Quality Control of Trace Gas Observations

Martin Steinbacher

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with contributions from NOAA-ESRL, ICOS & WCC-Empa

NIES technical training course on greenhouse gases and air pollutants monitoring in Indonesia
Tsukuba, 24 – 30 November 2019

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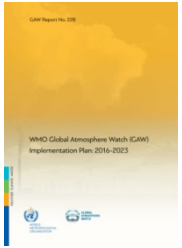
About me

- Meteorologist (University of Frankfurt, Germany)
- 2001 – 06/2004 PhD Fellow at the Laboratory of Atmospheric Chemistry, Paul Scherrer Institute, Villigen, Switzerland
- Summer 2004: PhD in Atmospheric Chemistry at ETH in Zurich
- Since July 2004: Scientist at Laboratory for Air Pollution / Environmental Technology, Empa, Duebendorf, Switzerland
    - Principal operator of the air quality observations within the Swiss National Air Pollution Monitoring Network at the GAW site Jungfraujoch
    - Head of WMO/GAW QA/SAC Switzerland
    - Chair of the Atmospheric Monitoring Station Assembly of the Integrated Carbon Observation System

Quality Assurance / Science Activity Centre Switzerland



GAW Implementation Plan 2016-2023, GAW Report Nr. 228, 2017

5.2.2 *Quality Assurance/Science Activity Centres (QA/SACs)*

Specific activities:

QA-1. Provide an operating framework for GAW quality assurance activities and calibration facilities for a specific variable and geographical area of responsibility (world, regional, national).

QA-2. Coordinate the activities of WCCs and RCCs in the area of their responsibility.

QA-3. Provide advice and support for the local QA system at individual GAW sites.

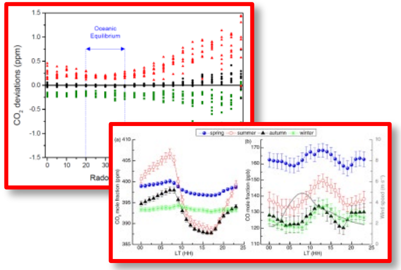
QA-4. Where appropriate, coordinate instrument calibrations and intercomparisons and other measurement activities.

QA-5. Perform or oversee regular system audits at GAW sites.

QA-6. Provide training, long-term technical help, and workshops for station scientists and technicians.

QA-7. Promote the scientific use of GAW data, and encourage and participate in scientific collaboration.

capacity building



science

Primary Tasks of QA/SAC-CH

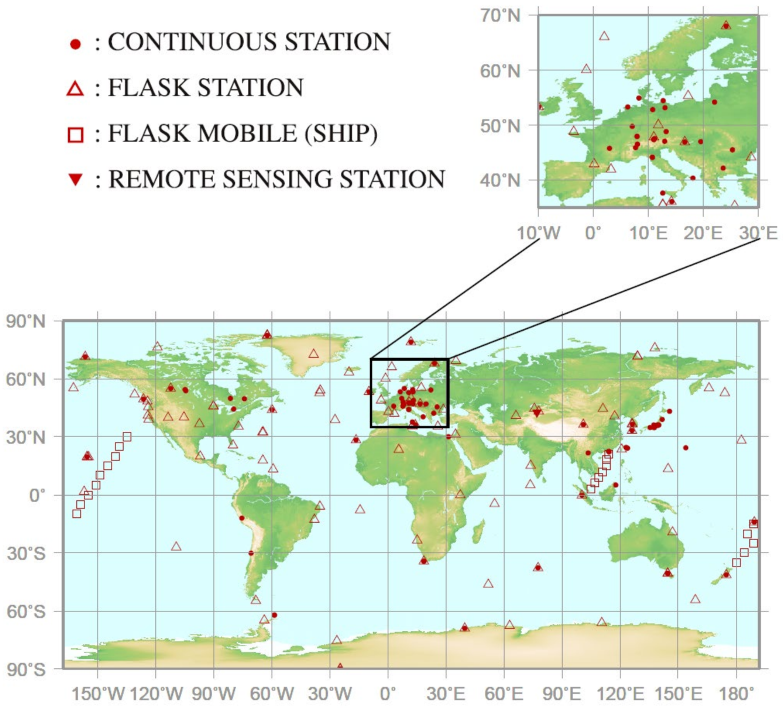
- research activities promoting technical progress and scientific data analysis,
- twinning, support, capacity building, and training
- contribution to GAW outreach,
- networking / cooperation with other programmes / projects in line with the GAW strategy

networking

outreach

Rationale for training and capacity building

Stations reporting CO_2 data



WDCGG Data Summary, No. 42, 2018

" … Building expertise in developing countries including the establishment of high-quality measurement capabilities remains a critical issue for achieving adequate spatial coverage of the globe in the coming decade. WMO and IAEA can make large contributions here through training courses, and stimulating partnerships between laboratories. …"

The long process of capacity building





<u>A-priori:</u> basic equipment / infrastructure available, willingness to perform high-precision air quality observations in a pristine environment

- advice for instrument selection
- technical support / advice to set up measurement capabilities
- regular on-site training
- remote support / trouble shooting
- facilitating the provision of spare parts
- support for data processing / data submission
- support for (research) proposal writing
- support for scientific data analysis and publication

> 10 years

<u>A-posteriori:</u> fully autonomous monitoring station, high-quality data, good visibility in the GAW and the scientific community

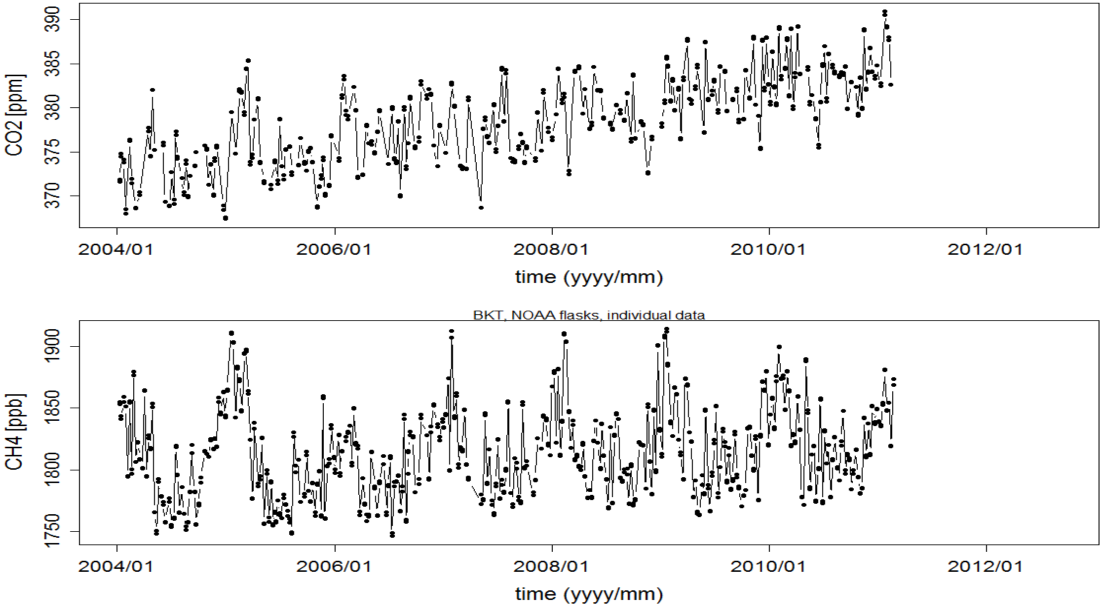
Planning of ambient air measurements

Planning of ambient air measurements

- Why are ambient air measurements needed?
- Which compounds are of interest?
  (gaseous compounds, particulates, deposition, meteorological parameters)
- What kind of data series are needed?
  (continuous, discrete, time resolution, concentration range)
- Where are measurements reasonable?
  (representatives of air, avoid influence of undesirable sources)
- When is the right time to measure?
  (annual cycles of compounds, special weather conditions)

Example – Bukit Koto Tabang

greenhouse gas observations
through flask sampling and in-situ monitoring



Example – Bukit Koto Tabang

greenhouse gas observations
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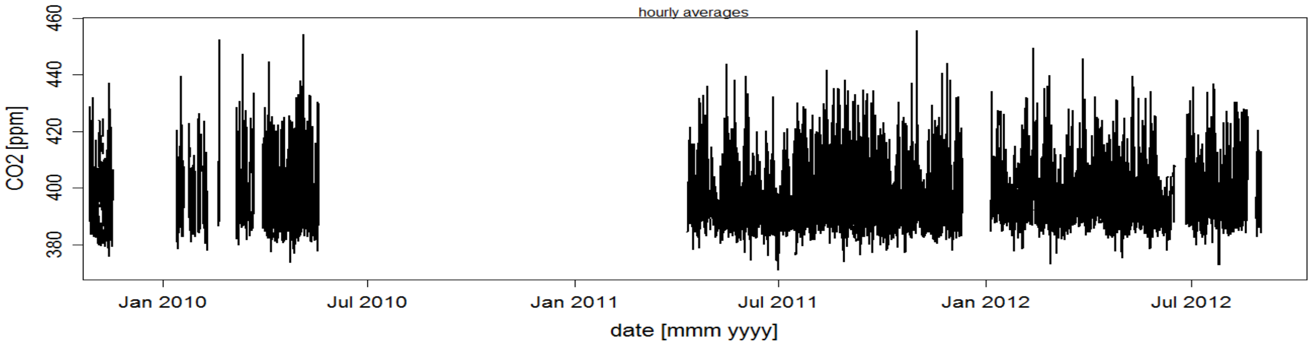

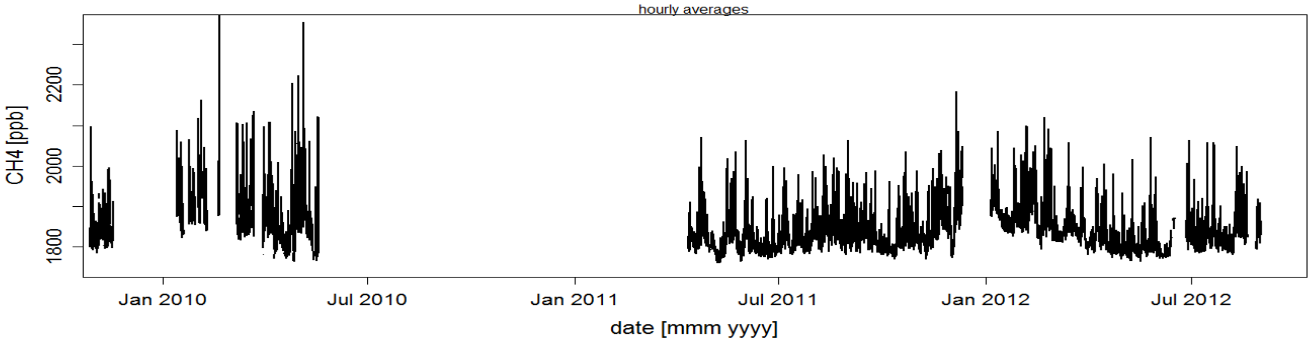

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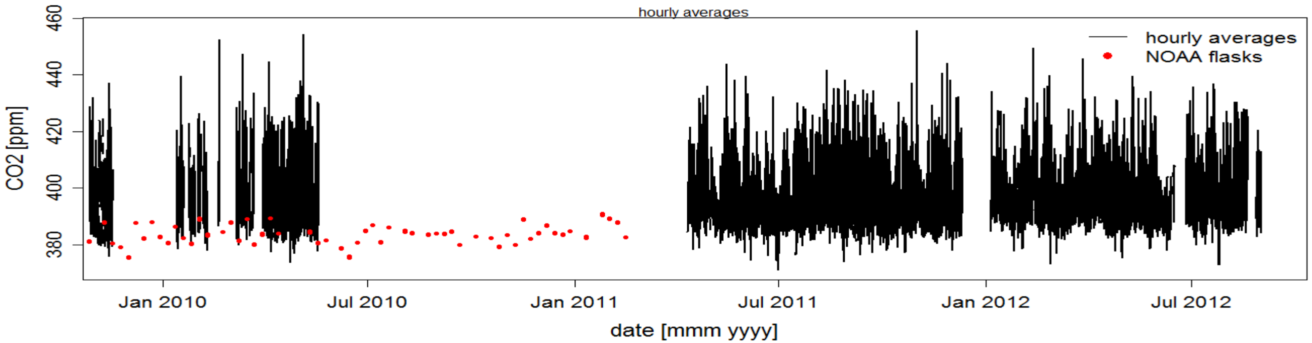

