ICOS | Atmosphere Thematic Centre

Document reference: ATC-CH-LA-RP-002-1.0

ICOS ATC Step 2 labelling report for the ICOS class 1 atmospheric station Jungfraujoch

Written by ATC
Approved by L. Rivier
Date: 2018/04/17

Document history

Version	Date	Actions
1.0	2018-04-17	Creation

Station associated documents

ID	Associated documents	Reference
AD1	ICOS atmospheric station specifications	ATC-GN-GN-SP-1.2_2016_08
AD2	ICOS step 1 report	ATC-CH-LA-RP-001-1.0
AD3	ICOS step 2 conference call minutes	ATC-GN-MT-MM-03-1.0_Step2_02Feb17; ATC-GN-MT-MM-04-1.0_Step2_24Feb17; ATC-GN-MT-MM-05-1.0_Step2_06Apr17;ATC-GN-MT-MM-06-1.0_Step2_31Jul17;ATC-GN-MT-MM-07-1.0_Step2_18Oct17;ATC-GN-MT-MM-08-1.0_Step2_11Dec17;ATC-GN-MT-MM-09-1.0_Step2_15Feb18;ATC-GN-MT-MM-10-1.0_Step2_19Mar18
AD4	Station piping and instrumentation diagram	ANET-CH-IN-PID-01-1.1-JFJ
AD5	ICOS ATC MLab water correction assessment report	ATC-ML-WC-RP-17-1.0-225
AD6	ICOS ANET Sampling system test report	ANET-CH-SS-RP-001-1.0-JFJ
AD7	ICOS ATC station website	https://icos-atc.lsce.ipsl.fr/JFJ

Diffusion

☐ ATC internal

☒ ICOS community

☐ Public

Repository

☒ Alfresco in Documents/Library/Common/ICOS-RI/ATC/MetrologyLab/Reports

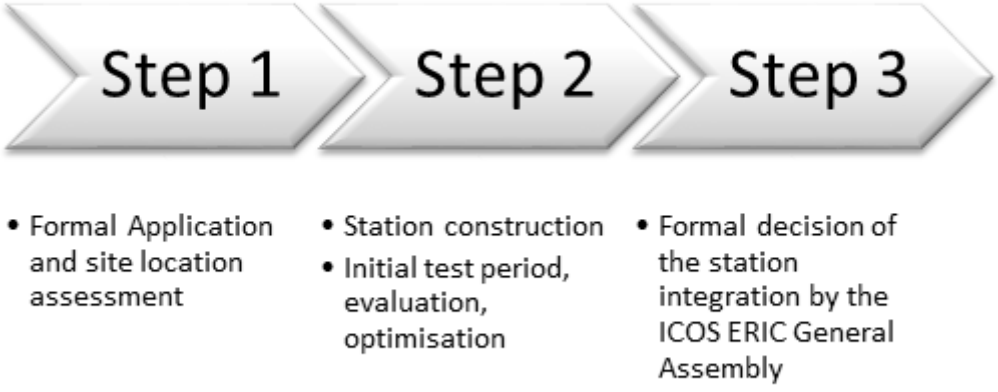
☒ ICOS ATC website: https://icos-atc.lsce.ipsl.fr/docs

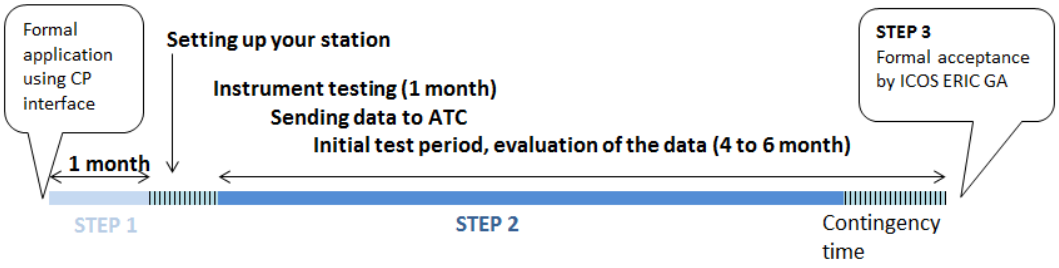
Disclaimer

Contents

1 Introduction

An atmospheric station officially becomes ICOS when it receives the ICOS label. ICOS Station Labelling is a 3 step process summarized in graph below.





Once the data flow from the station to the ATC is in place, a phase of measurement optimization starts, the so called initial test period. This is done in close collaboration between the station PI and the ATC. This period typically lasts 4 to 6 months to gather enough time-statistics. The period can be prolonged if need be.

Various measures, listed below, are used to assess the quality of the measurements:

- For gas measurements: Precision (CMR) / reproducibility (LTR) using target measurements (commensurate to ATC results)
- Temperature sensitivity of the gas instruments
- Bias assessment (based on the measurement of the target gas prepared and calibrated by ICOS FCL)
- Atmospheric signal variability (spike, local contamination detection)
- Drying system efficiency
- Data availability summary
- Flask- In-situ comparison when available
- Dedicated tests following discussion with ATC (eg. droplet test, ...)

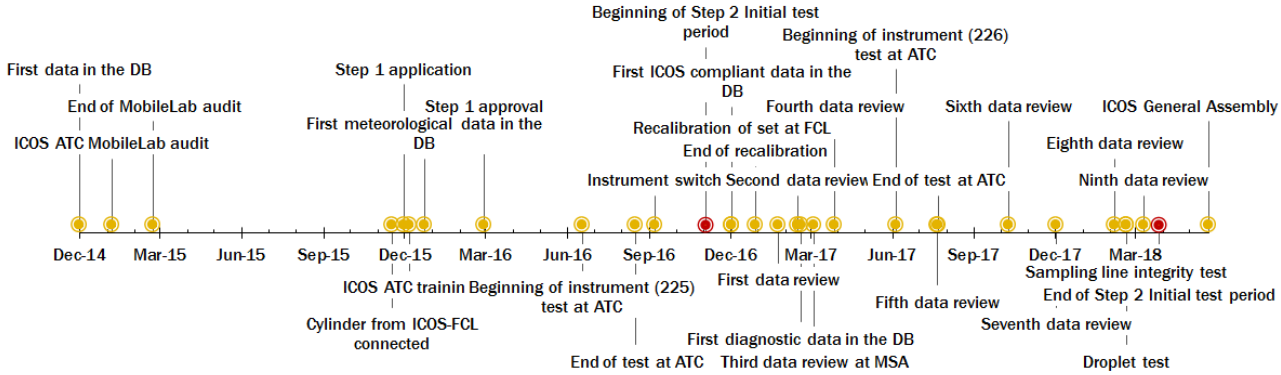
The step 2 finishes at the end of the initial test period.

In this report, we present the results of this initial testing period of labelling step 2 making use of data products to display various aspects of the measurements made at the station. We also check that all mandatory parameters and procedures are followed.

A short presentation of each data product is made, but for more details you can consult its dedicated webpage at https://icos-atc.lsce.ipsl.fr/dataproducts. Abbreviations as well as a glossary for technical terms can be found at the end of the document.

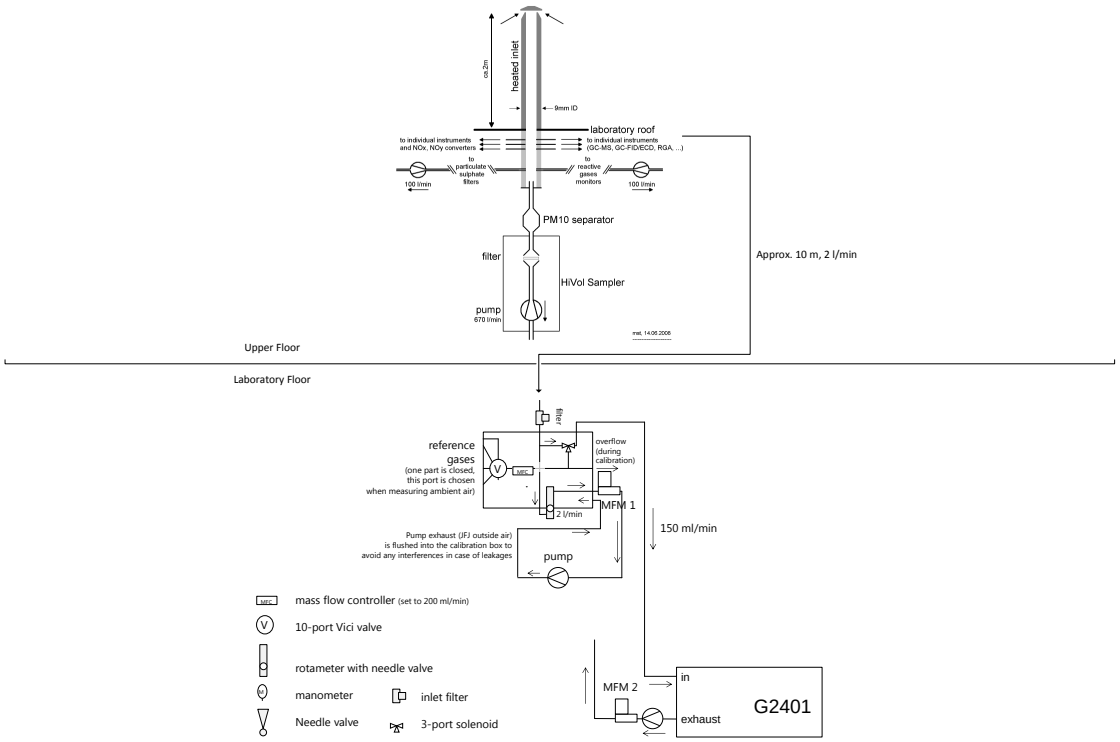
The recommendations found in this report are graded as minor, important or critical and are complemented with a priority (*** indicating highest priority) and a suggested completion date.

2 Station installation and operation timeline



DATE	MILESTONE
10-Dec-2014	First data in the DB
15-Jan-2015	ICOS ATC MobileLab audit
3-Mar-2015	End of MobileLab audit
26-Nov-2015	Cylinder from ICOS-FCL connected
9-Dec-2015	Step 1 application
15-Dec-2015	ICOS ATC training
1-Jan-2016	First meteorological data in the DB
8-Mar-2016	Step 1 approval
27-Jun-2016	Beginning of instrument (225) test at ATC
26-Aug-2016	End of test at ATC
16-Sep-2016	Instrument switch
12-Nov-2016	**Beginning of Step 2 Initial test period**
12-Dec-2016	First ICOS compliant data in the DB
12-Dec-2016	Recalibration of set at FCL
7-Jan-2017	End of recalibration
2-Feb-2017	First data review
24-Feb-2017	Second data review
27-Feb-2017	First diagnostic data in the DB
14-Mar-2017	Third data review at MSA
6-Apr-2017	Fourth data review
14-Jun-2017	Beginning of instrument (226) test at ATC
31-Jul-2017	Fifth data review
1-Aug-2017	End of test at ATC
19-Oct-2017	Sixth data review
11-Dec-2017	Seventh data review
15-Feb-2018	Eighth data review
28-Feb-2018	Droplet test
28-Feb-2018	Sampling line integrity test
19-Mar-2018	Ninth data review
6-Apr-2018	**End of Step 2 Initial test period**
31-May-2018	ICOS General Assembly

3 Station piping and instrumentation diagram



4 Station parameter availibility

Depending on the station class, different parameters are mandatory. Meteorological and diagnostic parameters (room temperature, flushing and instrument flow rates) must be reported. Having the GHG analyzers tested at ATC Metrology Laboratory (MLab) is also mandatory for every station. The reports from the tests made at the MLab are referenced in the table below and can be found on the ATC website. During the test at the ATC Mlab, an assessment of the following measures are performed.:

- Internal leakage
- Continuous measurement repeatability (CMR)
- Calibration linearity and drift
- Short term repeatability test (STR)
- Long term repeatability test (LTR)
- Extended range linearity
- Sensitivity to inlet pressure
- H_2O correction
- Temperature sensitivity
- Atmospheric pressure sensitivity
- Cold start stabilization time
- Cross talk measurements

At the end of the test, a certificate of compliance is delivered by the ATC together with the test report.

Parameter	Instrument ICOS ID	Initial test report
CO2	225	ATC-ML-IT-RP-54-2.0
CH4	225	ATC-ML-IT-RP-54-2.0
CO	225	ATC-ML-IT-RP-54-2.0
P, T, RH, WS, WD*	513, 514, 515	-
RoomT*, Flushing and instrument flow rates	522	-

*P, T, RH, WS, WD and RoomT stand for atmospheric pressure, temperature, relative humidity, wind speed, wind direction and room temperature respectively.

