-0.013	-0.01	0.008	

6.3 Measurement precision – Allan Variance

The measurement precision or repeatability for each instrument must be determined in the presence of real variations in the retrieved total column or X_{gas} data, so a standard deviation or similar statistic taken over a long time period is not an appropriate measure of precision. Allan variance (AV, or its square root, Allan deviation, AD) is the variance of the series of differences between time-adjacent measurements as a function of the averaging time of those measurements. Measured AV includes variance due to both measurement noise and any real change or drift in the true measured signal. If there is no real signal variability and the measurement noise is randomly distributed (as in the ideal case for detector noise), AV should decrease linearly with averaging time (and AD with the square root of averaging time). If there is real variability, the AV will decrease less than the random noise limit for averaging times longer than the timescale of the real variability. If the real variability of the measurand is slower in time than the timescale of the individual measurements, AV for single measurements should have only a small contribution from real variability and can be interpreted as an upper limit to the true variance of single measurements.

We have thus calculated Allan Deviations for the clear sky day of 6 Sept 2017, when the real variability was small, for X_{CO2} and X_{CH4} for all instruments. The Allan deviations as a function of averaging time for X_{CO2} are shown in Figure 15 and the single-measurement Allan deviations (ie the leftmost point in each AD plot) and measurement times are tabulated in Table 4.