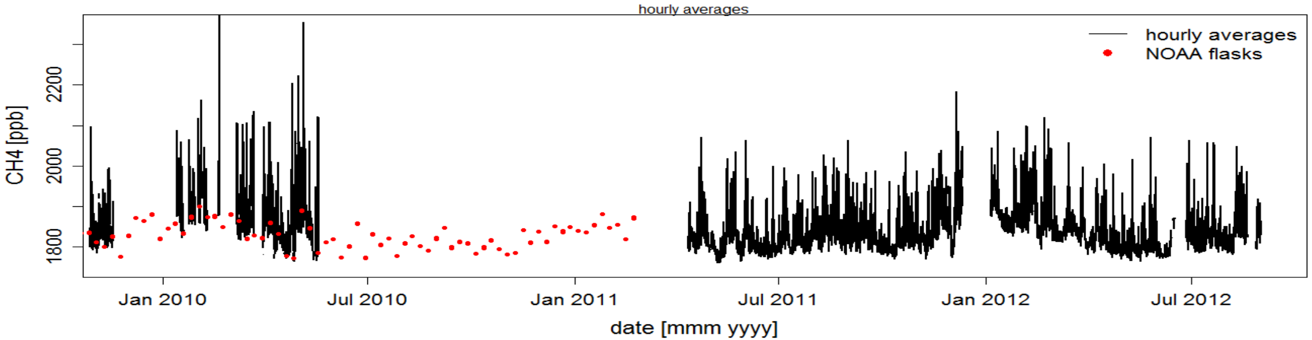

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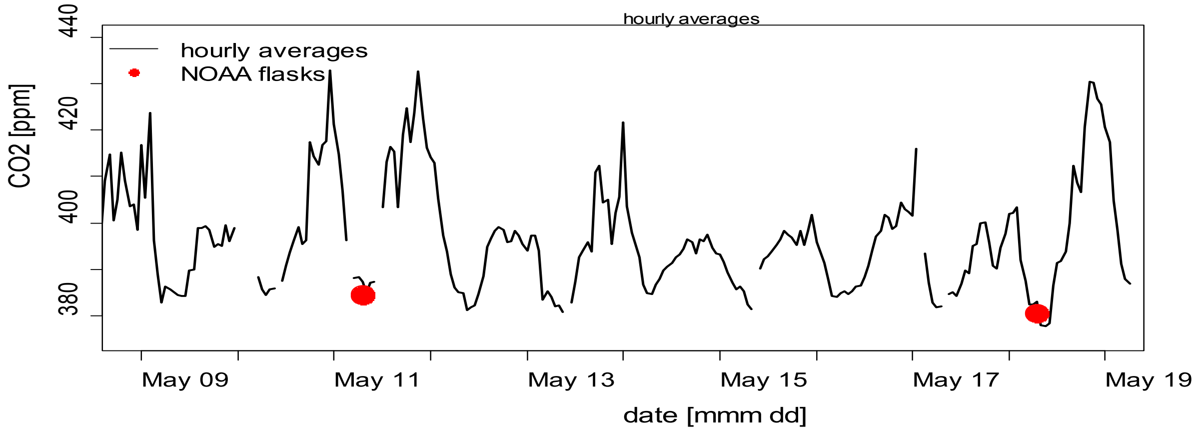

long-term flask observations suitable for trend estimates

continuous measurements allow gaining insight into local to regional processes

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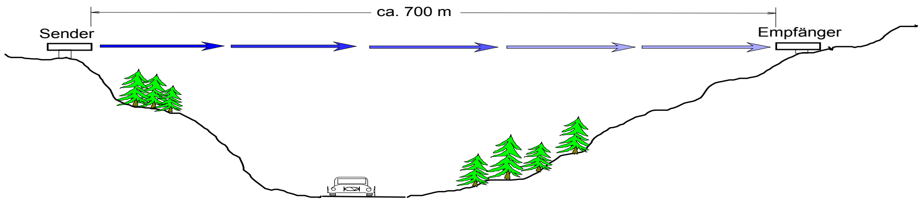
Measurement strategies

- **with sampling**
  - online, automatic analysis at site (monitor)
  - quasi-online (e.g. automated GC)
  - offline, sampling at site, analysis in laboratory
  - integral sampling
  - spot sampling

- **without sampling (remote sensing)**
  - DOAS (Differential Optical Absorption Spectroscopy)
  - FTIR (Fourier Transformation Infrared Spectroscopy)
  - LIDAR (Light Detection and Ranging)
  - TDLS (Tuneable Diode Laser Spectroscopy)
  - ...



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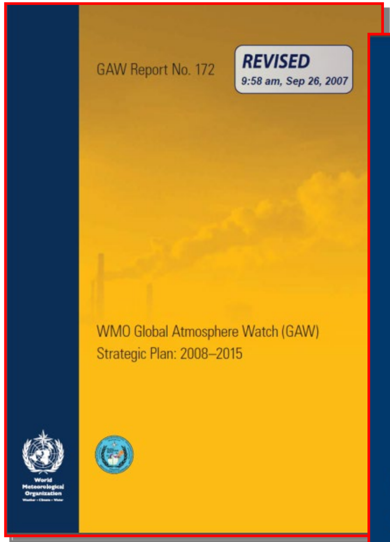
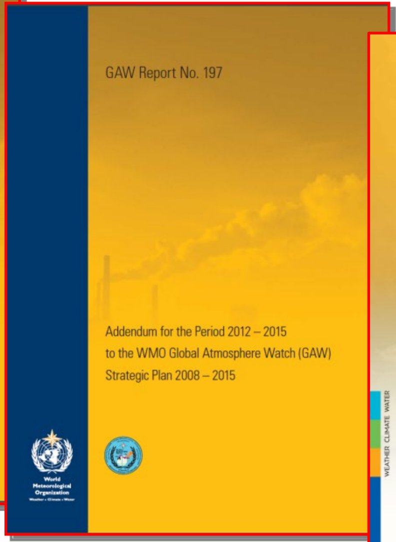
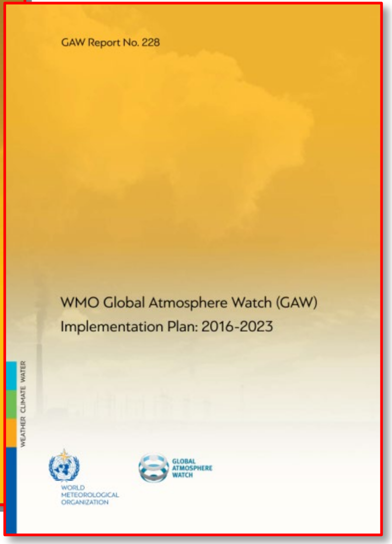
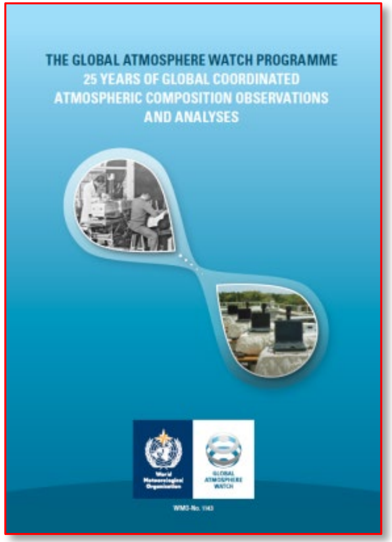
Useful documents







http://www.wmo.int/pages/prog/arep/gaw/gaw-reports.html



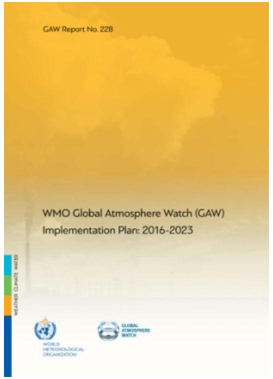
Global Atmosphere Watch (GAW) Programme: 25 years of global coordinated atmospheric composition observations and analyses
https://www.wmo.int/pages/prog/arep/gaw/documents/GAW25_brochure_wmo_1143_en.pdf

Useful documents

Requirements for Global Stations

These stations primarily observe GAW variables under background conditions, i.e. without permanent significant influence from local pollution sources. In addition to fulfilling the requirement of GAW Regional stations, Global stations must fulfil the following:

1. Measure at least two variables in at least three of the six GAW focal areas with the full implementation of GAW's Quality Assurance system (Box 7.1 (A)).
2. Have a strong scientific supporting programme with appropriate data analysis and interpretation within the country and, if possible, the support of more than one agency.
    a. The stations should have a confirmed track record of research campaigns and/or scientific products (within last 3 years) as a Regional station.
    b. The measurements at the station have been audited or the quality of the measurements has been documented through other means of verification.
    c. The data from at least two variables in at least three focal areas have been submitted to the respective World Data Centre(s) during at least three years within the data submission period of 1 year after measurement.
3. Provide a facility at which intensive campaign research can augment the long-term routine GAW observations and where testing and development of new GAW methods can be undertaken.
4. In case the measurements of some GAW variables are occasionally influenced by local pollution, the station shall subject the data to appropriate filter methods to extract the background concentrations and submit both a filtered and an unfiltered time series to the WDC. Also the station metadata on GAWSIS should describe the conditions under which pollution influences may be found and describe the applied filter methods.

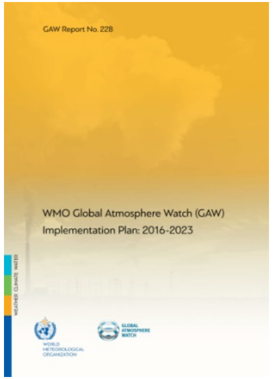


GAW Implementation Plan 2016-2023,
GAW Report Nr. 228, 2017

Useful documents

Requirements for GAW Regional stations in particular include:

1. The station location is chosen such that, for the variables measured, it is regionally representative and is normally free of the influence of significant local pollution sources or at least frequently experiences advection of pollution-free air from specific wind directions.
2. There is a commitment by the responsible agency to long-term observations of at least two variables in at least one GAW focal areas (ozone, aerosols, greenhouse gases, reactive gases, UV radiation, precipitation chemistry/total deposition). To address measurements for multiple applications in more than one focal area are recommended.
3. Adequate power, air conditioning, communication and building facilities are provided to sustain long-term observations with greater than 90% data capture[d] (i.e. <10% missing data).
4. Standard meteorological in situ observations (at least temperature, humidity, air pressure, and wind speed and direction), necessary for the accurate determination and interpretation of the GAW variables, are made of known quality.
5. Technical staff are trained to operate station equipment.
6. GAW observations are of known quality, follow GAW Quality Assurance principles and procedures, linked to the GAW Primary Standard where applicable and use the measurement methods recommended[e] by GAW.
7. A station logbook (i.e. record of observations made and activities that may affect observations) is maintained and is used in the data validation process.
8. The data and associated metadata must be submitted to one of the GAW World Data Centres at least on a yearly basis documenting Year N no later than end of Year N+1. Changes of metadata including instrumentation, traceability, observation procedures, must be reported to the responsible WDC and GAWSIS in a timely manner following the WIGOS metadata standards.
9. If feasible, data are submitted to a designated data distribution system in near-real-time.