5 Configuration of the station

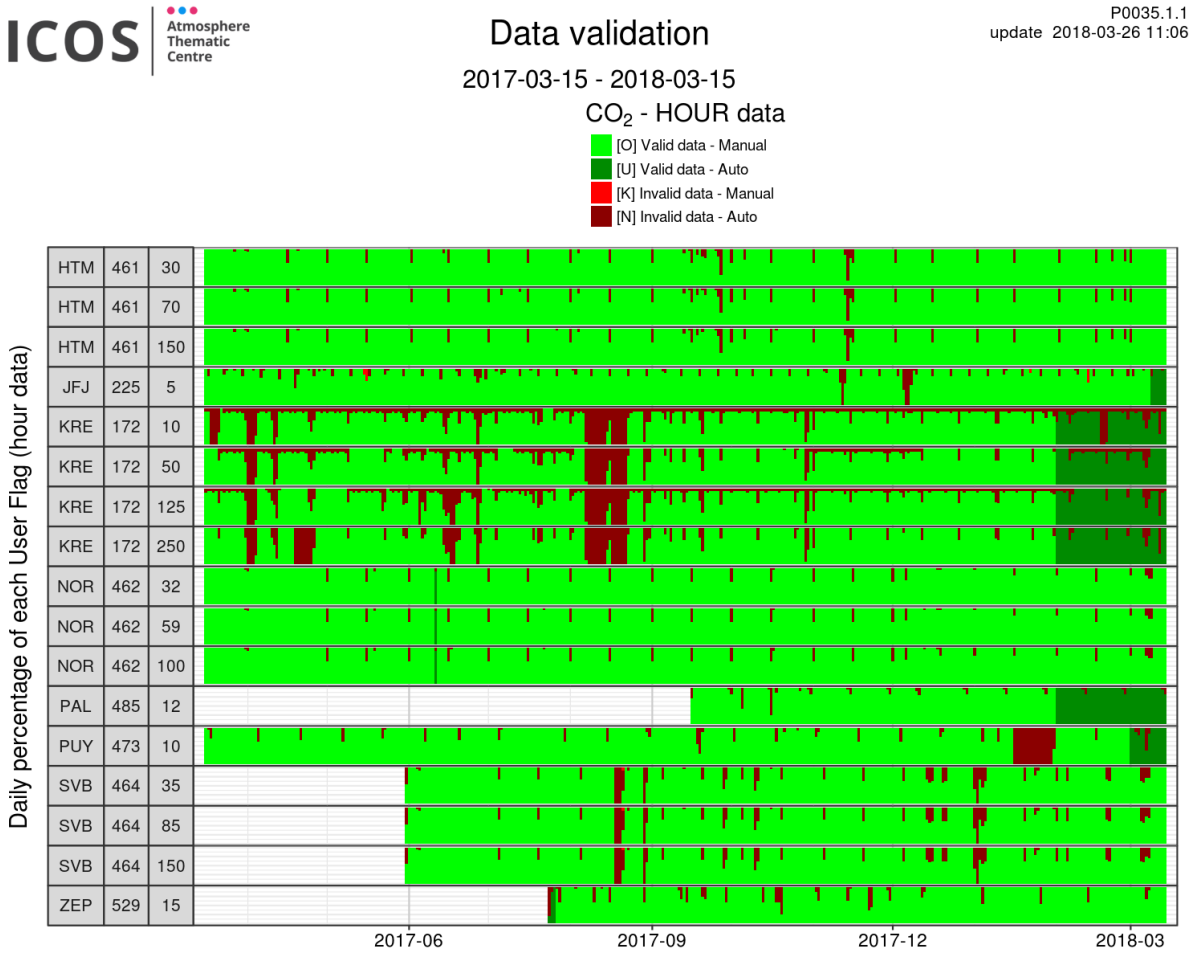
The station configuration defines in particular the calibration sequences. It is then used in the automatic data processing. It is adjusted during the step 2 test period.

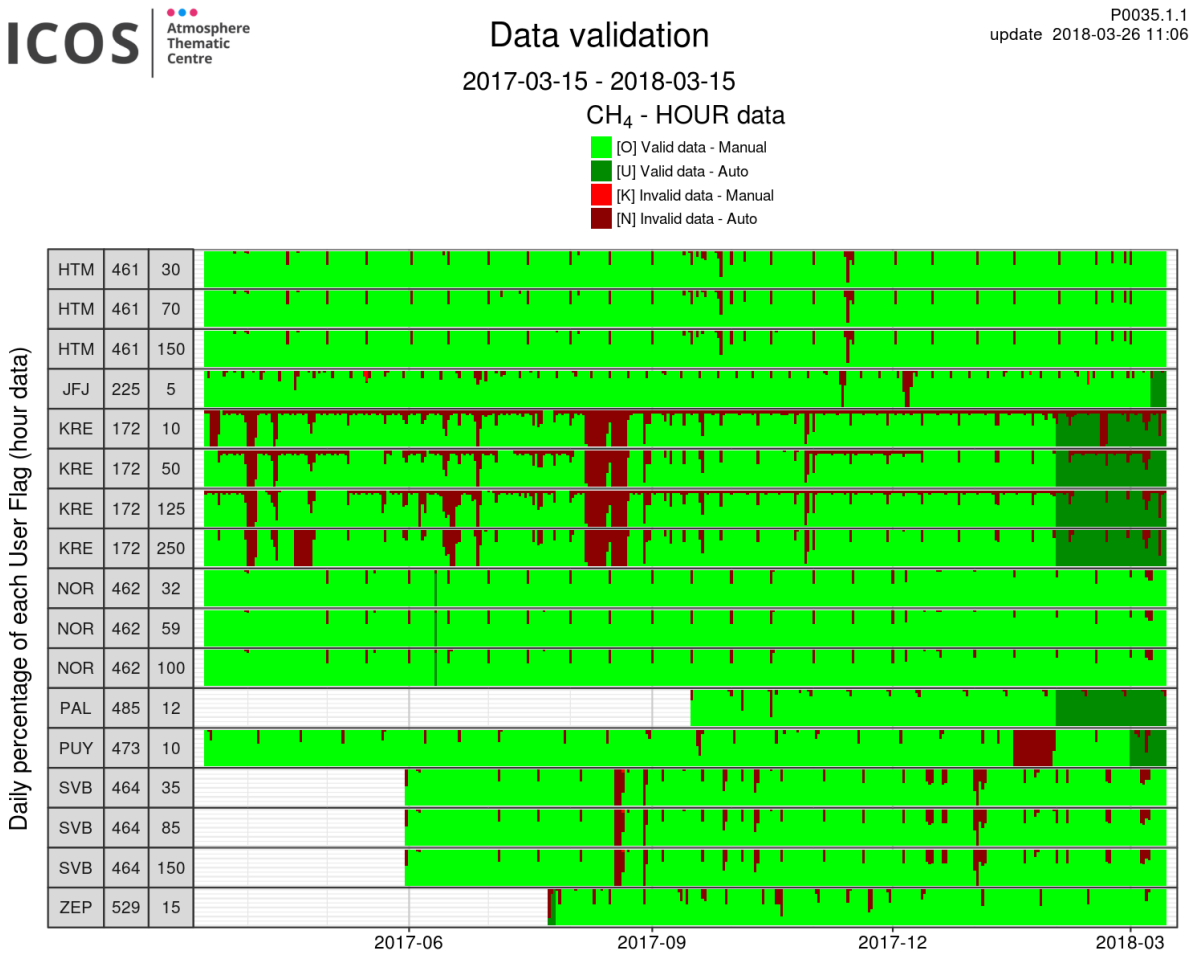
	225
Sampling level(s)	1
Min number of valid calibration cylinders	3
Number of stabilization cycles for the calibration	0
Minute standard deviation limit for valid calibration	CO2: 0.08ppm CH4: 0.8ppb CO: 14ppb
Cycle standard deviation limit for valid calibration	CO2: 0.06ppm CH4: 0.5ppb CO: 5ppb
Sequence standard deviation limit for valid calibration	CO2: 0.05ppm CH4: 0.3ppb CO: 1ppb
Calibration and target sampling duration	30min
Calibration frequency	7d
Stabilization time for TGTs and CALs	10min
Stabilization time for air	10min
Air sampling duration if multiple levels	
H2O coefficients from ATC MLab	Y
Dry or Wet	W
Use of a short term working standard	N

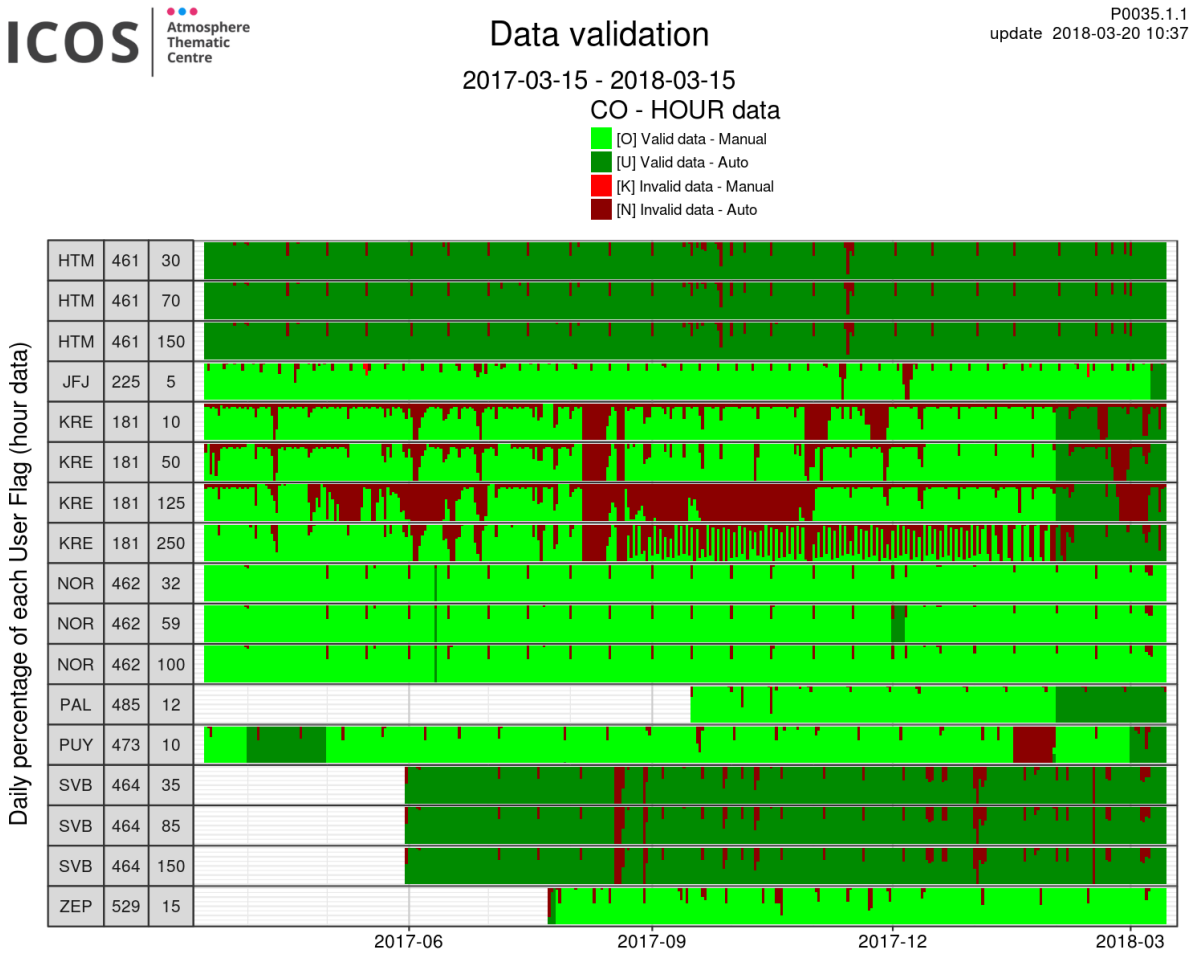
6 Data quality control

The following graphs present for CO_2, CH_4 and CO the amount of data that have been controlled by the station PI together with the other stations in step 2 over the last year. The first column indicates the station acronym, the second column is the instrument ICOS identifier and the third column is the sampling level. Data controlled by the station PI are in bright green (valid) or bright red (invalid).

As a reminder, the station has entered the step 2 since 2016-11-12 and the data are fully ICOS compliant since 2016-12-12.




ICOS
Atmosphere Thematic Centre
Data validation
P0035.1.1
update 2018-03-26 11:06
2017-03-15 - 2018-03-15
CH4 - HOUR data
[O] Valid data - Manual
[U] Valid data - Auto
[K] Invalid data - Manual
[N] Invalid data - Auto
Daily percentage of each User Flag (hour data)
HTM 461 30
HTM 461 70
HTM 461 150
JFJ 225 5
KRE 172 10
KRE 172 50
KRE 172 125
KRE 172 250
NOR 462 32
NOR 462 59
NOR 462 100
PAL 485 12
PUY 473 10
SVB 464 35
SVB 464 85
SVB 464 150
ZEP 529 15
2017-06
2017-09
2017-12
2018-03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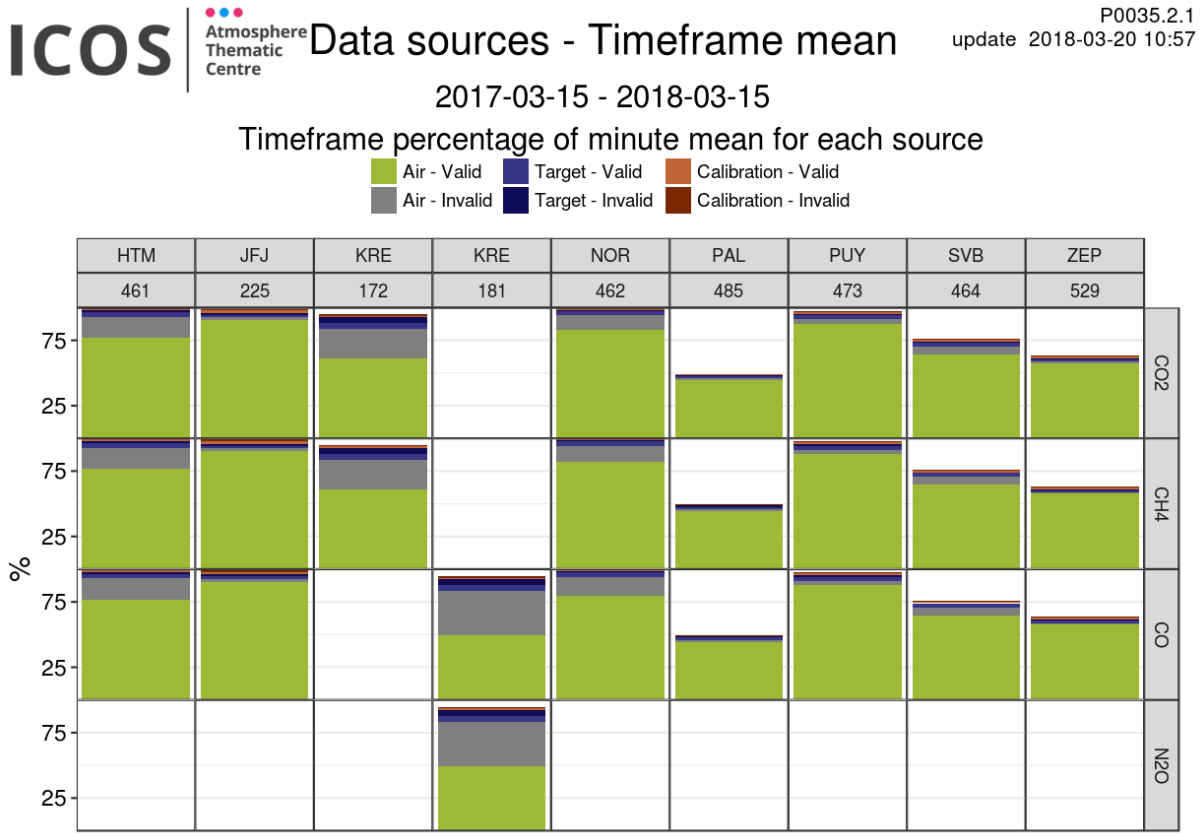
Atmosphere Thematic Centre
Data validation
P0035.1.1
update 2018-03-20 10:37
2017-03-15 - 2018-03-15
CO - HOUR data
[O] Valid data - Manual
[U] Valid data - Auto
[K] Invalid data - Manual
[N] Invalid data - Auto
Daily percentage of each User Flag (hour data)
HTM 461 30
HTM 461 70
HTM 461 150
JFJ 225 5
KRE 181 10
KRE 181 50
KRE 181 125
KRE 181 250
NOR 462 32
NOR 462 59
NOR 462 100
PAL 485 12
PUY 473 10
SVB 464 35
SVB 464 85
SVB 464 150
ZEP 529 15
2017-06
2017-09
2017-12
2018-03