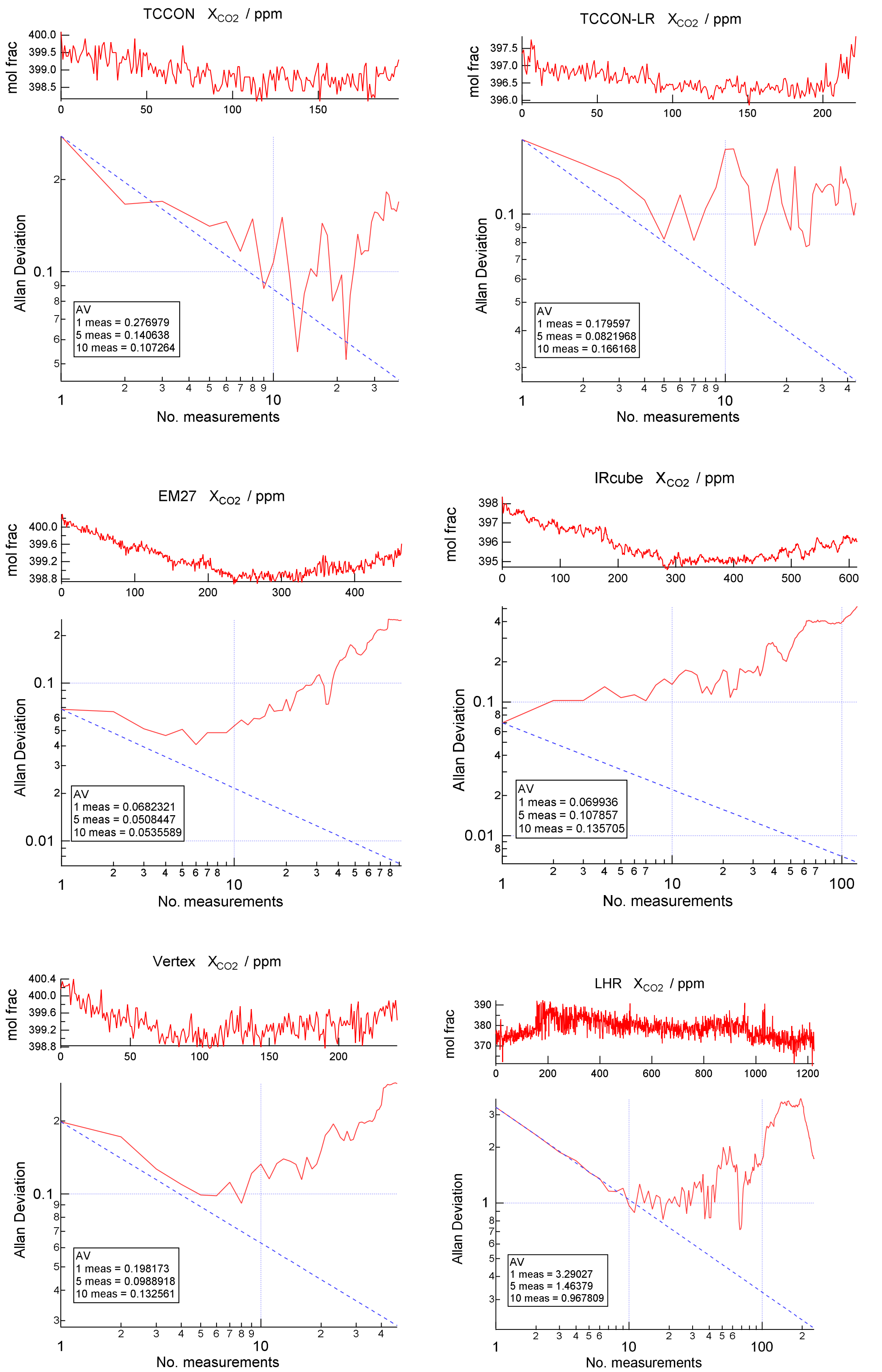

Figure 15. Allan deviation plots for X_{CO2} in ppm for 6 Sept 2017. The blue dotted lines represent the expected limit for random noise only.

Table 4. Single measurement times and Allan deviations for X_{CO2} and X_{CH4} for the raw data for each instrument.

Instrument	Averaging time single measurements (min)	Allan deviation single measurements	
		X_{CO2} / ppm	X_{CH4} / ppm
TCCON	1.3	0.28	0.0012
TCCON-LR	0.5	0.18	0.0008
EM27	1	0.07	0.0004
IRcube	1	0.07	0.0004
Vertex	2.5	0.20	0.0010
LHR	0.5	3.29	-

6.4 Aircore

A total of 10 AirCore profiles were made in 2017, see Figure 16. Due to logistical constrains, there were no AirCore flights in June or July, but instead four AirCore flights were made in September during a field campaign. The polar vortex was sampled by two flights in April, with the feature of very low CH_4 mole fractions between 20 and 25 km compared to other profiles. The CO profiles are noisy because of the analytical precision of the CRDS analyser used to analyse the air samples. Note that the CO profiles were only retrieved up to ~20 km because of the use of a fill gas with ~10 ppm CO mole fractions.

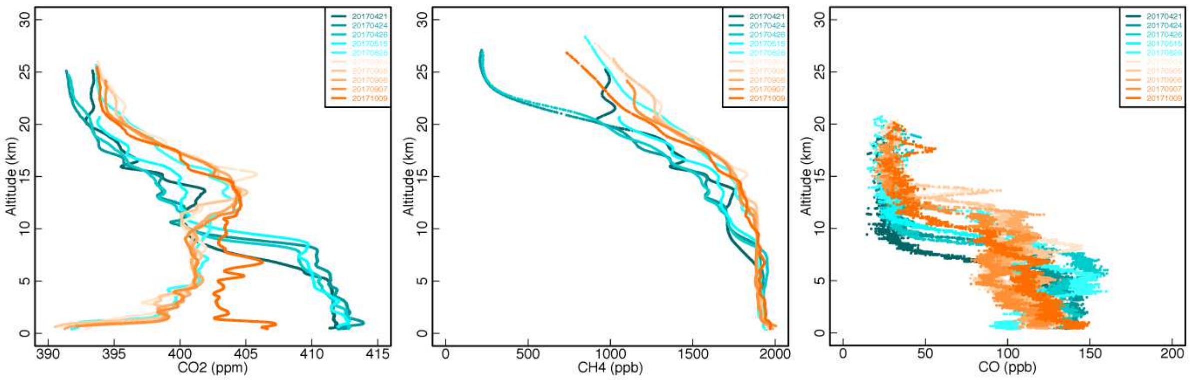

Figure 16. AirCore profiles of CO_2 (left), CH_4 (middle), and CO (right) mole fractions over Sodankyla in 2017. The CO profiles were only retrieved up to ~20 km because a fill gas with ~10 ppm CO mole fractions were used so that CO profiles above ~20 km were affected.

In addition, we have flown a recently developed lightweight stratospheric air (LISA) sampler together with AirCore in Sodankyla during four flights. The LISA sampler is capable of grabbing stratospheric air samples at an altitude of up to 30 km and provides a useful tool for validating AirCore measurements, especially the vertical altitude registration of AirCore profiles. A comparison of the four AirCore profiles and LISA sampler is shown in Figure 17.