GAW Implementation Plan 2016-2023,
GAW Report Nr. 228, 2017

Infrastructure Requirements

Measurement site infrastructure

- shelter
- mast for free exposure of the inlet
- reliable power supply
- air conditioning
- internet access
- access to the station (365 days a year)
- local support
- …

Instrument(s) and periphery

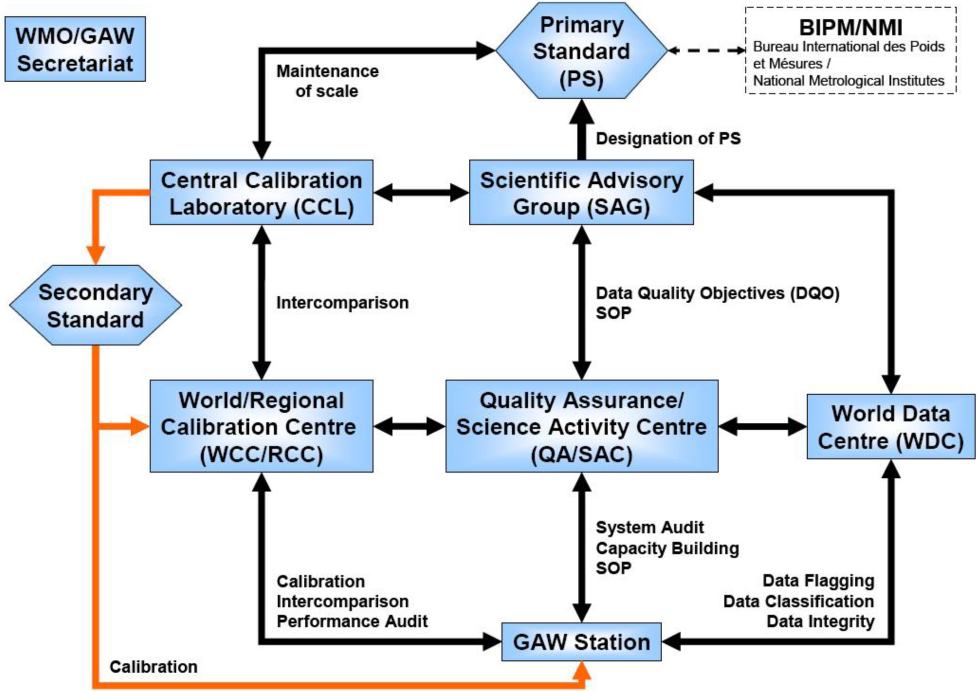
- adequate GHG analyzer
- periphery for automatic calibration
- reference gases (cals, targets)
- pressure reducers
- plumbing (additional pumps, tubing, connectors, inlet hat, drying unit, …)

- consumables, spare parts, backup instruments, …

Quality control of ambient air measurements

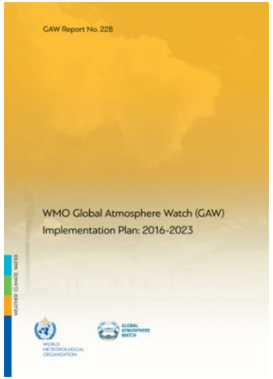
GAW Quality Management Framework

Elements of the Quality Assurance system,
QA activities and workflow in GAW



map of GAW stations

https://gawsis.meteoswiss.ch

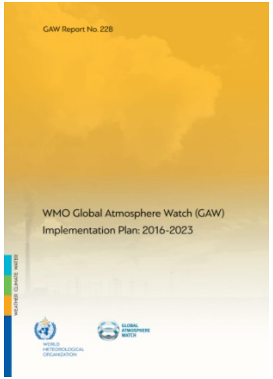


GAW Implementation Plan 2016-2023,
GAW Report Nr. 228, 2017

GAW's Central Facilities – the Trace Gas Perspective

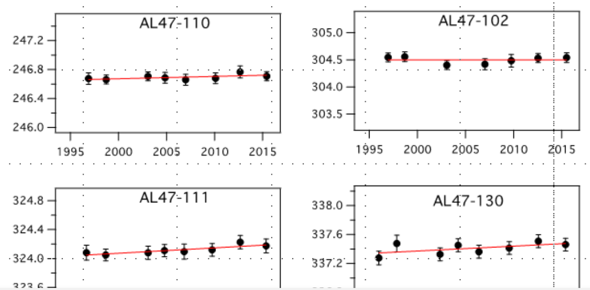
GAW Central Facilities

Variable	Quality Assurance / Science Activity Centre	Central Calibration Laboratory	World Calibration Centre	Regional Calibration Centres	World Data Centre
CO_2	JMA (Asia, South-West Pacific)	NOAA-ESRL	NOAA-ESRL (round robin) Empa (audits)		JMA
CO_2 Isotopes		MPI-BGC			JMA
CH_4	Empa (Americas, Europe, Africa) JMA (Asia, South-West Pacific)	NOAA-ESRL	Empa (Americas, Europe, Africa) JMA (Asia, South-West Pacific)		JMA
N_2O	UBA	NOAA-ESRL	KIT/IMK-IFU		JMA
SF_6		NOAA ESRL	KMA-KGAWC		JMA
CFCs, HCFCs, HFCs					JMA
Surface Ozone	Empa	NIST	Empa	OCBA (South America)	NILU
CO	Empa	NOAA-ESRL	Empa		JMA
VOCs	UBA	NPL (Ethane, Propane, n-butane, n-pentane, Acetylene, Toluene, Benzene, Isoprene) NIST (monoterpenes)	KIT/IMK-IFU		NILU
NO_X	UBA	NPL (NO)	FZJ (IEK-8) (NO)		NILU
SO_2					NILU



GAW Implementation Plan 2016-2023, GAW Report Nr. 228, 2017

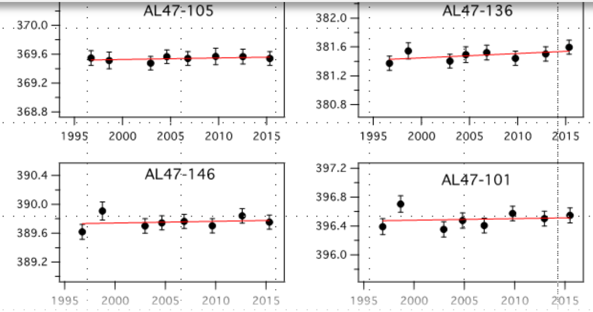
Example – CCL for CO2 (NOAA-ESRL)



Drift Assessment

	CO2	drift rate (ppm/yr)	Unc. 2-sd	N
AL47-110	246.69	0.0028	0.0099	8
AL47-102	304.45	0.0006	0.0144	7
AL47-111	324.11	0.0077	0.0133	8
AL47-130	337.41	0.0081	0.0133	8
AL47-106	412.25	0.0087	0.0169	8
AL47-123	423.27	0.0034	0.0158	8
AL47-107	453.25	-0.0099	0.0174	6
ND17440	479.74	0.0076	0.0456	5
AL47-132	521.7	0.0101	0.0201	8

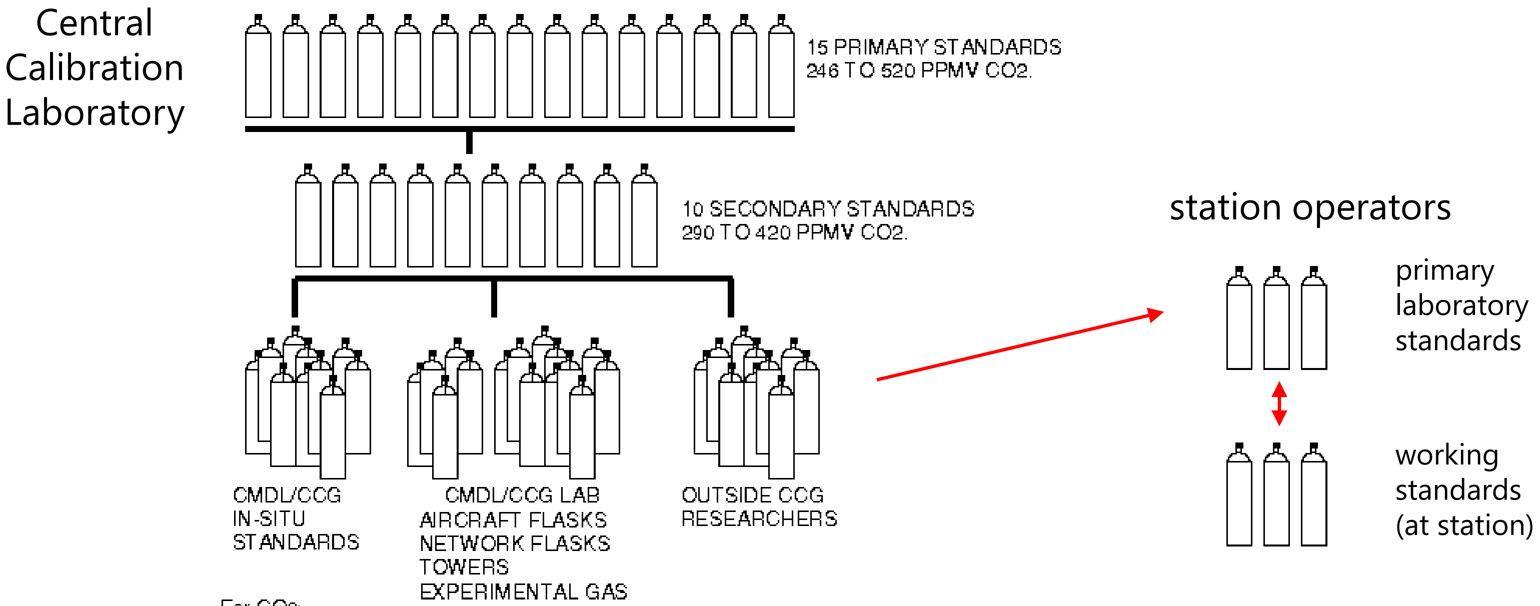
For greenhouse gases, primary standards are prepared gravimetrically by mixing aliquots of pure gaseous or liquid reagents with ultra-pure air, and are calibrated manometrically by measuring temperature and pressure in well-defined volumes of the whole air and the cryogenically trapped species of interest.