General comments: Raw and hourly data are regularly flagged since the beginning.

Recommendation 1 (***, important, -): It is recommended to continue the flagging of raw data on a weekly basis.

7 Data sampling distribution

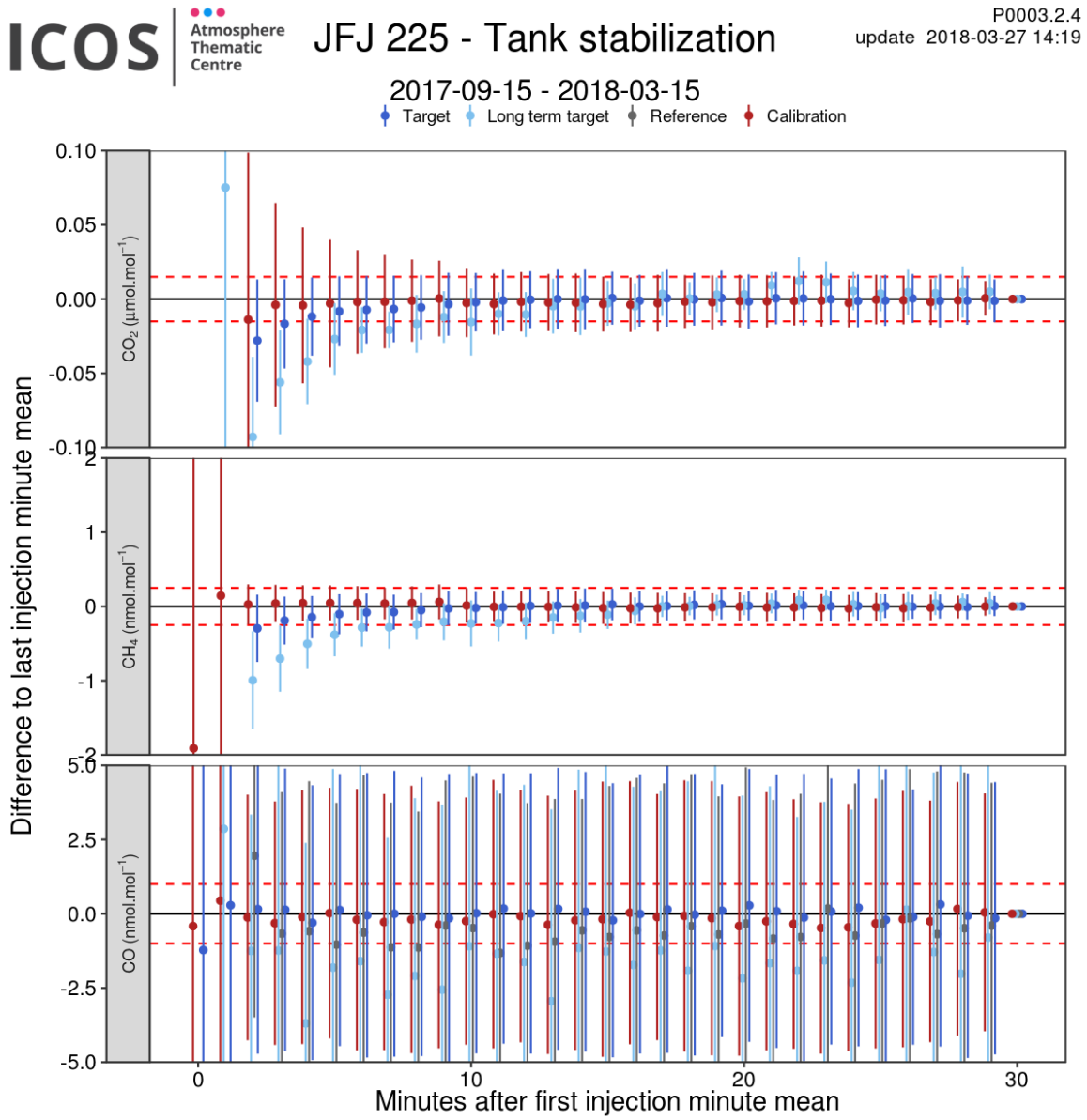
Goal: Present the time spent in sampling air, target gas or calibration gases. Invalid data mostly represent flushing time. This graphics can indicate if the station sampling sequence needs to be optimized, for example to reduce the flushing time.



General comments: More than 90% of the data is air sampled from the mast. Only a few percent of data are dedicated to flushing, target or calibration sampling.

8 Stabilization time

Goal: Evaluate the time needed for the instrument to flush the previous sample and be stable for the current one. We look at the short and long term target and calibration gases over the last 3-6 months. This allows to optimize the sampling strategy and can also help pinpoint problems on specific parts of the piping system.



	CO2	CH4	CO
Treshold (ppm for CO2, ppb for CH4 and CO)	0.015	0.25	1
Flushing time for target (min) - 211 injections	4	3	1
Flushing time for long term target (min) - 12 injections	11	8	29
Flushing time for calibration (min) - 252 injections	2	1	1

The flushing time is estimated as the time necessary for the difference between each injection and the last injection to be under the defined threshold. Thresholds are estimated relative to WMO goals and usual performances of instruments.

General comments: In the present situation we recommend to keep the 10mn flushing time for target gases and for calibration gases. The longer time of stabilisation of the long term target is probably due to the low number of injections (poor representative statistics). Taking into account this stabilization time, we recommend to set the tank measurement duration at least at 25 minutes in order to have a 15 minute average which provide a good precision for CO.

Recommendation 2 (*, minor, 2018): Cylinder measurement duration can be decreased to 25 minutes with 10 minute flushing.

9 Calibration

9.1 Instrument drift

Goal: Identify a calibration cylinder that would behave differently from the others or one calibration sequence that needs further inspection and quality control.

General comments: The calibration tanks do not show a drift trend. All the calibration tanks show a similar variability. The CO_2 shows a significant "jump" end of October 2017 which might be related to the Nafion removal (the initial sampling setup was equipped with Nafion dryer). This change might imply a calibration interpolation break. Due to the observed variability, ATC recommends to perform a calibration at least every 2 weeks. Many calibrations have been rejected, mainly due to sequencer issue.

Recommendation 3 (*, important, -): Due to the CO variability, the calibration intervals should be kept at two weeks.