The comparison results show that the AirCore altitude registration matches well with the LISA sampler measurements up to ~20 km. However, due to the lack of measurements of either AirCore or the LISA sampler, a direct comparison between AirCore and the LISA sampler measurements above 20 km were not possible.

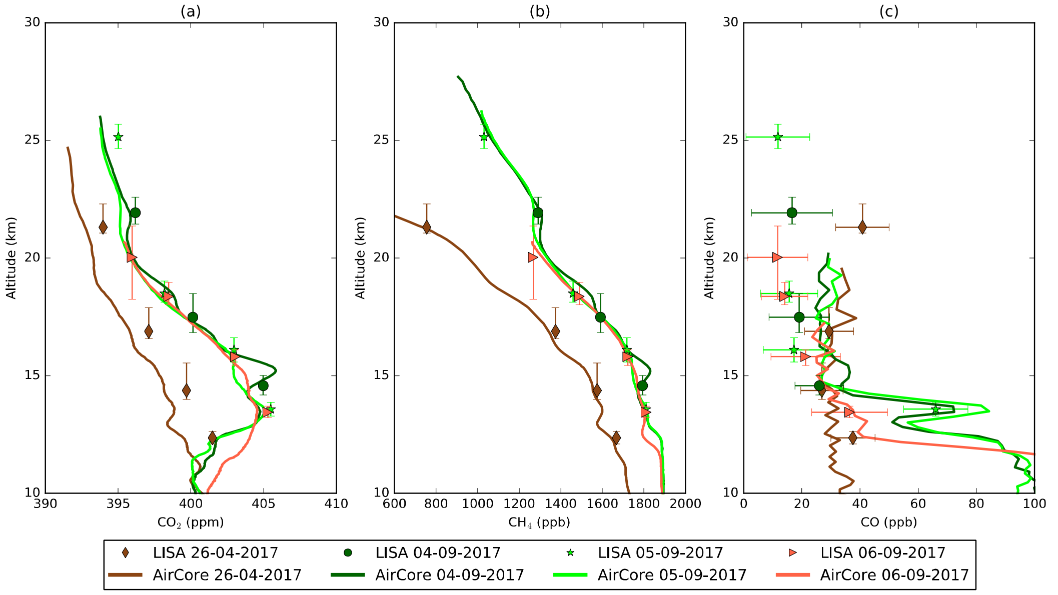

Figure 17. Comparison of AirCore and LISA measurements of (a) CO_2, (b) CH_4 and (c) CO mole fractions. The AirCore CO profiles are averaged in 100 meter bins to smooth the relatively large noise of the measurements due to the analytical precision of 7 ppb (1 sigma) of the CRDS analyser. Different colours and symbols are used to label the samples from different flights shown in the legend.

6.5 Comments and comparisons by instrument

6.5.1 TCCON - EM27

The EM27 was run throughout the campaign without any reported problems or departures from normal operational procedures as documented in a recent publication by Frey et al. (AMTD, submitted May 2018).

- Instrumental drifts were low with respect to TCCON for X_{air} and X_{CO2}
- The March-May X_{CH4} data with respect to TCCON show some positive bias, Figure 18, indicating that this is more likely a retrieval issue.