Mean: 0.05 ppm/decade

slide: courtesy of Brad Hall (NOAA)

Propagation of the scale, from CCL to station



For CO_2:
CALIBRATION PRECISION; 0.014 µmol/mol [1 sd of calibrations < 6 months apart].
precision for < 325 approx. 0.1
precision for > 425 approx. 0.25

Absolute Uncertainty; 0.1 µmol/mol
Internal consistency [325-425 µmol/mol]; 0.04 µmol/mol [2 sigma] [< 2 years]

https://www.esrl.noaa.gov/gmd/ccl/airstandard.html

Traceability

- make sure that you know your traceability chain
- add this information to your data / metadata

Data header

```
# ORG_QCflag_description :
# intake_height_total_listed : 1
# intake_height_1 : 5
# intake_height_1_units : m
# intake_height_1_start_date : 2013-05-01T00:00:00Z
# intake_height_1_end_date : 2015-12-30T00:00:00Z
# instrument_total_listed : 1
# instrument_1 : Picarro Inc., G2401, S/N CFKADS2031
# instrument_1_measurement_method_type_code : 18
# instrument_1_measurement_method_name : CRDS
# instrument_1_start_date : 2013-05-01T00:00:00Z
# instrument_1_end_date : 2015-12-30T00:00:00Z
# scale_total_listed : 1
# scale_1_code : 1
# scale_1_name : WMO CO2 X2007
# scale_1_start_date : 2013-05-01T00:00:00Z
# scale_1_end_date : 2015-12-30T00:00:00Z
```

File | Contact | Observation | Reference(s) | Gallery

Organization

NO	17
Acronym	DMC
Name	Direccion Meteorologica de Chile
Address 1	
Address 2	Dirección Meteorológica de Chile
Address 3	Av. Portales 3450, Estación Central - Santiago
Country/Territory	Chile
Website	http://www.meteochile.gob.cl/

Contact(s)

Name	Gaston Torres
Prefix	
Email	gtorres@meteochile.cl
Organization No	17
Organization acronym	DMC
Organization name	Direccion Meteorologica de Chile
Organization country/territory	Chile
Address 1	

CO2 _ TLL _

File | Contact | Observation | Reference(s)

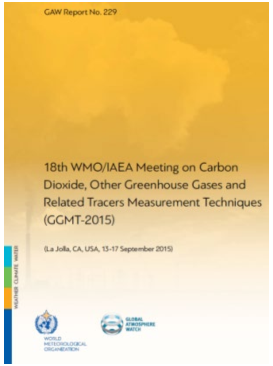
Search by a keyword: (start typing)

Collaborator(s)	NO: 23; Acronym: Empa; Name: Swiss Federal Laboratories for Materials Science and Technology
Aim of Observation	Background observation
Data Time zone	UTC
Unit	ppm
Calibration Scale	9999-12-31 00:00:00 - 9999-12-31 23:59:59: WMO CO2 X2007
Instruments(s)	9999-12-31 00:00:00 - 9999-12-31 23:59:59: Picarro Inc., G2401, S/N CFKADS2031(CRDS)
Intake Height above ground level	9999-12-31 00:00:00 - 9999-12-31 23:59:59: 5 (m)
Sampling Frequency	1 second
Measurement Calibration	Four calibration tanks are measured automatically every 2 to 9 days. Three of them are tanks purchased from the GAW Central Calibration Laboratory (NOAA ESRL), the mole fractions of the fourth tank are determined by the GAW World Calibration Centre for CH4, CO2, CO and surface O3 (WCC-Empa). WCC-Empa also assigned the mole fractions of an additional target cylinder that is measured every second day for quality control. the analyzer is regularly calibrated with four reference gases. All assigned mole fractions are reported on the WMO CO2 X2007 scale. The quality of the calibration is verified with a fifth reference gas (target cylinder).
Data Processing	Quality assurance procedures involve time series plots, target tank (i.e. cylinders containing natural air with assigned trace gas mole fractions that are treated as (unknown) sample in a sequence of analyses) measurements, and consistency checks.
Processing for averaging	[Hourly] high-resolution data are aggregated to 1min averages before hourly averages are calculated. Thus, ND (the number of detections) refers to the number of available 1min averages within the respective hour. [Daily] hourly averages are aggregated to daily means. Thus, ND (the number of detections) refers to the number of available hourly averages within the respective day. [Monthly] daily data are aggregated to monthly means. Thus, ND (the number of detections) refers to the number of available

Targeted compatibility for greenhouse gases within GAW

Recommended compatibility of greenhouse gas measurements

Component	*Compatibility goal 1-sigma*	*Extended compatibility goal*[1]	*Range in unpolluted troposphere (approx. range for 2015)*	*Range covered by the WMO scale*
CO_2	± 0.1 ppm (North.Hem.) ± 0.05 ppm (So.Hemisph)	± 0.2 ppm	380 - 450 ppm	250 – 520 ppm
CH_4	± 2 ppb	± 5 ppb	1750 – 2100 ppb	300 – 5900 ppb
CO	± 2 ppb	± 5 ppb	30 – 300 ppb	30 -500 ppb
N_2O	± 0.1 ppb	± 0.3 ppb	325 – 335 ppb	260 – 370 ppb
SF_6	± 0.02 ppt	± 0.05 ppt	8 – 10 ppt	2.0 – 20 ppt
H_2	± 2 ppb	± 5 ppb	400 – 600 ppb	140 –1200 ppb
$\delta^{13}C$-CO_2	± 0.01‰	± 0.1‰	-9.5 to -7.5‰ (VPDB)	
$\delta\,^{18}O$-CO_2	± 0.05‰	± 0.1‰	-2 to +2‰ ($VPDB$-CO_2)	
$\Delta^{14}C$-CO_2	± 0.5‰	± 3‰	-50 to 50‰	
$\Delta\,^{14}C$-CH_4	± 0.5‰		50-350‰	
$\Delta\,^{14}C$-CO	± 2 molecules cm^{-3}		0-25 molecules cm^{-3}	
$\delta\,^{13}C$-CH_4	± 0.02‰	± 0.2‰		
δ D-CH_4	± 1‰	± 5‰		
O_2/N_2	± 2 per meg	± 10 per meg	-900 to -400 per meg (vs. SIO scale)	



GGMT-2015 Report, GAW Report Nr. 229, 2016

rule of thumb: internal reproducibility goals is one half the network compatibility goals

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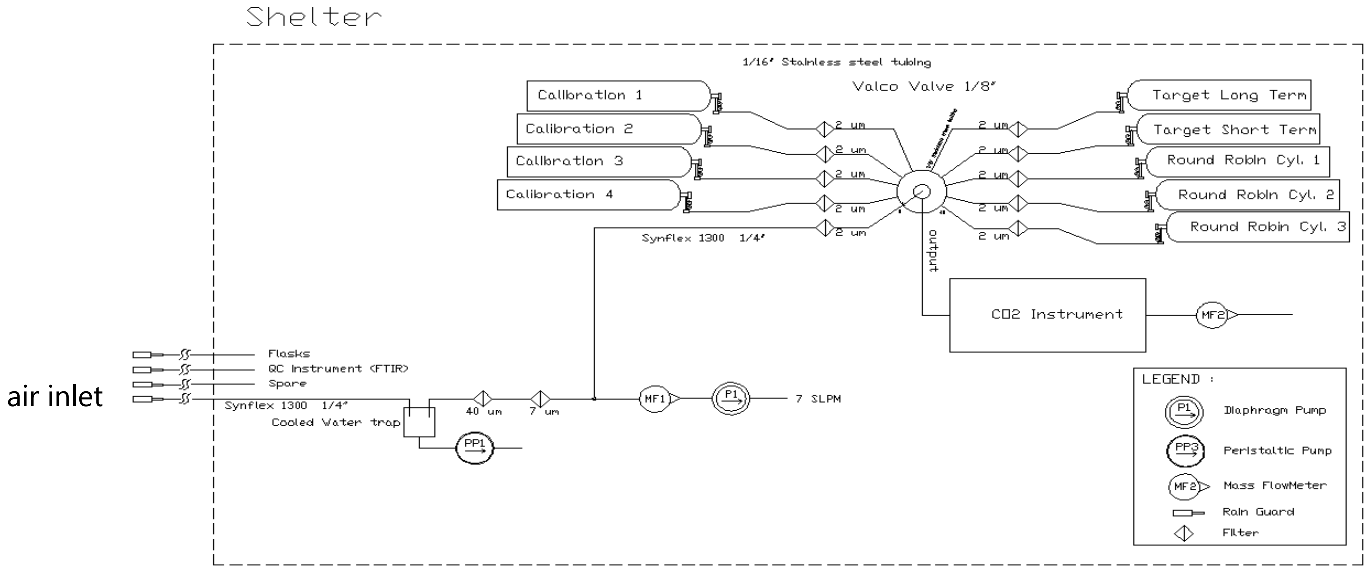
Typical plumbing design for CO2 observations

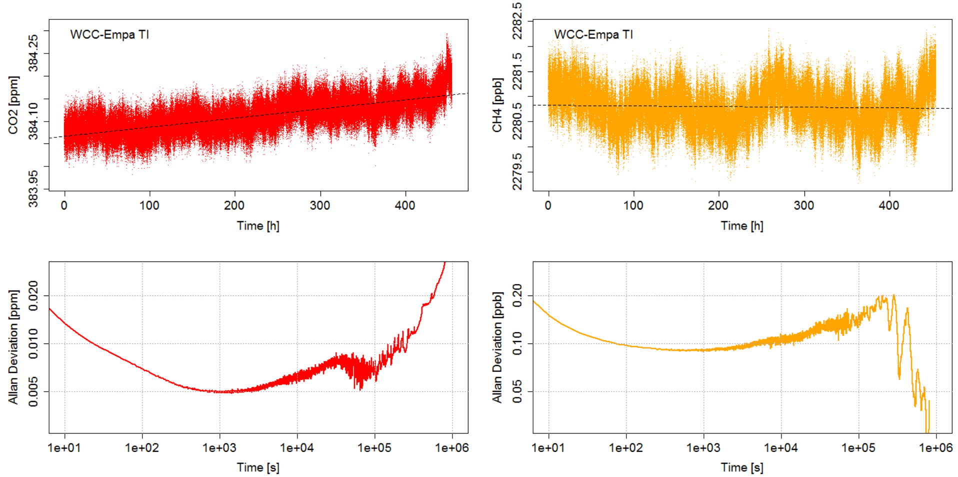


ICOS Atmospheric Station Specification Document
https://www.icos-ri.eu/documents/ATC%20Public

Frequency of calibrations depending on the time-scale of sensitivity changes of the analyzer