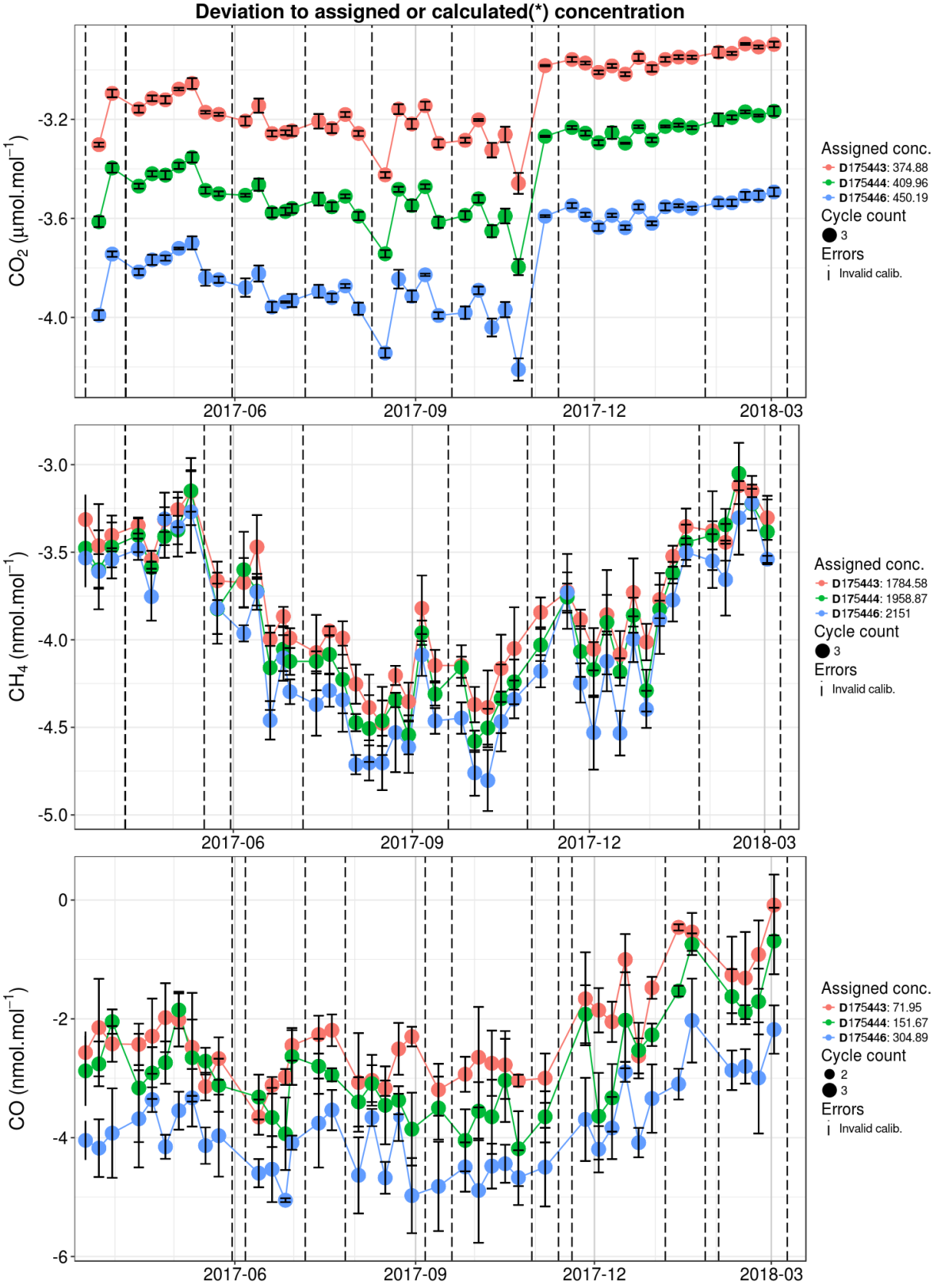
ICOS Atmosphere Thematic Centre

JFJ 225 - Calibration tank drift

P0002.2
update 2018-03-16 15:49

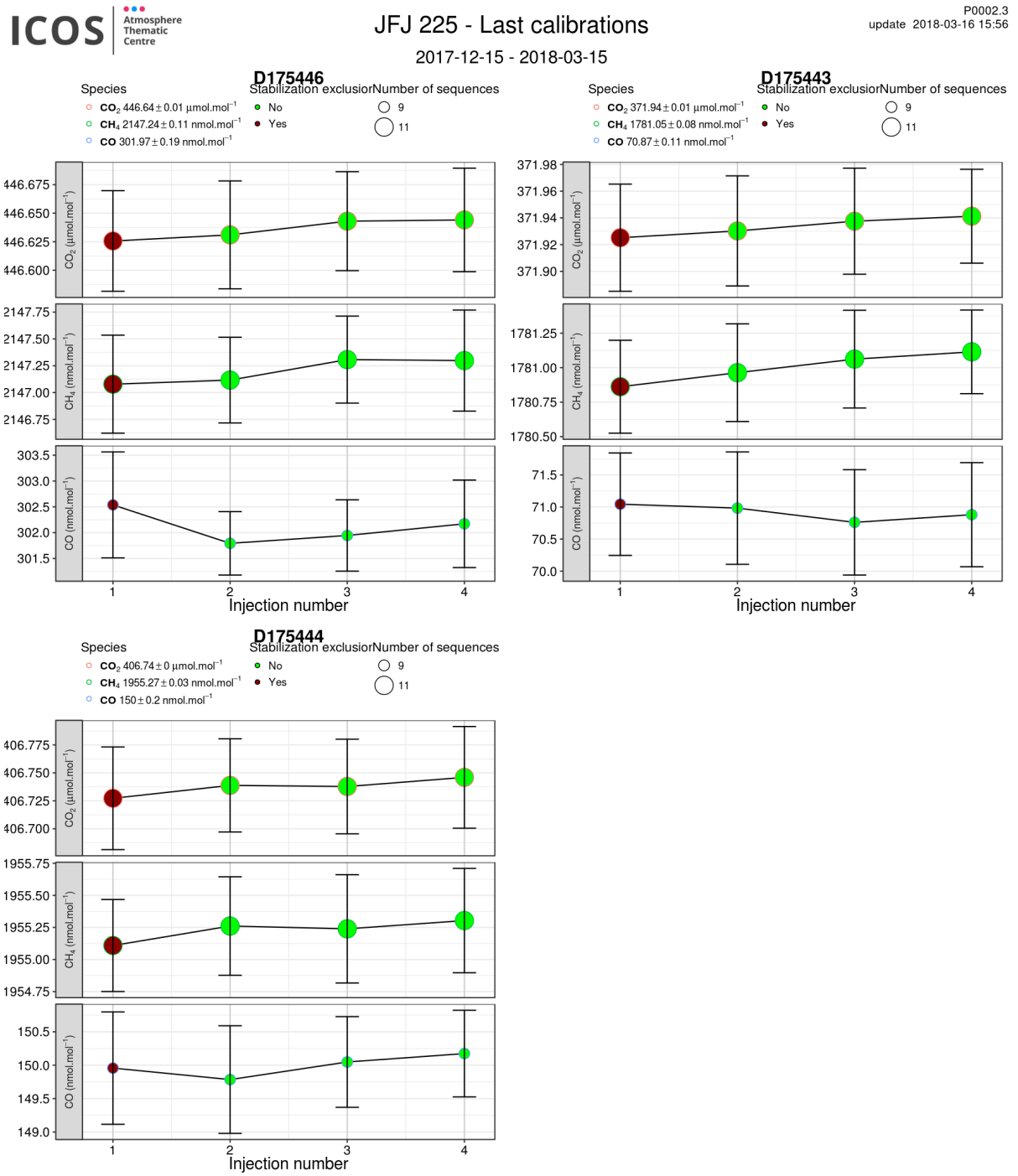
2017-03-15 - 2018-03-15

Deviation to assigned or calculated(*) concentration



9.2 Calibration quality control

Goal: Evaluate the quality of the calibrations by checking the mean standard deviation and difference between the different cycles of all the calibrations run during the ICOS labelling step 2. One graph by calibration cylinder is shown.

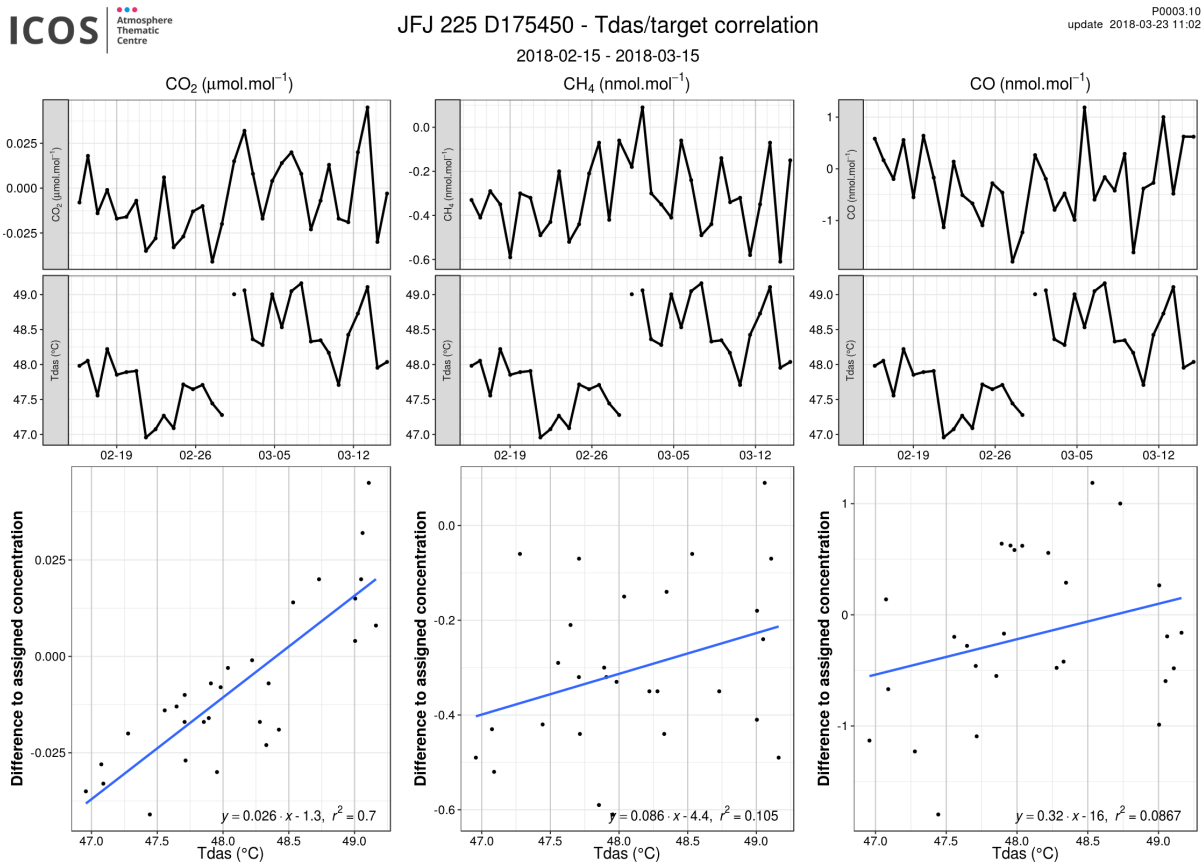


General comments: The overall quality of the calibration cycles is good. The setup of automatic quality control is well adapted.

Recommendation 4 (*, minor, 2018): It is possible to reduce to three calibration cycles instead of four (keeping the rejection of the first cycle in the ATC configuration)

10 Temperature dependence

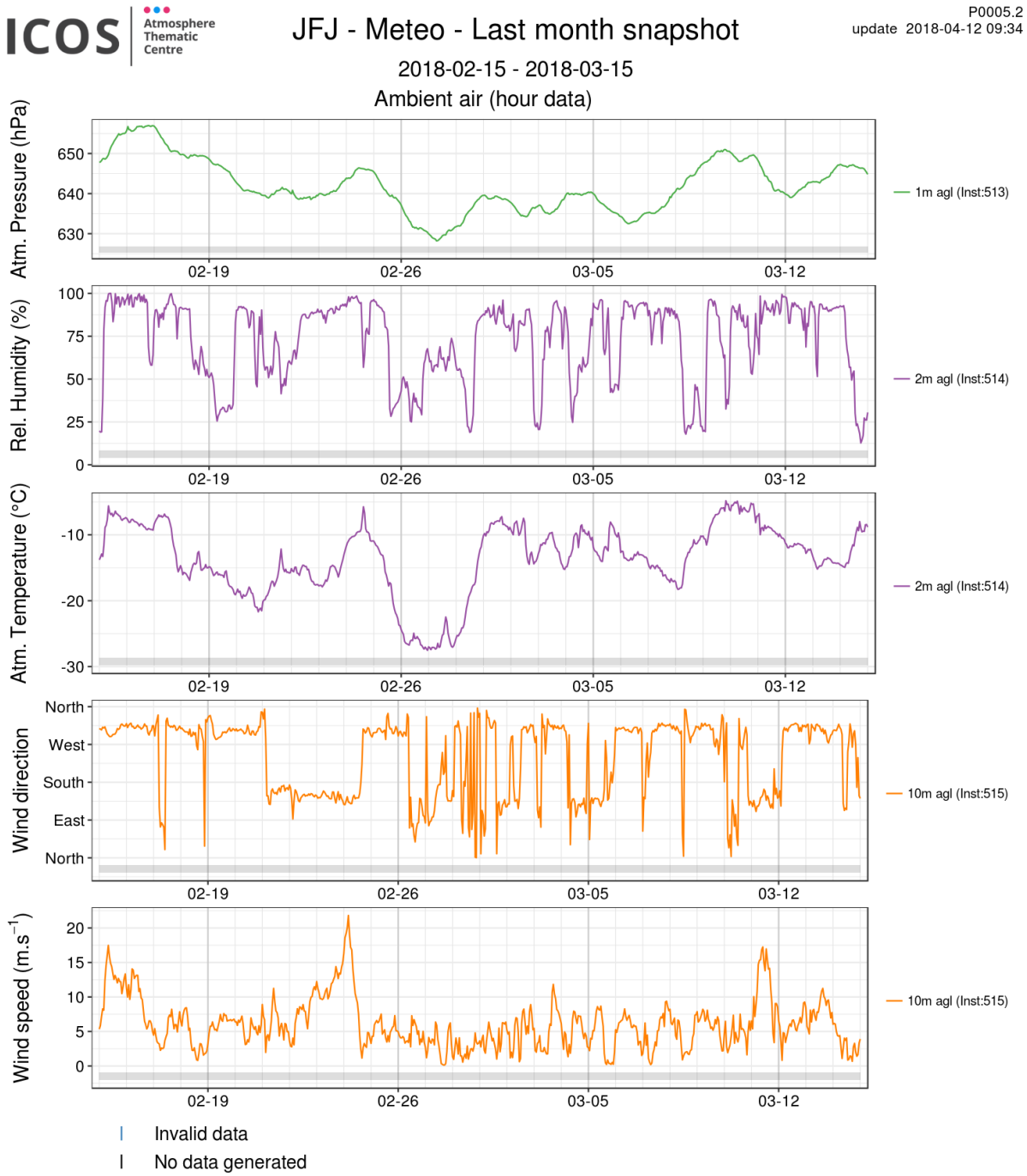
Goal: Control the temperature influence on the instrument. We use the target gas measurement and the temperature measured inside the instrument (which usually follow closely the room temperature modifications).



General comments: The temperature of the instrument is varying within 2°C. We do not detect any significant variability of the short-term target gas measurements with temperature for CO_2, CH_4 and CO.

11 Meteorological parameters

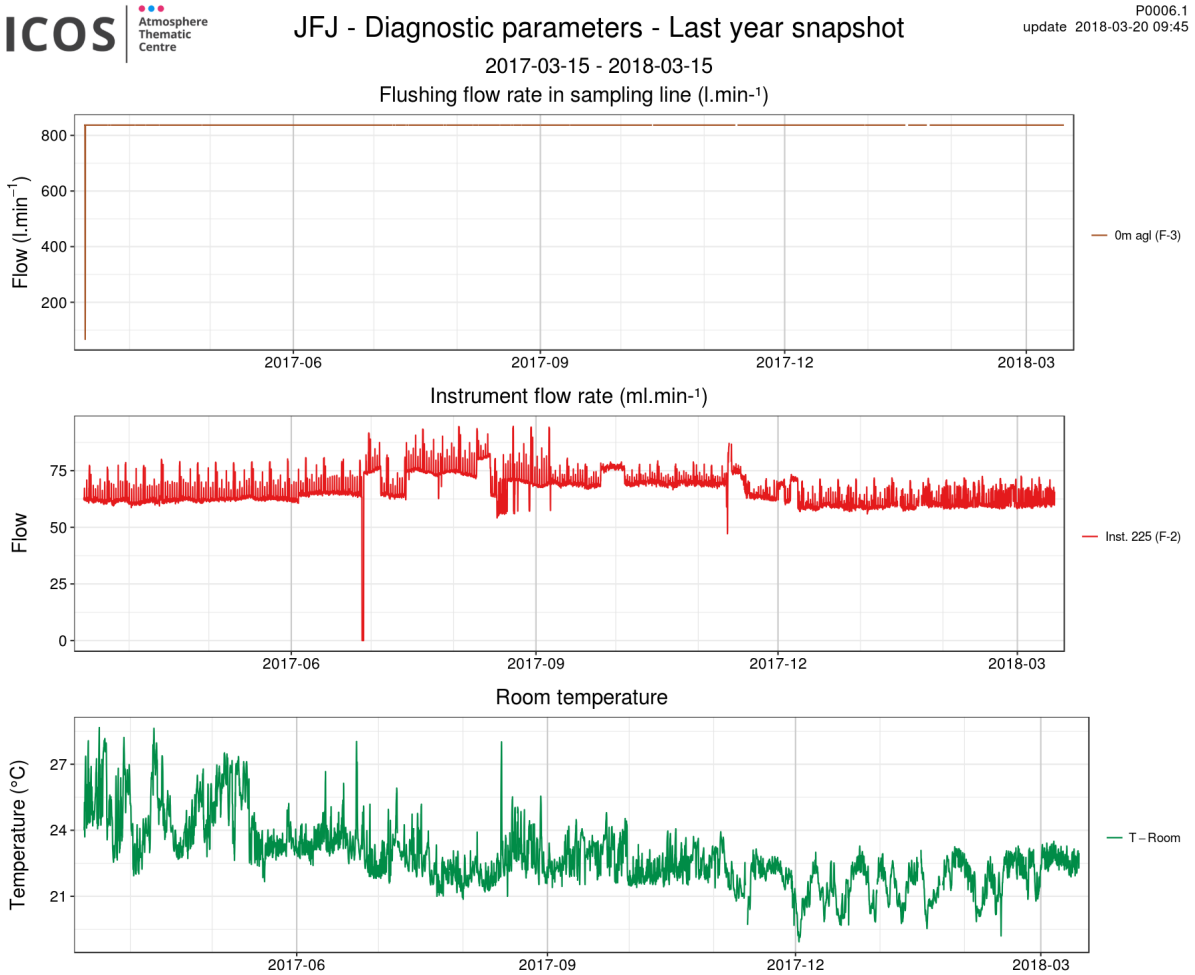
The meteorological parameters from the last month are shown here.