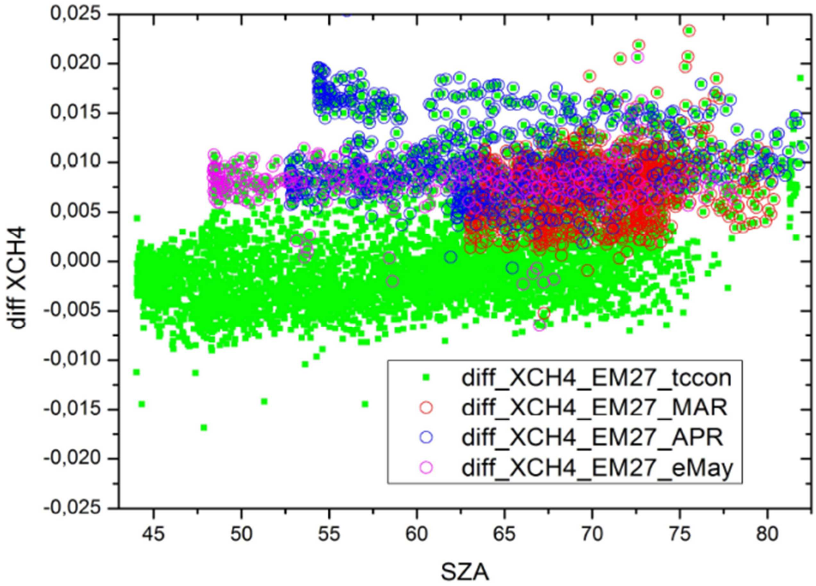

Figure 18. EM27 X_{CH4} data wrt TCCON showing March-May positive bias.

- Some of this X_{CH4} March-May bias is due to differing sensitivities between TCCON and low-res spectrometers and a-prioris not matching well with the actual profile shape

6.5.2 TCCON - IRcube

A broken optical fibre optic in March led to a possible step change in X_{CO2} after replacement, though the change could also be due to seasonal dependence. Other than this early event in March, there were no significant instrument changes or problems throughout the campaign.

- The IRCube ran autonomously throughout the campaign (once the FO was replaced), apart from ILS measurements and parking of the tracker during wet weather.

6.5.3 TCCON - Vertex

The Vertex data must be viewed in two temporal parts, before and after the addition of an external aperture stop in July 2017.

- There is a clear improvement in all gas biases after the change
- For all gases, no clear trend in the seasonal bias but this is difficult to judge based on the step change mid-year.
- Post instrument alignment, the Vertex bias appears to be close to zero for X_{CO2}, and slightly positive for both X_{CH4} and X_{CO}

6.5.4 TCCON - LHR

The LHR is an instrument in under development. Refer to document on the FRM4GHG website[2] for a more detailed description of the instrument's ongoing development.

- LHR has strong systematic negative bias and diurnal bias variation
- diurnal-varying bias affecting the LHR data has not been identified
- current LHR data are therefore not yet able to provide meaningful geophysical information but have proven invaluable to characterize and understand the LHR instrument

6.6 Analysis software

Some differences between instruments could be due to the retrieval software adopted by the different groups, PROFFIT and GFIT. It is beyond the scope of this project, but recommended for further analysis in the extension project in 2018.

The EM27/SUN analysis applies an empirical airmass correction derived before the campaign from independent measurements with another EM27/SUN during a ship cruise. This measure is an integral part of the EM27/SUN approach under consideration (as the predetermined calibration factors for the low-res network and each individual spectrometer, the use of measured ILS parameters, etc).

7 Applicable documents

Statement of Work: Fiducial Reference Measurements for Ground-Based FTIR Greenhouse Gas Observations (FRM4GHG)
Prepared by: T. Fehr/B. Bojkov (EOP-GMQ), Reference: ESA-EOPG-MOM-SOW-0007

8 Reference documents

FRM4GHG deliverable D2.3: Description of measurement strategy to ensure comparable observations, made available via the project website **http://frm4ghg.aeronomie.be/index.php/outreach/deliverables**

FRM4GHG deliverable D2.5: Retrieval strategy & Intercomparison strategy and protocol, made available via the project website **http://frm4ghg.aeronomie.be/index.php/outreach/deliverables**

FRM4GHG deliverable D3.1: Preliminary datasets & results distributed among partners via project Web portal (Semi-blind intercomparison), made available via the project website **http://frm4ghg.aeronomie.be/index.php/outreach/deliverables**

FRM4GHG deliverable D4.1: Final datasets from individual instruments delivered to ESA, made available via the project website **http://frm4ghg.aeronomie.be/index.php/outreach/deliverables**

Tabulated data in files FRM4GHG_2017_Xair.csv, FRM4GHG_2017_XCO.csv, FRM4GHG_2017_XCH4.csv, and FRM4GHG_2017_XCH4.csv included with this deliverable.

Documents available online at http://frm4ghg.aeronomie.be/index.php/documents/results: FRM4GHG_2017_TCCON_LHR_Vertex70_IRcube_EM27SUN.pdf

[2] The retrieval strategy is described in a document provided by RAL. See http://frm4ghg.aeronomie.be/index.php/documents, in Results section: **Laser Heterodyne Radiometer (LHR)**