Calibration frequency for CO2 observations

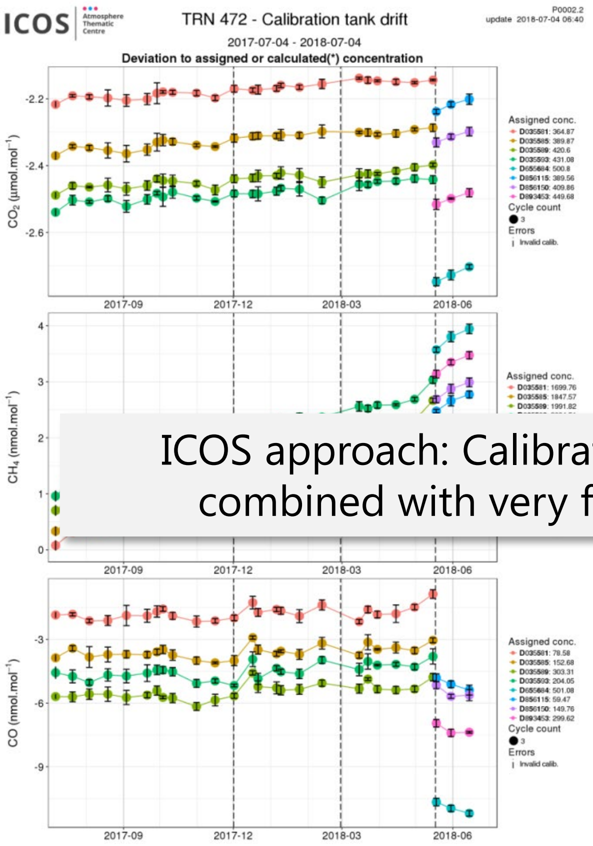
Allan deviation plots

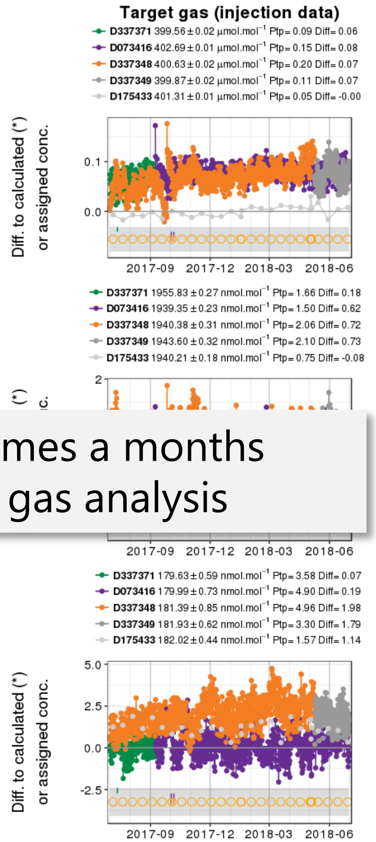


Zellweger et al., AMT, 2016

"A thorough analysis of the CO2 and CH4 stability of [this type of cavity enhanced laser spectrometer] indicates that the optimal calibration frequency is approximately 30 h."

Calibration frequency for CO2 observations



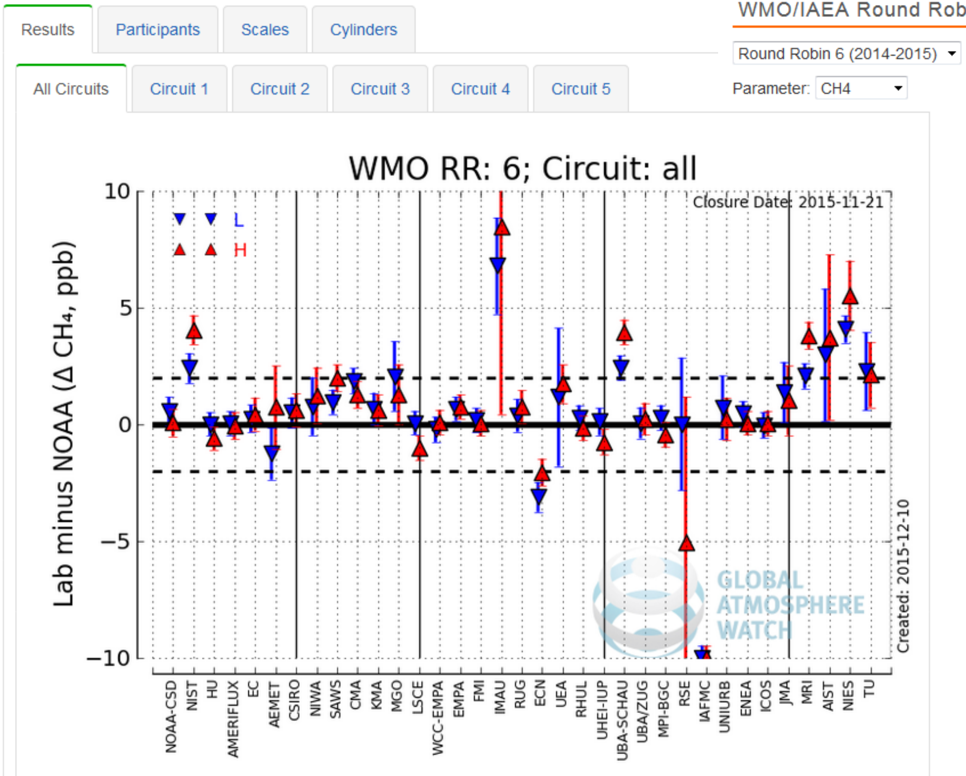


ICOS approach: Calibration only 2-3 times a months combined with very frequent target gas analysis

ICOS ATC (Atmospheric Thematic Center), screenshots

Network wide quality control

- Round Robin Exercises for Greenhouse Gases

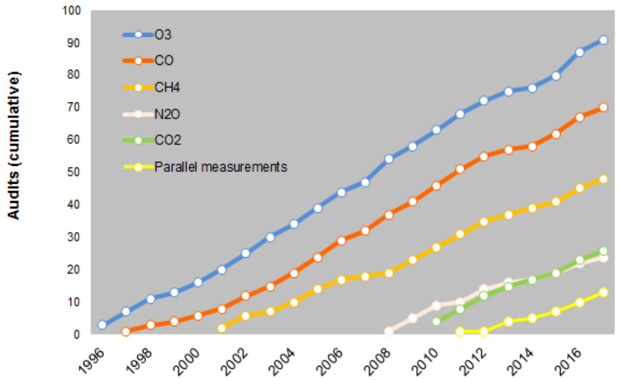


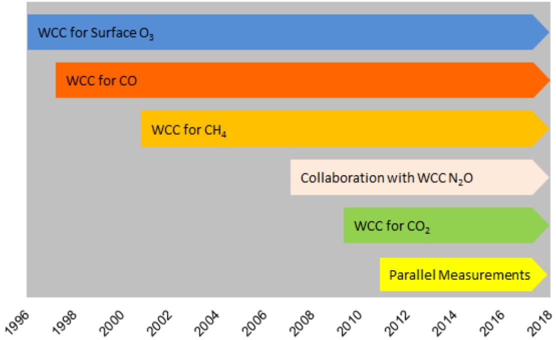
5 circuits of 2 cylinders travelling around the world; 44 participating labs (RR6)

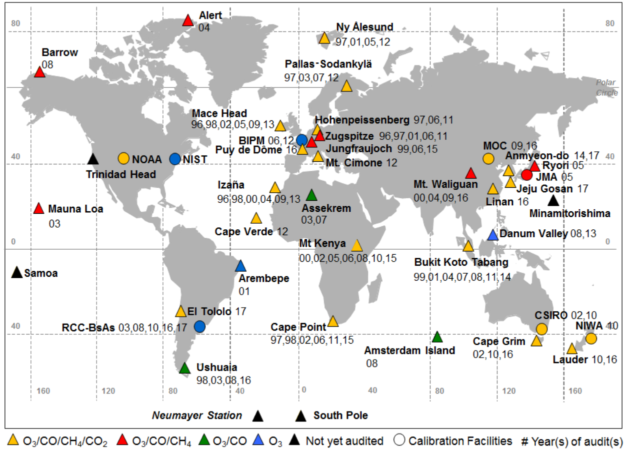
https://www.esrl.noaa.gov/gmd/ccgg/wmorr/

Network wide quality control

- World Calibration Centre for Surface O3, CO, CH4, and CO2 (WCC-Empa)



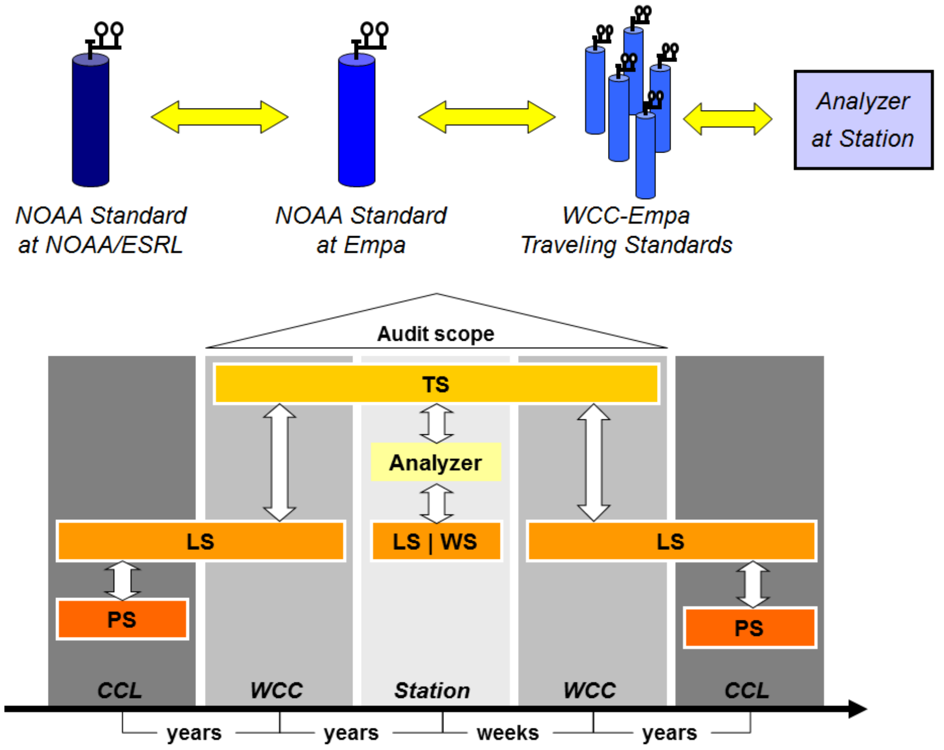


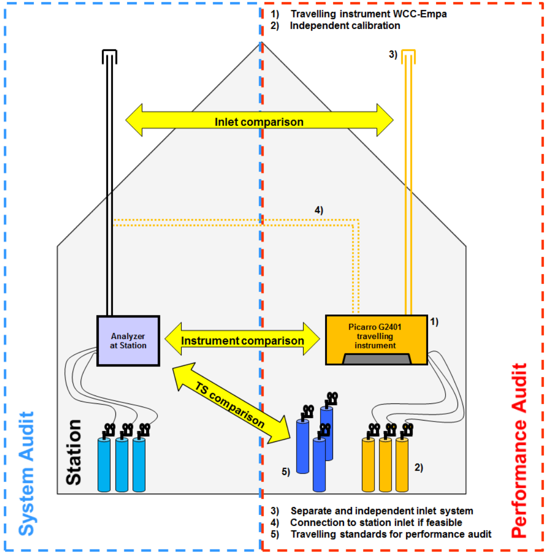


- established in 1996, more than 90 audits since then
- ensures traceability to the GAW reference and determines compatibility
- assists stations with regards to instruments and measurement issues (WCC-Empa & QA/SAC-CH)
- improves technical know-how at stations through on-site training (WCC-Empa & QA/SAC-CH)