General comments: The sensors at three levels are providing data to the database once a month after being controlled by the Swiss meteorological agency.

12 Diagnostic parameters

The diagnostic parameters from up to a year are presented here.



General comments: The three mandatory diagnostic parameters (flushing flowrate, instrument flow rate, and room temperature) are properly recorded and transferred to the database. Records show pretty stable values, without gap.

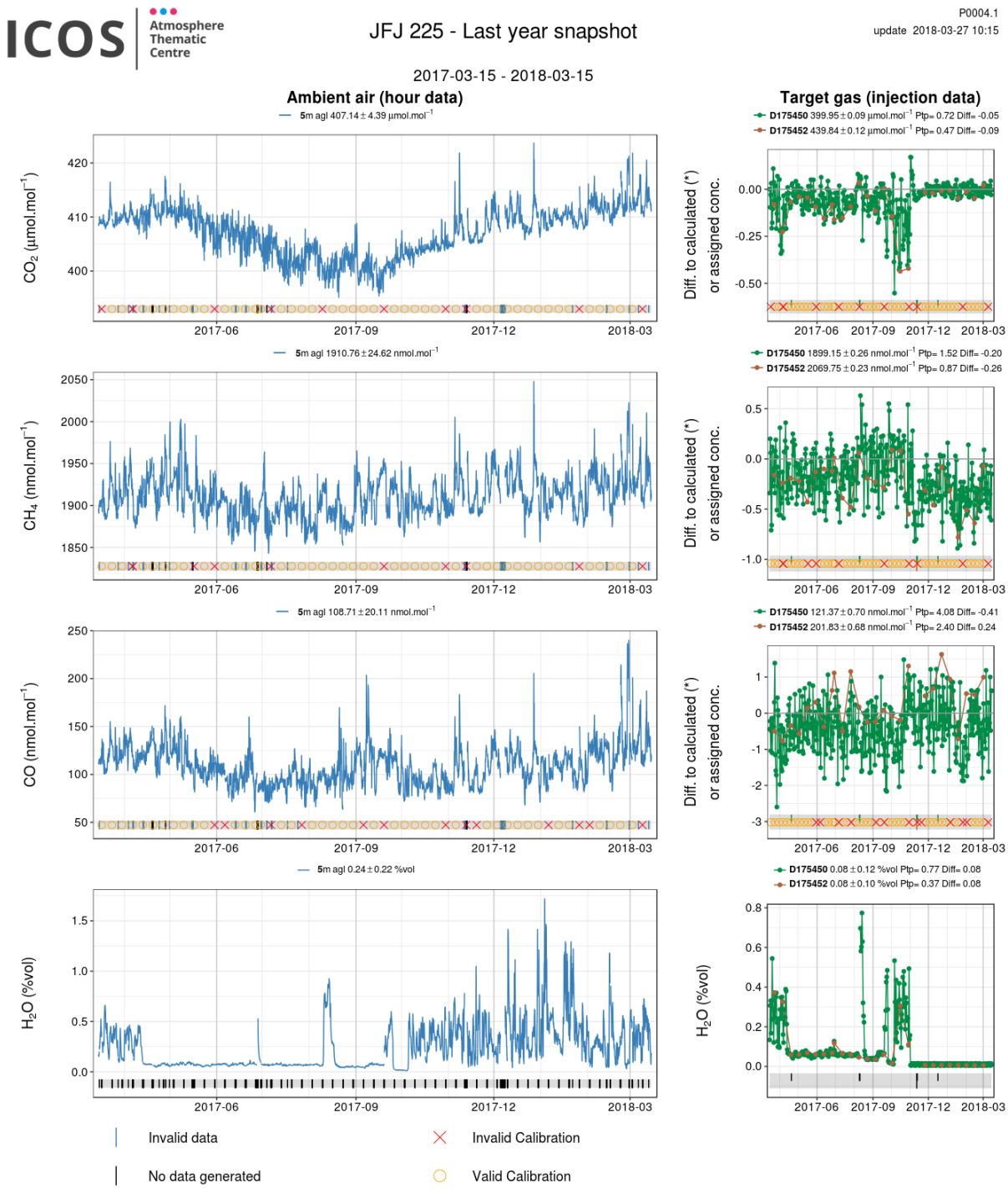
13 Greenhouse gas series

Goal: Evaluate the ambient air and target data over different periods of time.

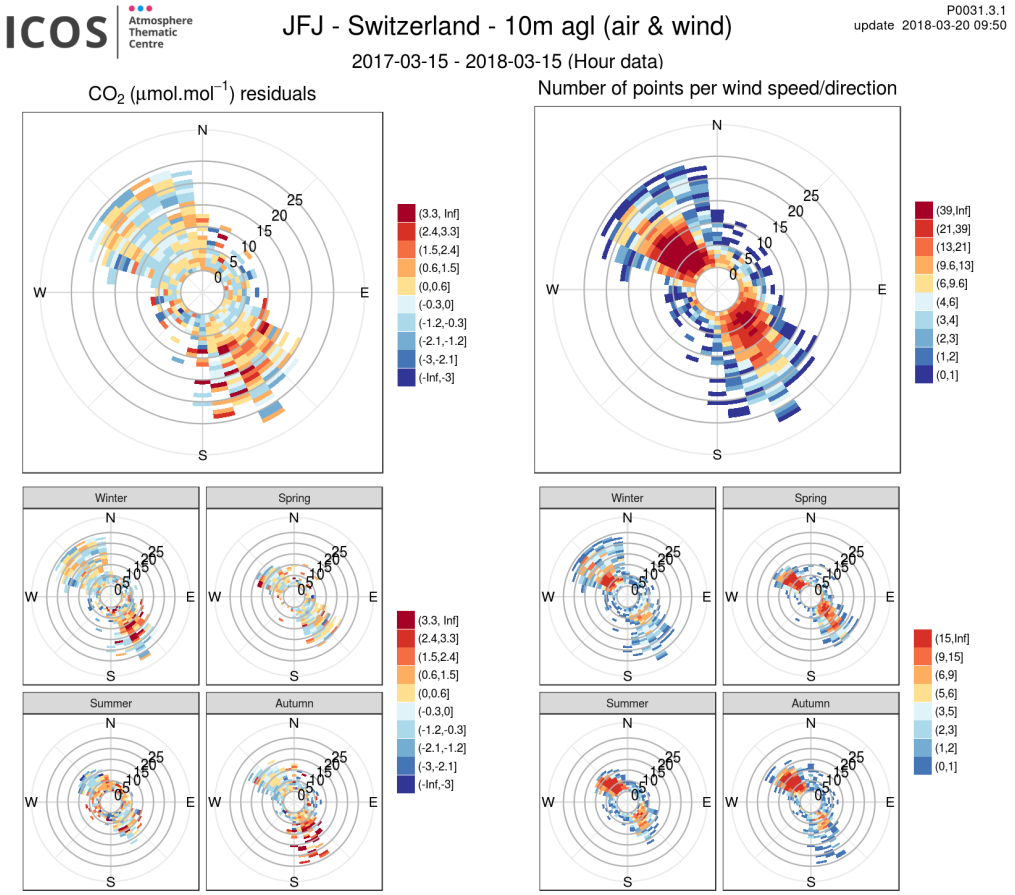
The data from last year and month are presented here. On the first plot, on the left panels are the ambient air measurement, on the right the target measurements. For the yearly data, a second plot shows data as windroses. The GHG residuals (deduced from the fitted smooth curve using CCGVU) and the data frequency depending on wind direction and speed are shown.

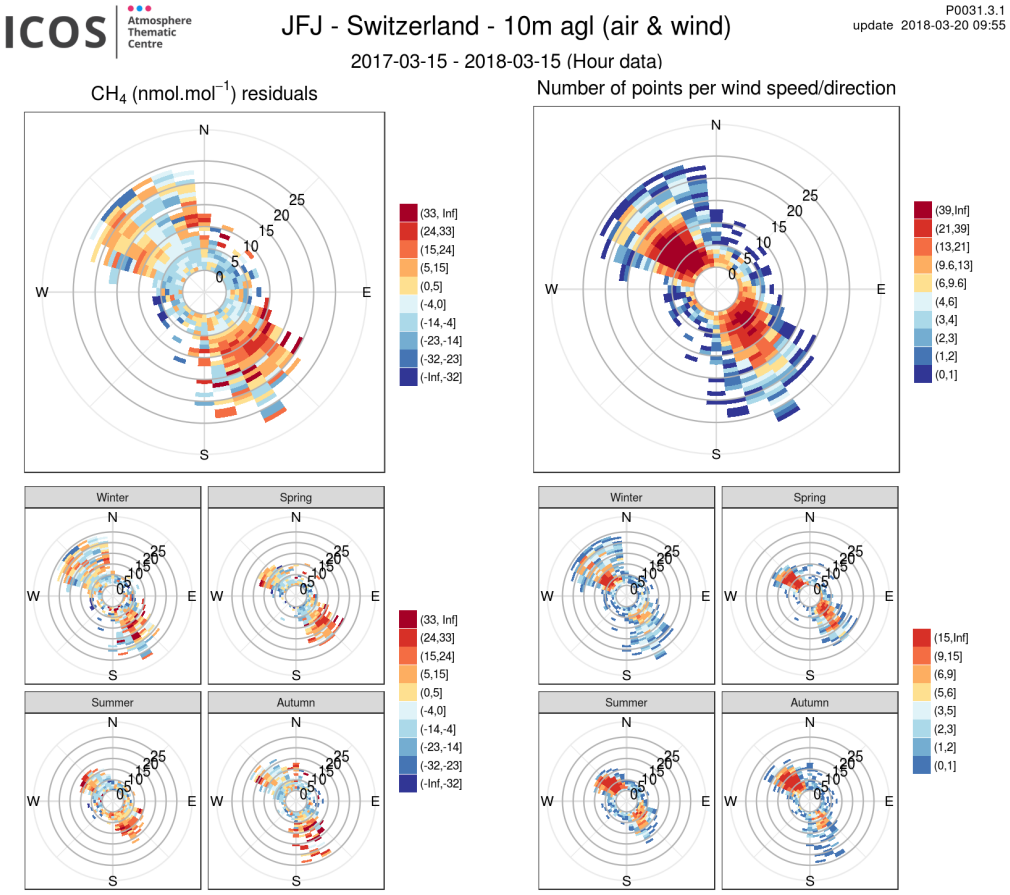
As a reminder, the data are ICOS compliant since 2016-12-12.

13.1 Last Year



General comments: The time series show a good record, without significant gap. Calibrations and target gases measurements are performed regularly following the ICOS recommendations. The short term target gas do not show significant bias in CO_2, CH4 and CO. The Long term target does not show any significant bias. The short term target shows a significant variability in CO_2 up to end of October 2017 while sampling the air (ambient air and all the tanks) through a Nafion dryer. After ATC recommendation to remove the Nafion, the CO_2 variability improved.




ICOS
Atmosphere Thematic Centre
JFJ - Switzerland - 10m agl (air & wind)
P0031.3.1
update 2018-03-20 09:55
2017-03-15 - 2018-03-15 (Hour data)
CH4 (nmol.mol−1) residuals
Number of points per wind speed/direction
Winter
Spring
Summer
Autumn
N
E
S
W
(33, Inf]
(24,33]
(15,24]
(5,15]
(0,5]
(-4,0]
(-14,-4]
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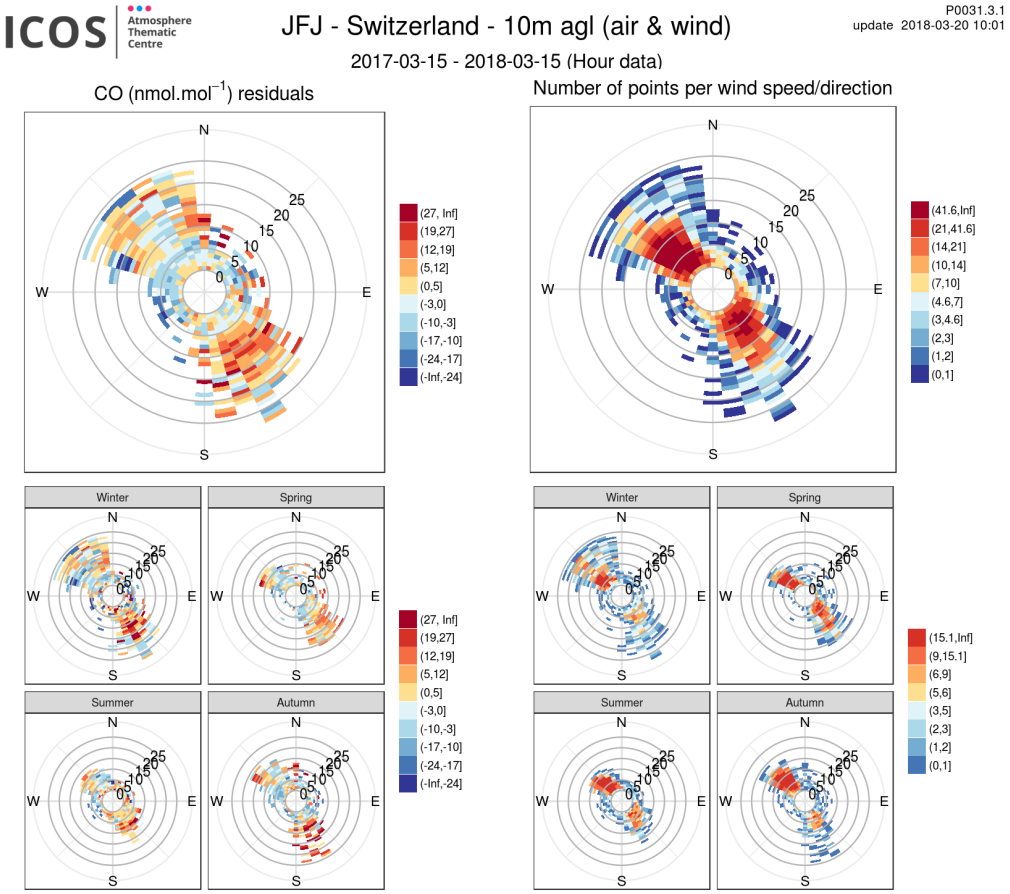
ICOS
Atmosphere Thematic Centre
JFJ - Switzerland - 10m agl (air & wind)
P0031.3.1
update 2018-03-20 10:01
2017-03-15 - 2018-03-15 (Hour data)
CO (nmol.mol−1) residuals
Number of points per wind speed/direction
Winter
Spring
Summer
Autumn
N
E
S
W
(27, Inf]
(19,27]
(12,19]
(5,12]
(0,5]
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(1,2]
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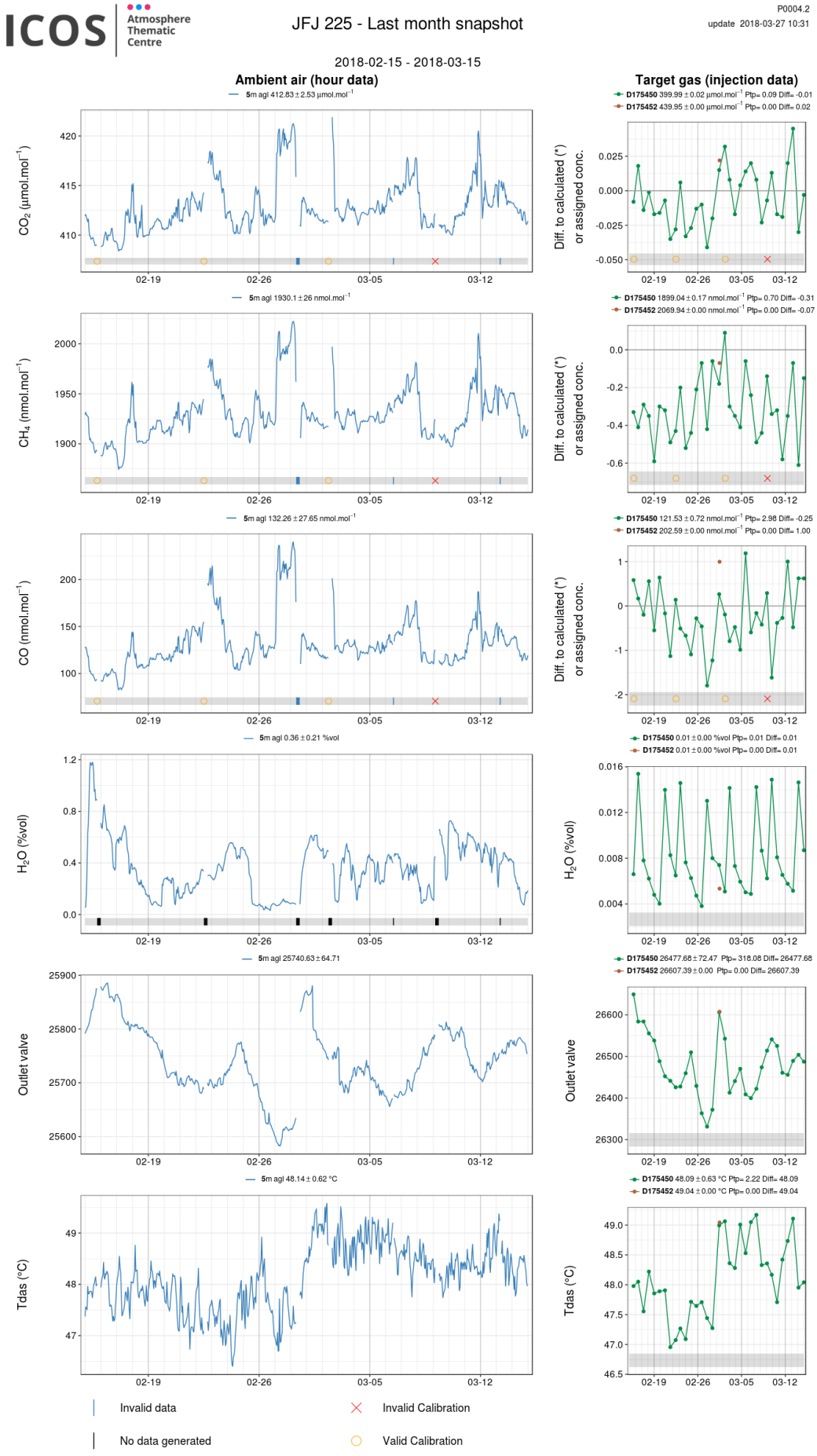
13.2 Last month

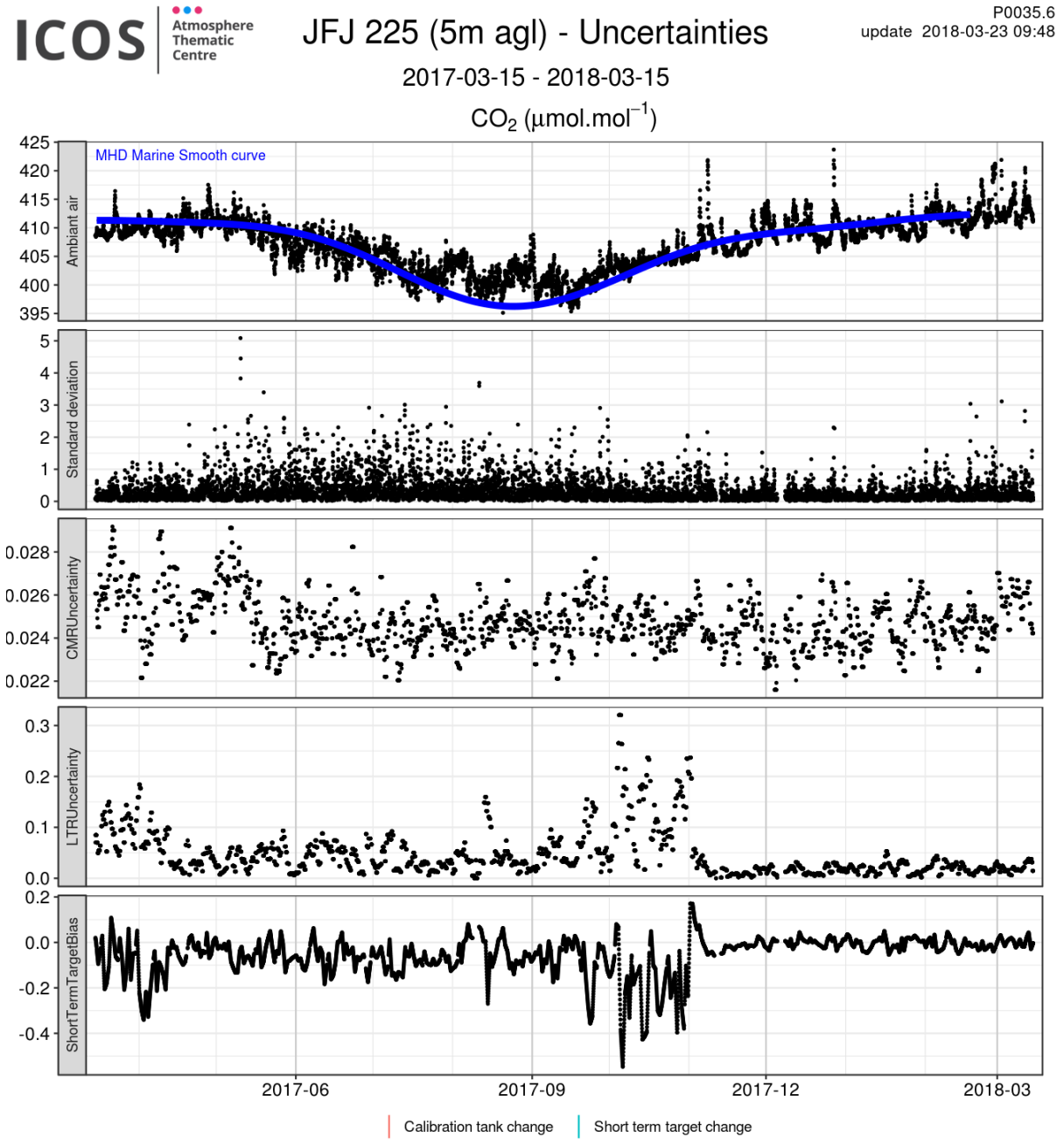


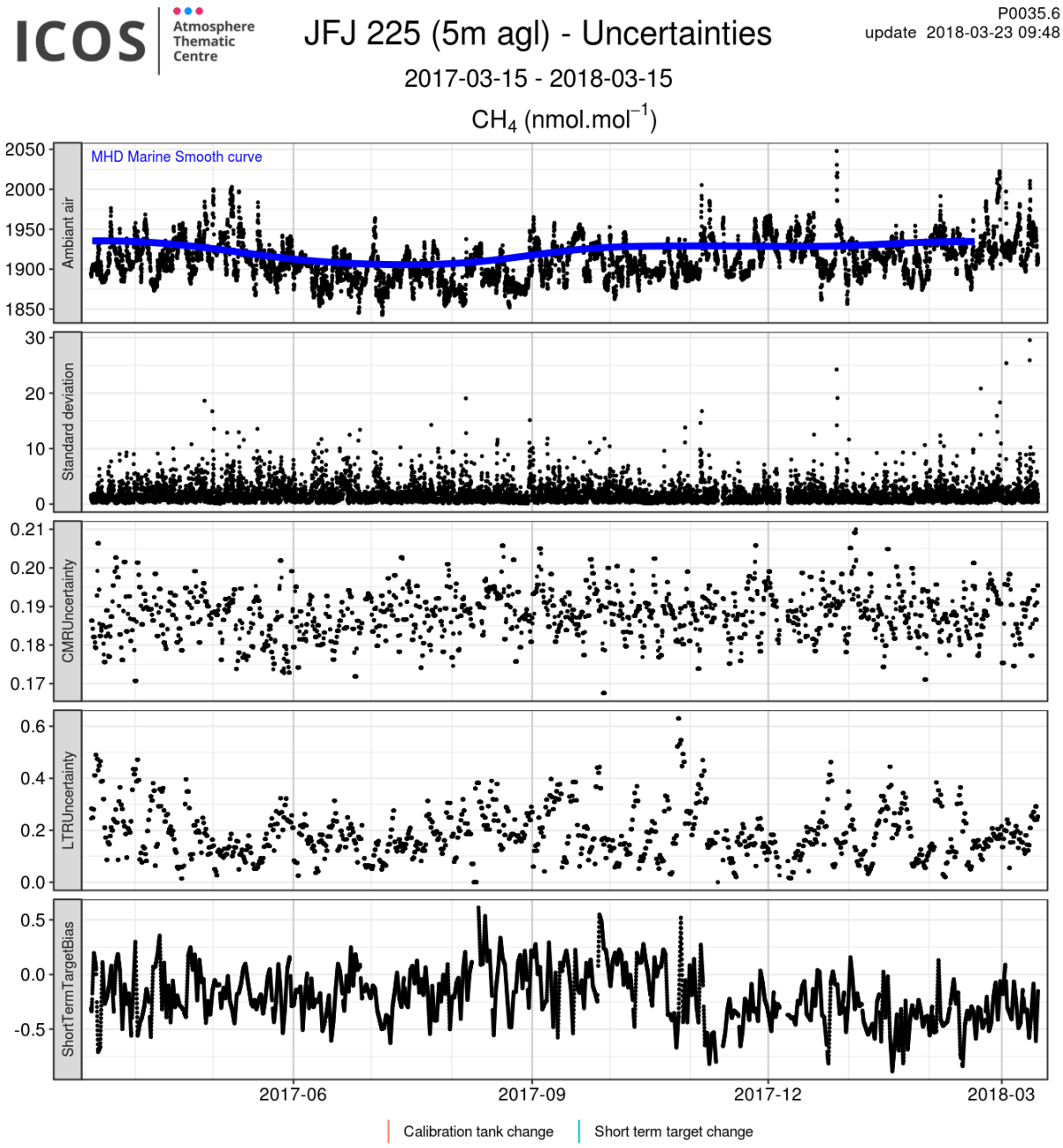
General comments: The outletvalve value during ambient air and target measurement are consistent and stable.