Network wide quality control

- World Calibration Centre for Surface O3, CO, CH4, and CO2 (WCC-Empa)





https://www.empa.ch/web/s503/wcc-empa

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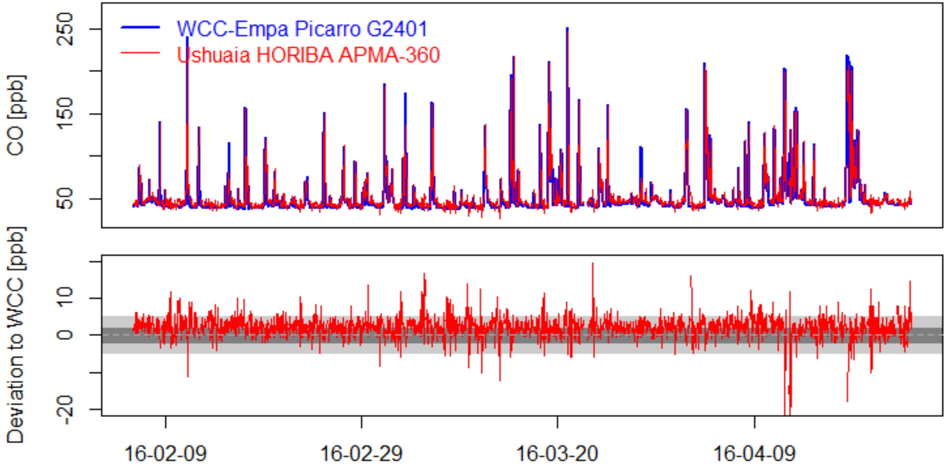
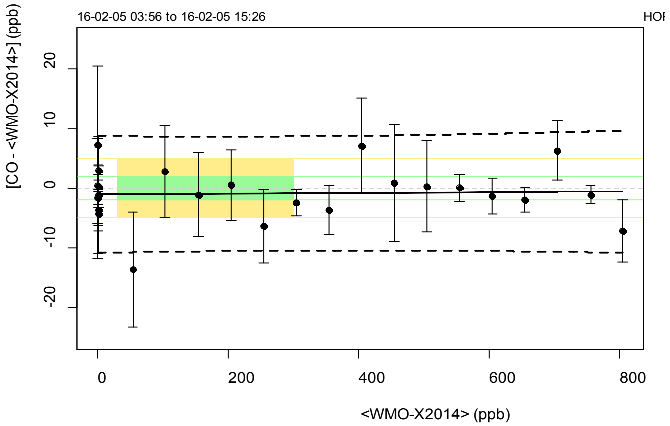
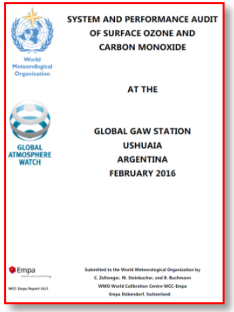


WCC-Empa audit in Ushuaia (Argentina) (February 2016)




SYSTEM AND PERFORMANCE AUDIT
OF SURFACE OZONE AND
CARBON MONOXIDE

AT THE

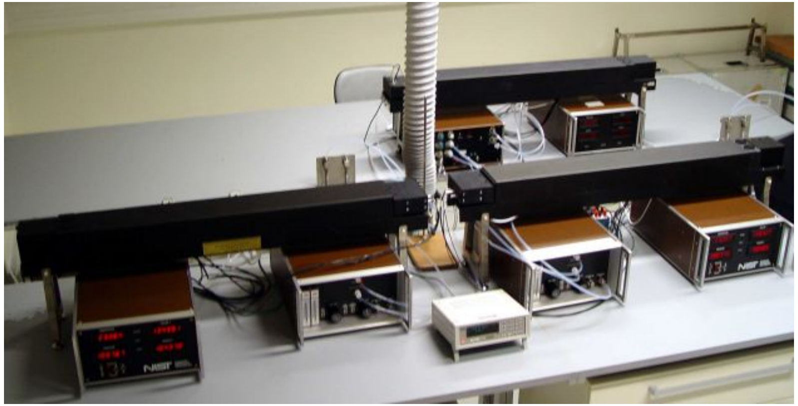
GLOBAL GAW STATION
USHUAIA
ARGENTINA
FEBRUARY 2016

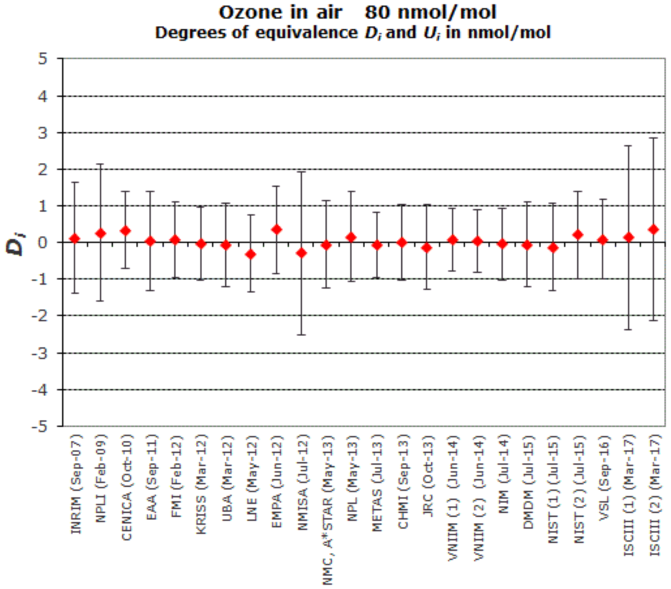
Audit reports are publicly available at

- https://gawsis.meteoswiss.ch/
- www.empa.ch/gaw, and
- http://www.wmo.int/pages/prog/arep/gaw/other_pub.html

Traceability for surface ozone measurements

- Each NIST Standard Reference Photometer (SRP) is a realisation of a Primary Standard
- CCL is NIST, which maintains SRP#2 (=reference for GAW), but SRP#X is also a primary standard
- The 'SRP family', which defines the O_3 reference, is inter-compared in an ongoing Key Comparison organized by BIPM (www.bipm.org)





Calibration (and auditing) of surface O3 analyzers

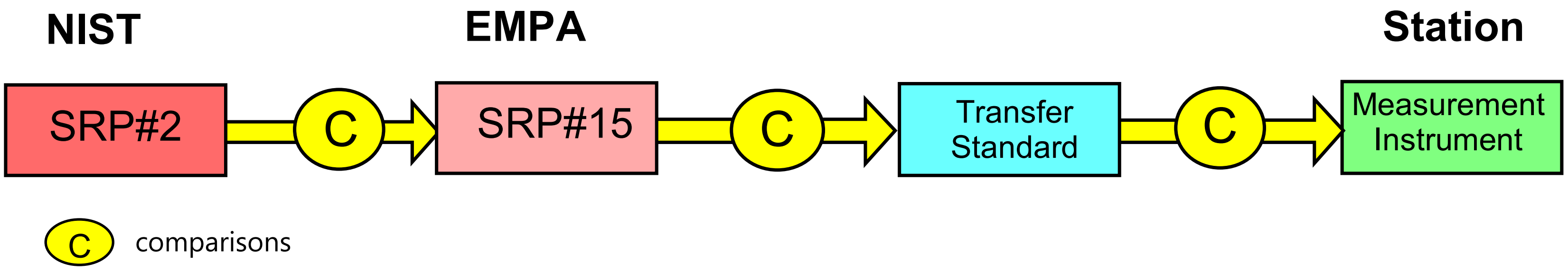
Reference: Standard Reference Photometer (SRP)

World reference: SRP #2 at National Institute for Standards and Technology

Currently: approx. 60 SRPs worldwide

Transfer standard / calibrator is calibrated against a reference photometer and used for the calibration of ozone instruments

Traceability chain:



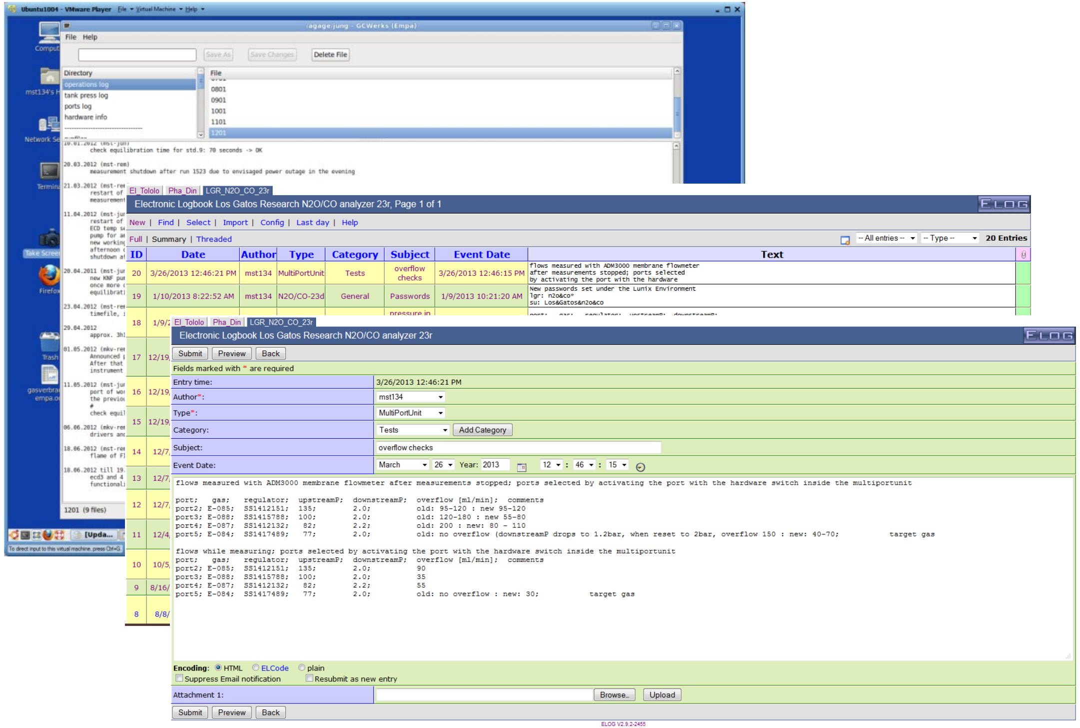
martin.steinbacher@empa.ch

Operation and maintenance

Operation and maintenance

Measurements and beyond

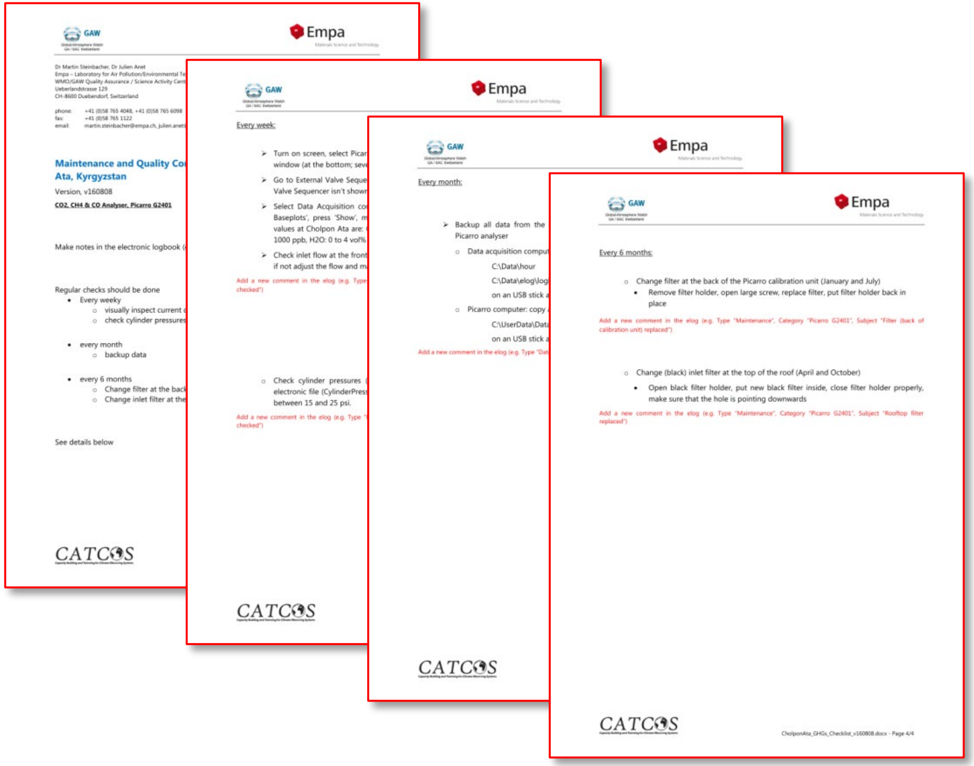
- documentation, log books
- metadata management