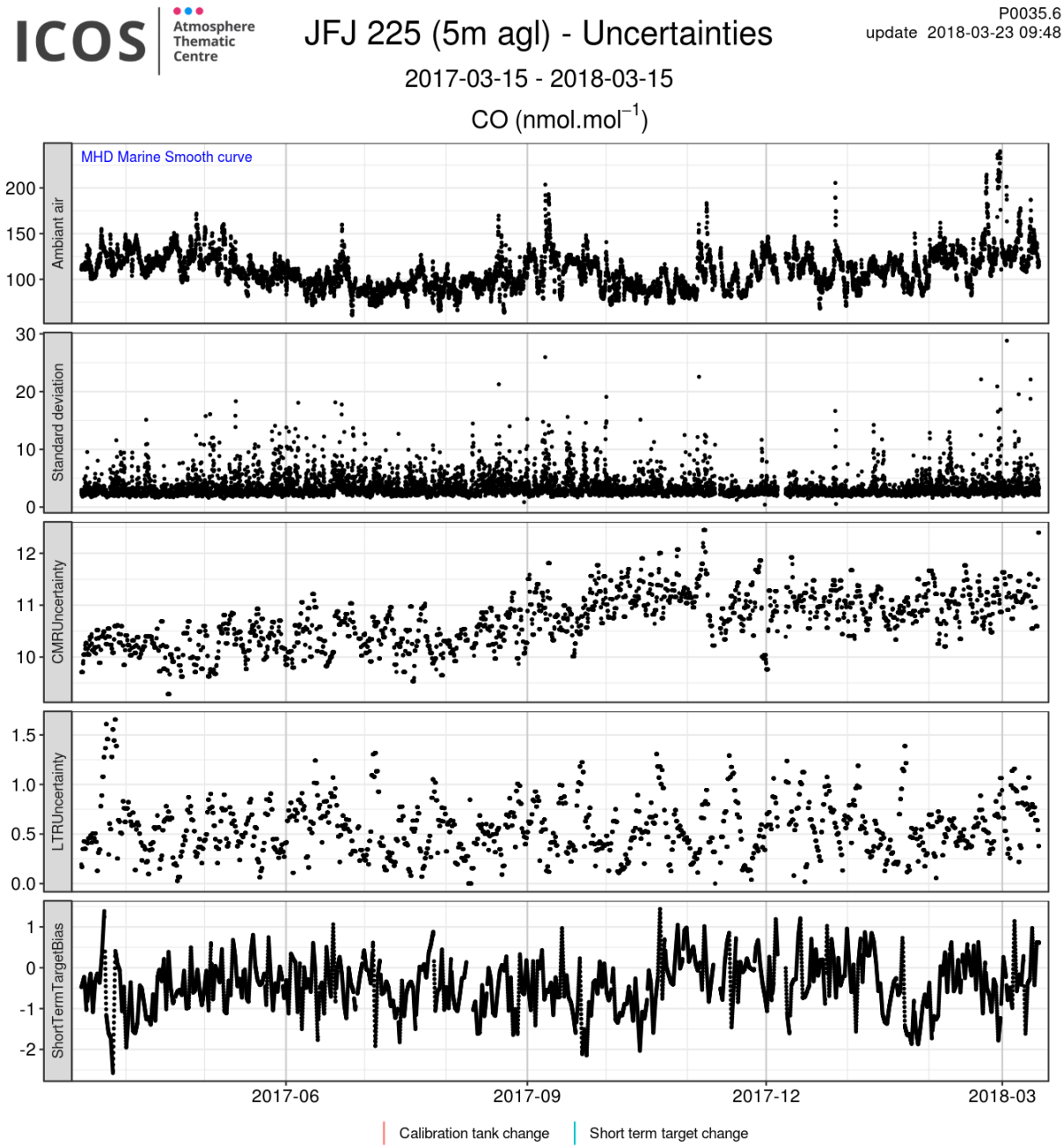
14 Uncertainties

Goal: Present the data alongside the estimated uncertainties.

The uncertainties shown are calculated using the target gas measurements and the air measurements at the highest level of the station mast. On the top panel, the data are shown with the marine baseline measured at Mace Head (Ireland) as a visual perspective. On the second panel, we show the standard deviation of the hourly air data (after removing the baseline calculated using CCGVU). The next panels are produced using the target data. We show the CMR, STR and LTR as defined in Yver Kwok et al., 2014.




ICOS
Atmosphere Thematic Centre
JFJ 225 (5m agl) - Uncertainties
P0035.6
update 2018-03-23 09:48
2017-03-15 - 2018-03-15
CH4 (nmol.mol−1)
MHD Marine Smooth curve
Ambiant air
Standard deviation
CMRUncertainty
LTRUncertainty
ShortTermTargetBias
2017-06
2017-09
2017-12
2018-03
Calibration tank change
Short term target change



	CO2	CH4	CO
MLab CMR (ppb)	22	0.19	8.94
MLab LTR (ppb)	50	0.64	3.30

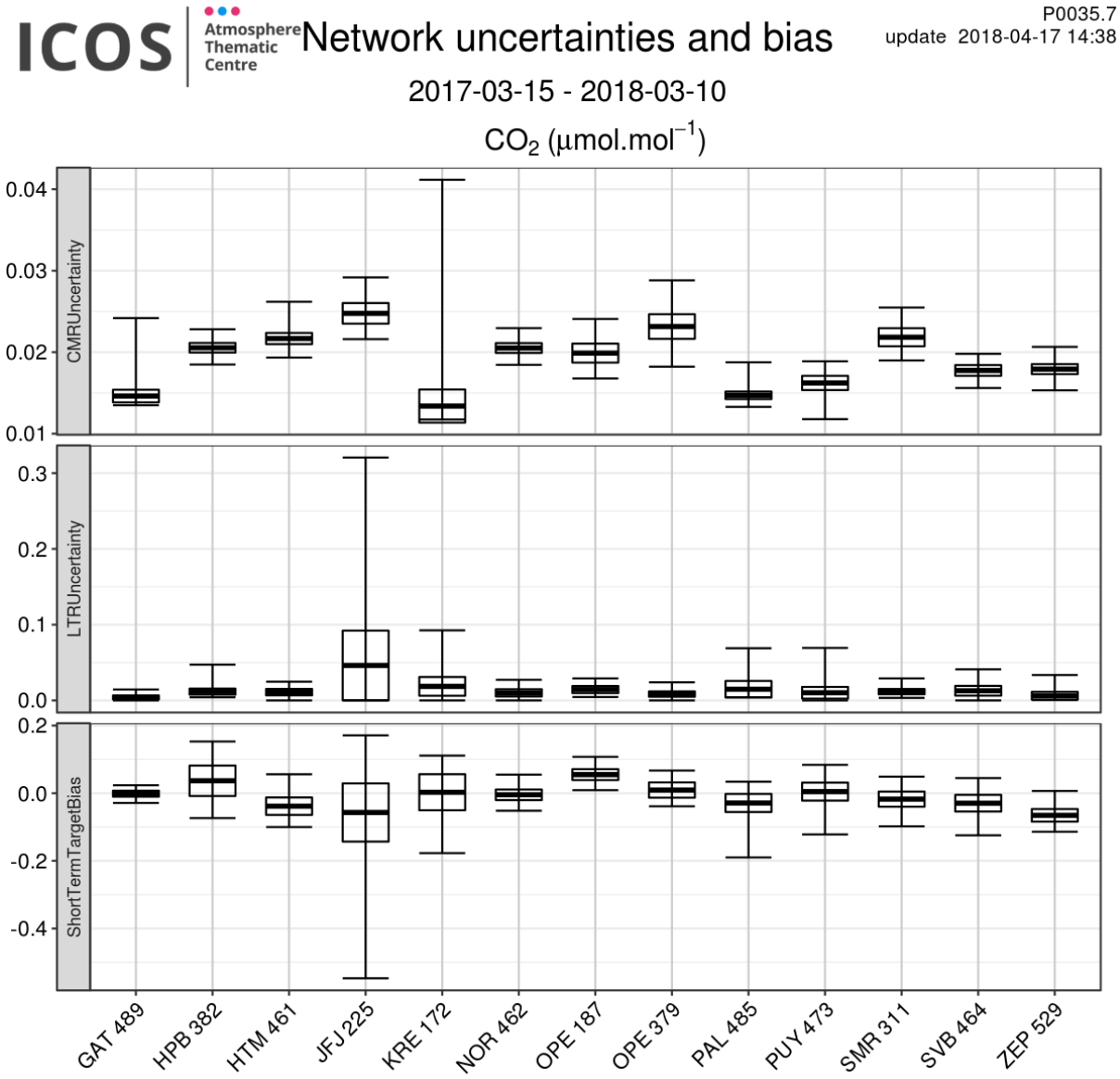
Uncertainties (CMR and LTR) estimated during the initial instrument test at the MLab

General comments: Since the Nafion removal, uncertainties show stable values in line with ICOS expectations. The CMR and LTR repeatability show consistent values with the initial test done at ATC lab indicating that the installation at the station has not generated additional noise in the measurements. The LTR CO performance is even better onsite than at ATC MLab.

15 Comparison within the network

Goal: Evaluate the target performances at the station.

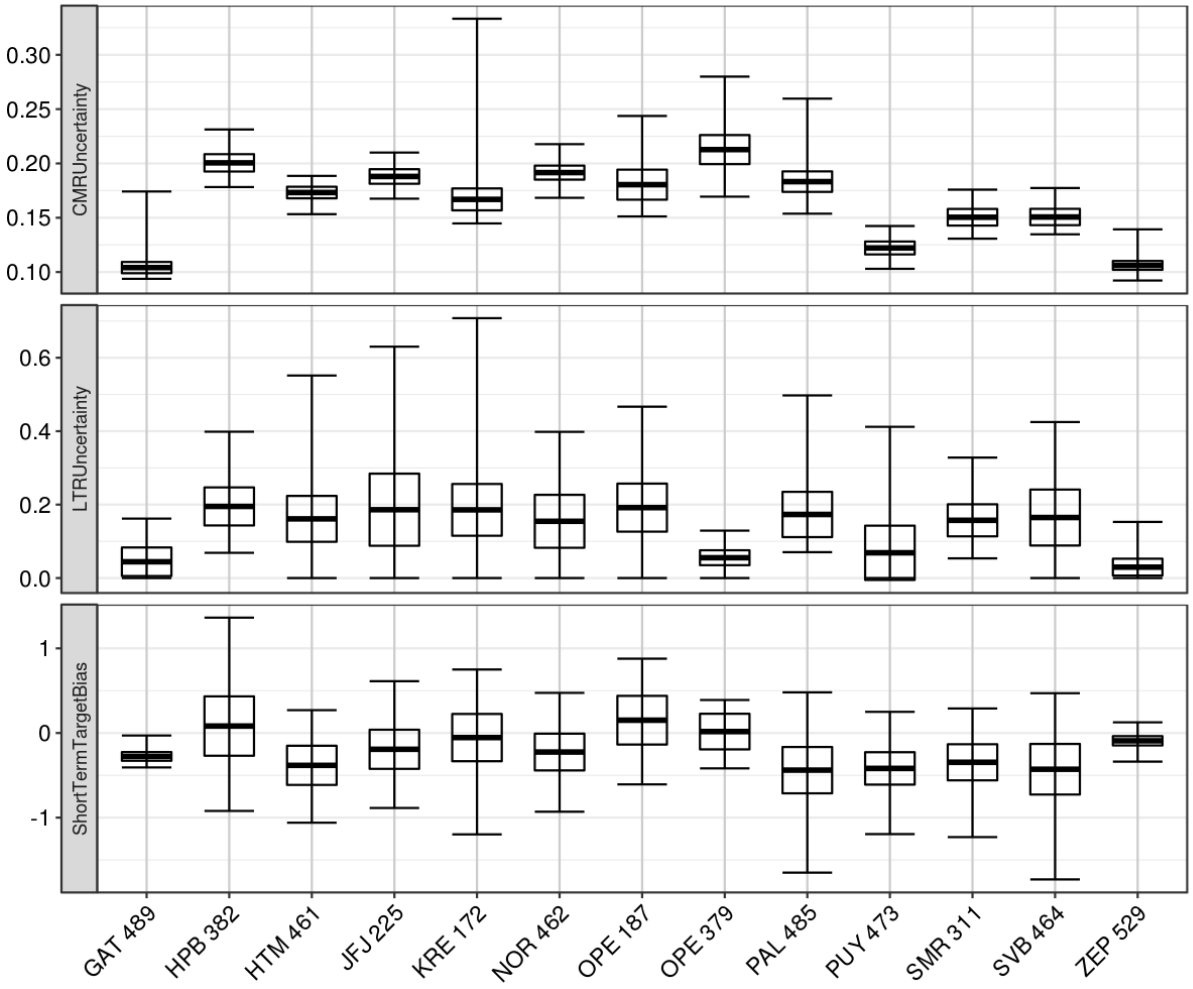
In these plots, the target performances of the different stations labelled or in step 2 are shown.



Network uncertainties and bias

2017-03-15 - 2018-03-10

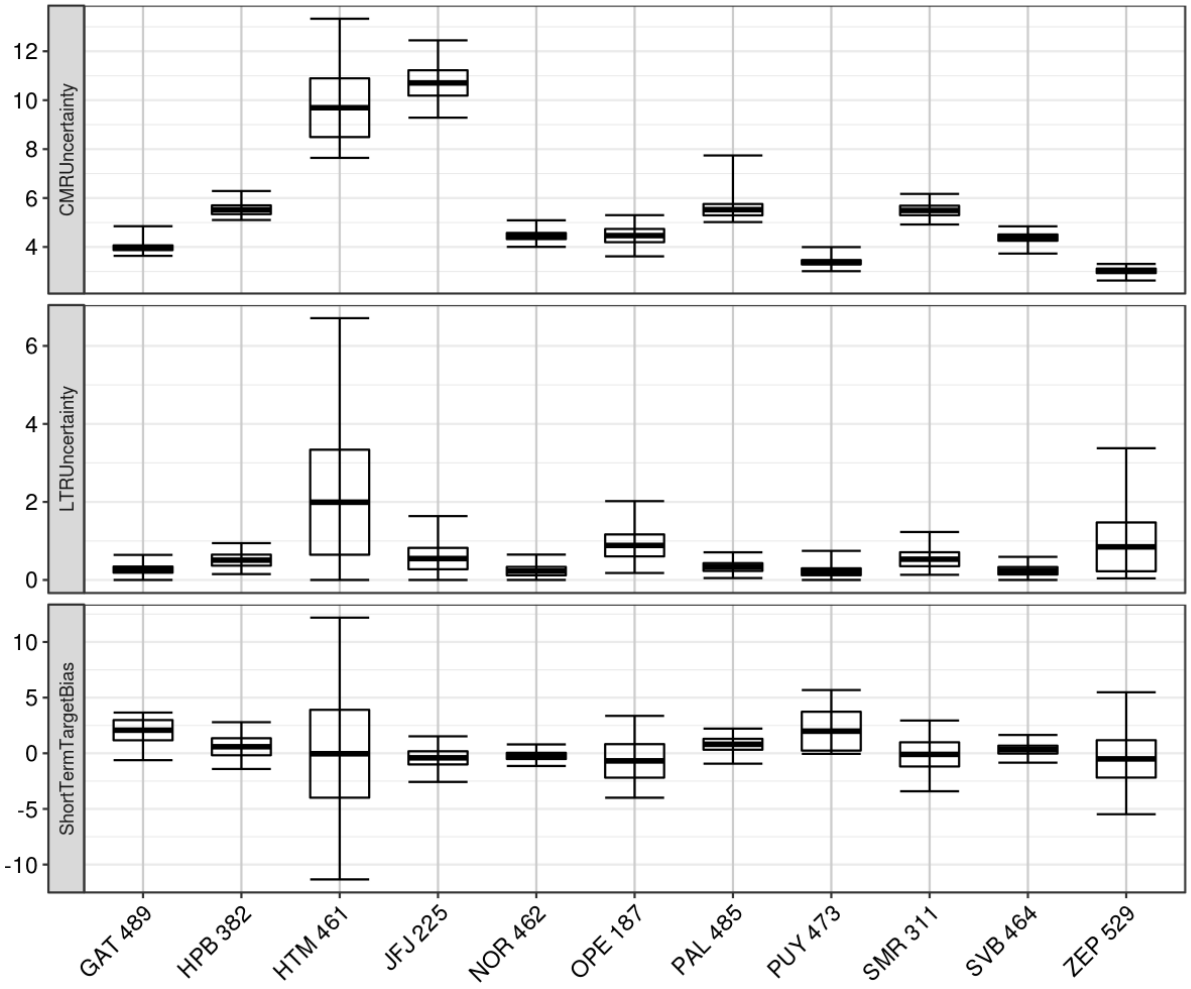
CH_4 (nmol.mol^{-1})

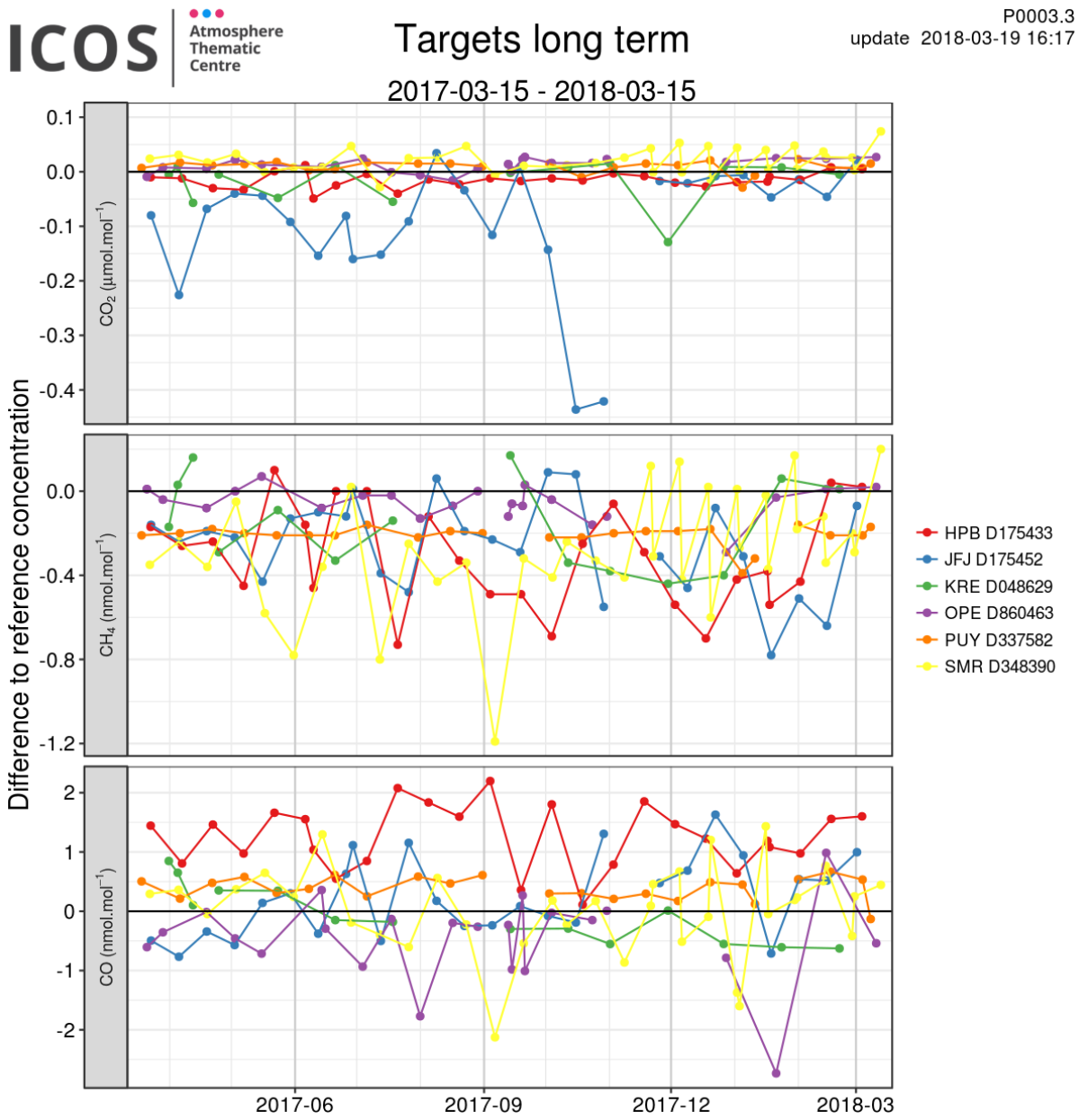


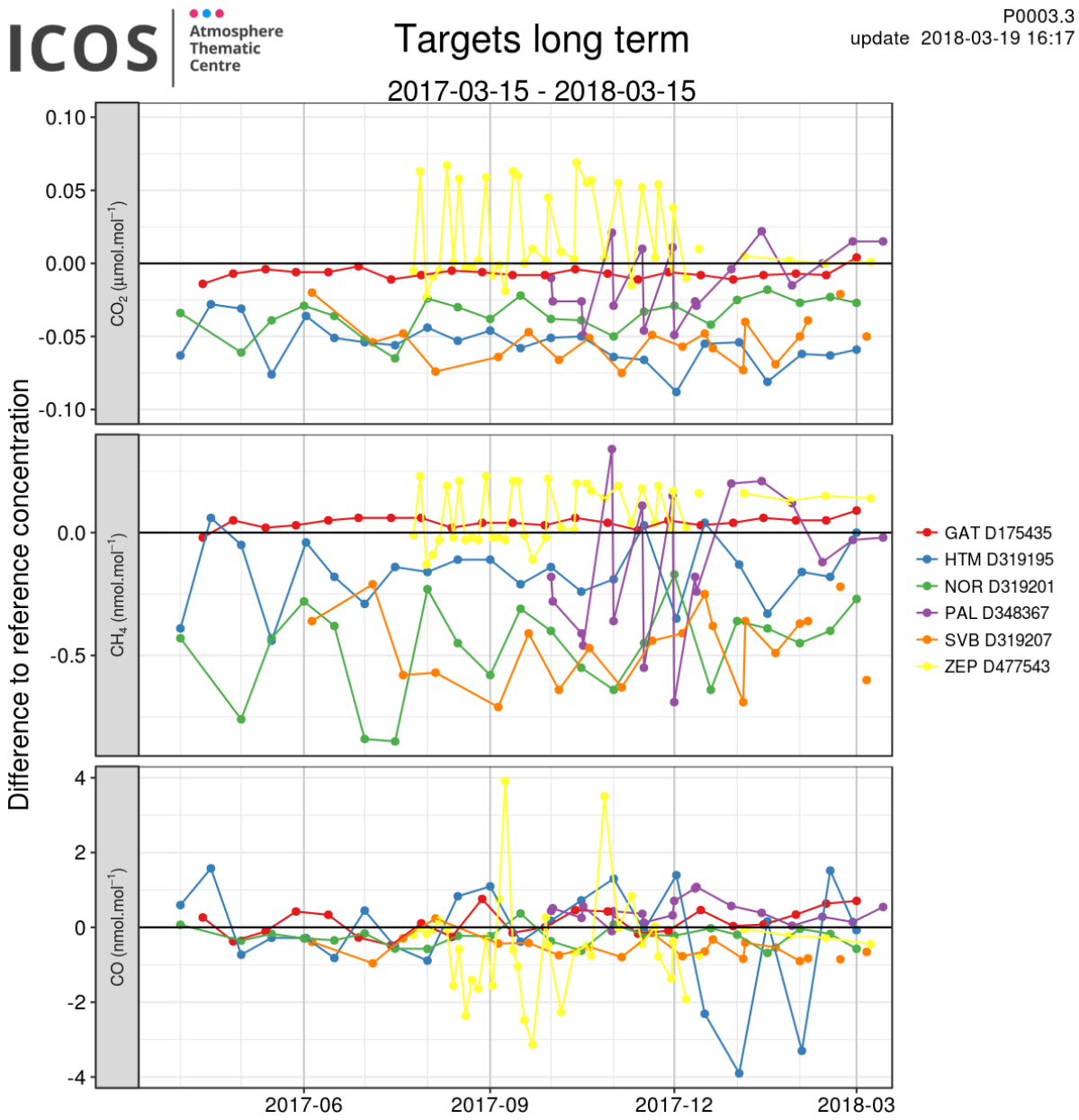
Network uncertainties and bias

2017-03-15 - 2018-03-10

CO (nmol.mol^{-1})




ICOS
Atmosphere Thematic Centre
Targets long term
2017-03-15 - 2018-03-15
P0003.3
update 2018-03-19 16:17
Difference to reference concentration
CO2 (µmol.mol−1)
CH4 (nmol.mol−1)
CO (nmol.mol−1)
0.1
0.0
-0.1
-0.2
-0.3
-0.4
0.0
-0.4
-0.8
-1.2
2
1
0
-1
-2
2017-06
2017-09
2017-12
2018-03
HPB D175433
JFJ D175452
KRE D048629
OPE D860463
PUY D337582
SMR D348390



General comments: The JFJ station shows average performance in term of bias for all species (based on long term target study). The improvement on CO_2 after Nafion removal is well observed.

16 Recommendation summary and conclusion

Jungfraujoch is providing ICOS specifications compatible data since 2016-12-12.

The following recommendations have been made:

- (***, important, -): It is recommended to continue the flagging of raw data on a weekly basis.
- (*, minor, 2018): Cylinder measurement duration can be decreased to 25 minutes with 10 minute flushing.
- (*, important, -): Due to the CO variability, the calibration intervals should be kept at two weeks.
- (*, minor, 2018): It is possible to reduce to three calibration cycles instead of four (keeping the rejection of the first cycle in the ATC configuration)

Based on the data provided during the initial test period, we recommend that the Jungfraujoch station (JFJ) is labelled as part of the ICOS Atmospheric Network.

17 List of abbreviations and glossary

ATC: Atmospheric Thematic Center

CMR: Continuous Measurement Reproductibility

CP: Carbon Portal

GAW: Global Atmosphere Watch

GHG: GreenHouse Gas

ICOS: Integrated Carbon Observation System

ICOS-FCL: ICOS Flask and Calibration Laboratory

LTR: Long-Term Repeatability

STR: Short-Term Repeatability

TGT: Target

WMO: World Meteorological Organization

Calibration: As detailed in the ICOS specifications, three to four standard gases (known concentrations calibrated at the ICOS-FCL) are measured one after the other at least four times for 30 min each calibration sequence (each set of the three to four cylinders measurement is called a cycle). Usually the first cycle is used to flush the calibration lines.The calibration function using a linear fit is calculated.

CCGVU: Smoothing curve algorithm (Thoning, K. W., Tans, P. P., and Komhyr, W. D.: Atmospheric carbon dioxide at Mauna Loa Observatory: 2. Analysis of the NOAA GMCC data, 1974–1985, J. Geophys. Res., 94, 8549, https://doi.org/10.1029/JD094iD06p08549, 1989)

CMR: In the MLab, the continuous measurement repeatability is evaluated with the standard deviation of the continuous measurements of a cylinder over 24 hours. Using the station data, the CMR is calculated using regular but not continuous measurements of the short term target gas. We calculate the moving monthly average of the standard deviations of raw data over 1 min intervals.

Flushing flow rate: Flow rate measured in the sampling air lines.

Instrument flow rate: Flow rate measured at the outlet of the instrument.

Long term target: gas with known concentrations (calibrated at the ICOS-FCL) that is measured on a monthly basis to insure data quality continuity through the different short term target changes

LTR: In the MLab, a target gas is measured for 30 min bracketed by around 5 hours of wet ambient air over 72 hours of total measurements. For each measure, only the last 10 min are averaged. The long-term repeatability is then expressed through the standard deviation of these averaged measures. Using the station data, we calculate the moving standard deviation of the averaged short term target measurement intervals over 3 days as in the MLab.

Outlet valve: Measure of the opening of the outlet valve on Picarro instrument, in arbitrary units.

Short term target: gas with known concentrations (calibrated at the ICOS-FCL) that is measured frequently (two to three times a day) to follow short term instrument variability.

Short term target bias: difference between the short term target injection average and its assigned value.

STR: In the MLab, a target gas is measured 10 times (15 min bracketed by 5 min of wet ambient air measurements). For each measure, only the last 9 min are averaged. The repeatability is then expressed through the mean and standard deviation of these averaged measures.

Short term working standard: gas that is measured frequently to correct for the short term variability.

Tdas: Temperature inside the Picarro instruments.