Operation and maintenance

Measurements and beyond

- documentation, log books
- metadata management
- preparation of checklists



NIES technical training course, Tsukuba, November 2019

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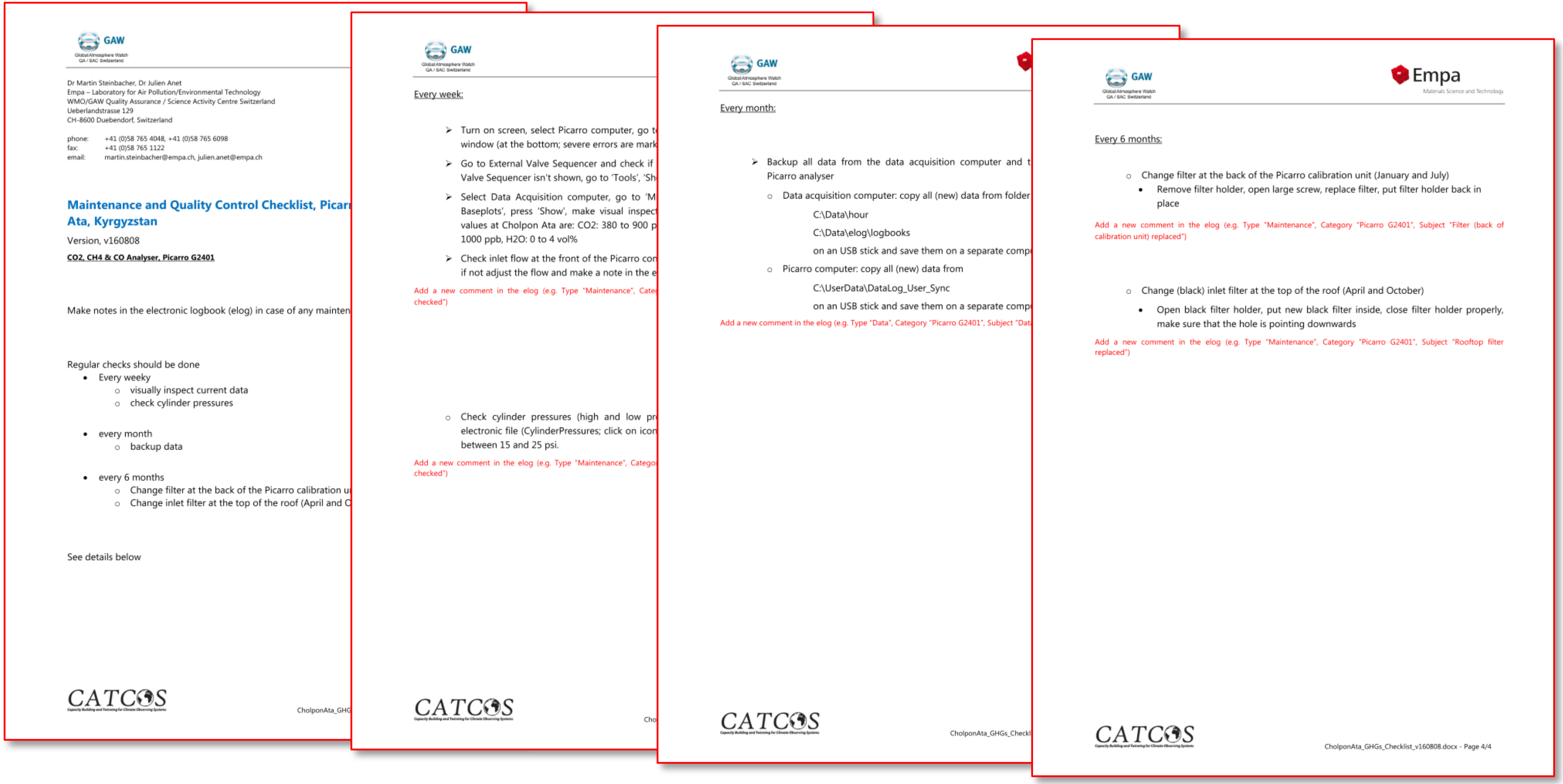
Standard Operation Procedures and Checklists



GAW
Global Atmosphere Watch
QA / SAC Switzerland

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Empa – Laboratory for Air Pollution/Environmental Technology
WMO/GAW Quality Assurance / Science Activity Centre Switzerland
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fax: +41 (0)58 765 1122
email: martin.steinbacher@empa.ch, julien.anet@empa.ch

Maintenance and Quality Control Checklist, Picarr Ata, Kyrgyzstan

Version, v160808

CO2, CH4 & CO Analyser, Picarro G2401

Make notes in the electronic logbook (elog) in case of any mainten

Regular checks should be done

- Every weeky
  - visually inspect current data
  - check cylinder pressures
- every month
  - backup data
- every 6 months
  - Change filter at the back of the Picarro calibration u
  - Change inlet filter at the top of the roof (April and O

See details below

CATCOS Capacity Building and Twinning for Climate Observing Systems

CholponAta_GHG

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Every week:

- Turn on screen, select Picarro computer, go t window (at the bottom; severe errors are mark
- Go to External Valve Sequencer and check if Valve Sequencer isn't shown, go to 'Tools', 'Sh
- Select Data Acquisition computer, go to 'M Baseplots', press 'Show', make visual inspec values at Cholpon Ata are: CO2: 380 to 900 p 1000 ppb, H2O: 0 to 4 vol%
- Check inlet flow at the front of the Picarro cor if not adjust the flow and make a note in the e

Add a new comment in the elog (e.g. Type "Maintenance", Cate checked")

- Check cylinder pressures (high and low pr electronic file (CylinderPressures; click on icon between 15 and 25 psi.

Add a new comment in the elog (e.g. Type "Maintenance", Catego checked")

CATCOS Capacity Building and Twinning for Climate Observing Systems

Cho

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Every month:

- Backup all data from the data acquisition computer and t Picarro analyser
  - Data acquisition computer: copy all (new) data from folder
    - C:\Data\hour
    - C:\Data\elog\logbooks
    - on an USB stick and save them on a separate comp
  - Picarro computer: copy all (new) data from
    - C:\UserData\DataLog_User_Sync
    - on an USB stick and save them on a separate comp

Add a new comment in the elog (e.g. Type "Data", Category "Picarro G2401", Subject "Dat

CATCOS Capacity Building and Twinning for Climate Observing Systems

CholponAta_GHGs_Checkl

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Every 6 months:

- Change filter at the back of the Picarro calibration unit (January and July)
  - Remove filter holder, open large screw, replace filter, put filter holder back in place

Add a new comment in the elog (e.g. Type "Maintenance", Category "Picarro G2401", Subject "Filter (back of calibration unit) replaced")

- Change (black) inlet filter at the top of the roof (April and October)
  - Open black filter holder, put new black filter inside, close filter holder properly, make sure that the hole is pointing downwards

Add a new comment in the elog (e.g. Type "Maintenance", Category "Picarro G2401", Subject "Rooftop filter replaced")

CATCOS Capacity Building and Twinning for Climate Observing Systems

Standard Operation Procedures and Checklists

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fax: +41 (0)58 765 1122
email: martin.steinbacher@empa.ch

Example for a Maintenance Checklist, Ozone analyser TE49i

Version, v171027

OZONE ANALYZER (Thermo Environmental Instruments Model 49i)

Make notes in the logbook in case of any maintenance !

Regular checks should be done

- every week
  - checking instrument performance and verification of principal instrument parameters
  - zero and span check (if technically possible)
- every month
  - Replace inlet filter
- every 3 months
  - A/B test
  - Check / clean ventilation instrument filter
  - Check pressure sensor
- every 6 months
  - Cell cleaning
  - Leak check
  - Check coarse filter on the roof (if available)

See details below

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Every week

Checking instrument performance and verification of principal instrument parameters

Date ...., Time (UTC) ...., Operator ....

Ambient pressure	.... hPa = ... mm Hg (1 mbar := 0.75006 mm Hg)		
Instrument runs fine	(or alarm ....)	Y / N	
Temperatures:	Bench: 15 - 45°C (approx. 5°C above lab temperature)	(.................. °C)	Y /
	Bench Lamp: 50 - 60°C	(.................. °C)	Y /
Pressure:	a few mm Hg below ambient pressure	(.................. mm Hg)	Y /
Flows:	each 0.4 - 1.2 l/Min (Cell A: .... l/Min. / Cell B: .... l/Min.)		Y /
Intensities:	65 000 – 150 000 Hz (Cell A: .... kHz / Cell B: .... kHz)		Y /

Notes: ....

How to do:

Check Alarms, press "ALARM", go back with ► button

Press "DIAGS", go to Temperatures, enter numbers into form above, go back with MAIN MENU button

Go to Pressures, enter number into form above, go back with MAIN MENU button

Go to Flows, enter numbers into form above, go back with MAIN MENU button

Go to Intensities, enter numbers into form above, go back with MAIN MENU button

Go to main screen by pressing ► button

Add a new comment in the elog (e.g. Type "Maintenance", Category "Thermo 49I", Subject "O3 Parameters checked")

- If possible, visually inspect the time series of ozone (and the diagnostic parameters (tperatures, flows, intensities), if available) of the last week on the data acquisition system

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Every week

Zero and Span Check

Date ...., Time (UTC) ...., Operator ....

Zero .... ppb (from .... to .... Time (UTC))

Span (Level1) .... ppb (from .... to .... Time (UTC))

How to do (in case of TE49i instrument with internal ozone generator):

plug in pump of O3 zero air unit

open instrument, check (and adjust of necessary) the pressure to 15 psi

push ► button on front of the instrument, reading on the display (lower left) will change from "Sample" to "Zero"; wait for approximately 20 minutes until the signals stabilizes, write down the measured O3 value

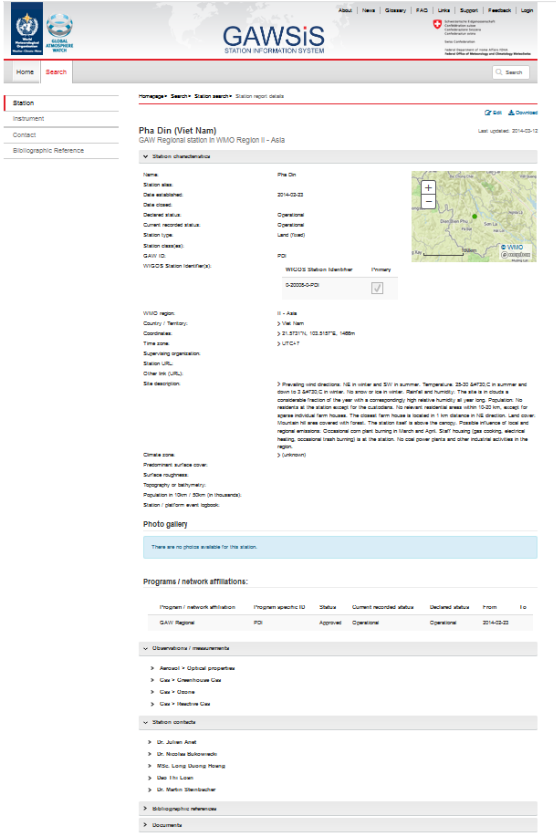
push ► button again, until "Level1" is displayed; wait for 20 minutes, write down the measured value

push ► button again until "Sample" is displayed again, unplug pump of zero air unit

Operation and maintenance

Measurements and beyond

- documentation, log books
- metadata management
- preparation of checklists
- regular station updates in GAWSIS

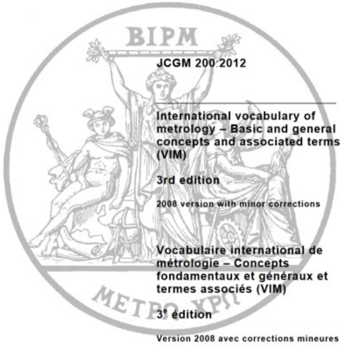


Operation and maintenance

Measurements and beyond

- documentation, log books
- metadata management
- preparation of checklists
- regular station updates in GAWSIS

- use of common terminology



EN DE FR KONTAKT INTRANET LOGIN SEARCH

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OVERVIEW RESEARCH PUBLICATIONS TEAM

Empa > 500 - Mobility, Energy and Environment > 503 - Air Pollution / Environmental Technology > Research > Global Atmosphere Watch > gaw_glossary

Empa > 500 - Mobility, Energy and Environment > 503 - Air Pollution / Environmental Technology > Research > Global Atmosphere Watch > gaw_glossary

WMO/GAW Glossary of QA/QC-Related Terminology

Version 1.0 2010-09-14 (last update: 2016-05-26 (minor changes, see Version history for details))

Editors: J. Klausen, H.-E. Scheel and M. Steinbacher

Table of Contents

Glossary

Alphabetical list of terms

accuracy | adjustment of a measuring system | audit | calibration | calibration curve | calibration hierarchy | Central Calibration Laboratory (CCL) | certified reference material | combined standard measurement uncertainty | concentration | conventional quantity value | conventional reference scale | correction | coverage factor | coverage interval | coverage probability | data quality objectives (DQOs) | definitional uncertainty | expanded measurement uncertainty | indication | input quantity in a measurement model | international system of units | laboratory standard | measurand | measured quantity value | measurement | measurement accuracy | measurement bias | measurement error | measurement guideline (MG) | measuring instrument | measurement precision | measurement procedure | measurement repeatability | measurement reproducibility | measurement result | measurement trueness | measurement standard | measuring system | measurement uncertainty | metrological comparability of measurement results | metrological compatibility of measurement results | metrological traceability | metrological traceability chain | (mass) mixing ratio | (volume) mixing ratio | mole fraction | nominal quantity value | ordinal quantity | output quantity in a measurement model | precision | primary measurement standard | quality assurance | quality control | quantity | quantity value | random measurement error | reference material | reference measurement standard | reference quantity value | reference scale | repeatability condition of measurement | reproducibility condition of measurement | resolution | secondary measurement standard | sensitivity of a measuring system | selectivity of a measuring system | (measurement) standard | standard measurement uncertainty | standard operating procedure (SOP) | standard scale | surveillance cylinder | systematic measurement error | target cylinder (target gas) | tertiary standard | transfer measurement device | travelling measurement standard | true quantity value | Type A evaluation of measurement uncertainty | Type B evaluation of measurement uncertainty | World Calibration Centre (WCC) | working measurement standard | zero adjustment of a measuring system

https://www.empa.ch/web/s503/gaw_glossary

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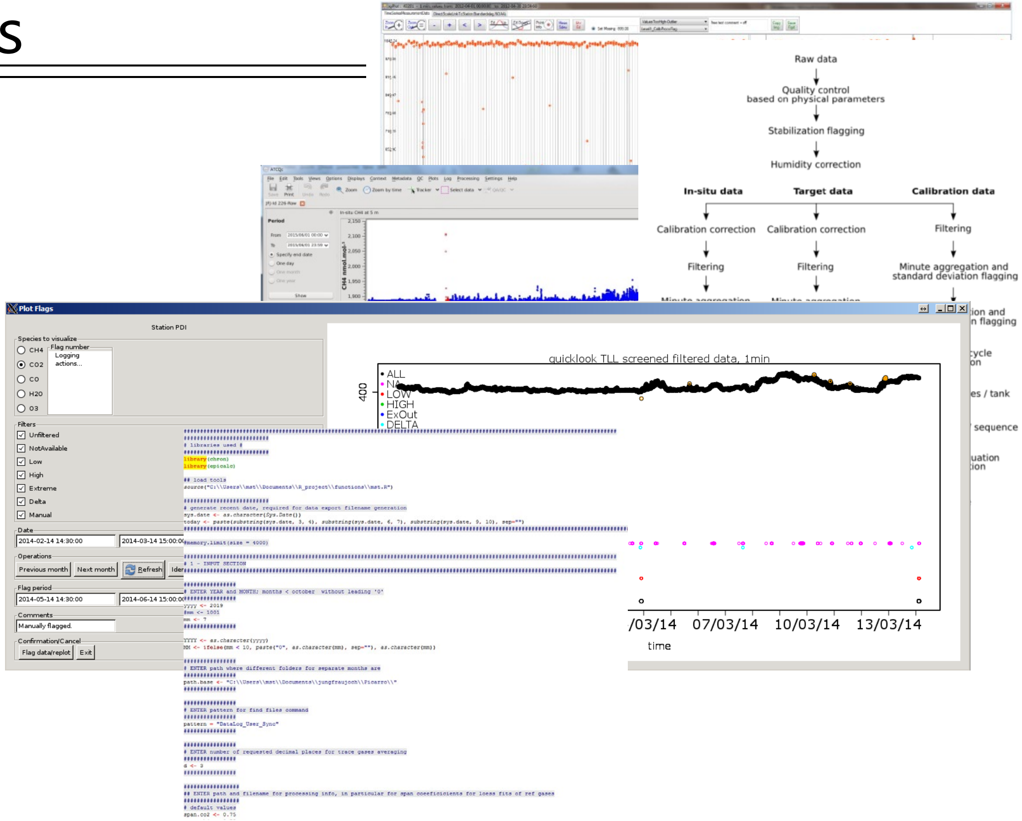
Data handling and analysis

Data processing

- automated procedures are encouraged
- facilitates diagnostics and quality control
- allows for re-processing of the data (e.g. in case of scale changes)



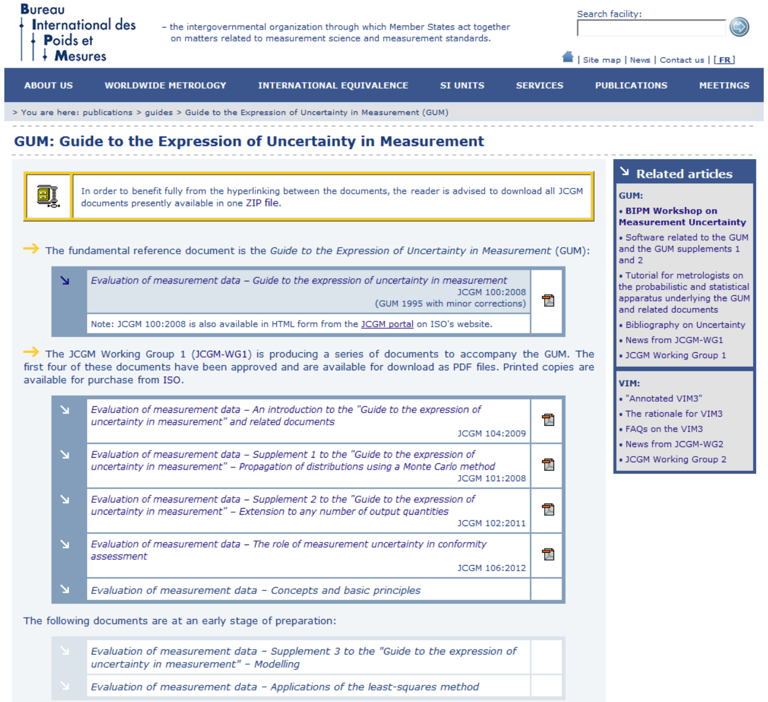
source codes w/o graphical user interface

Data handling and analysis

Data processing

- automated procedures are encouraged
- facilitates diagnostics and quality control
- allows for re-processing of the data (e.g. in case of scale changes)

- estimation of measurement uncertainty



https://www.bipm.org/en/publications/guides/gum.html

Measurement uncertainty – ozone measurements

Table 1 - Example of an uncertainty budget of an ozone analyser

Component (*y*)	Source	Distribution	Contribution to *u(x)*
Imperfect calibration / linearity	Comparison between TS and OA	Rectangular	$0.0017 \cdot x^{*}$
Repeatability	Instrument stability	Rectangular	$0.0016 \cdot x$
Span drift	Instrument stability	Rectangular	$0.0040 \cdot x$
Zero drift	Instrument stability	Rectangular	0.17
Pressure *P*	Pressure measurement	Rectangular	$0.0002 \cdot x$
Temperature *T*	Temp. measurement	Rectangular	$0.0005 \cdot x$
H_2O interference	Interference in the UV		$0.0060 \cdot x$
Other interferences	Interference in the UV		0.6
Sampling loss (Inlet)	Inlet material, dirt	Rectangular	$0.0014 \cdot x$

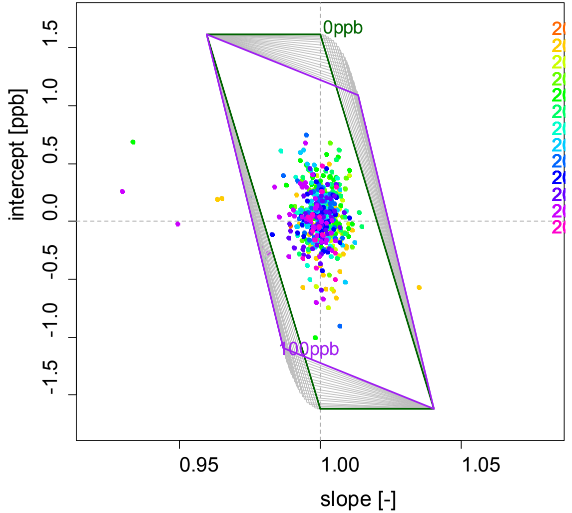
* *where x refers to ozone mole fraction*

A conservative estimate of the total uncertainty can now be obtained by combing the uncertainties of the ozone analyser (13), the transfer standard (12) and the primary reference (11).

$$u(O_3) = \sqrt{(0.81)^2 + (0.0089 \times O_3)^2} \text{ nmol mol}^{-1} \qquad (14)$$

O3 measurement guidelines, GAW Report Nr. 209, 2013

Intercept vs. slope plot for 559 calibrations of various ozone analysers with transfer standards within the Swiss National Air Pollution Monitoring Network between November 2005 and April 2017



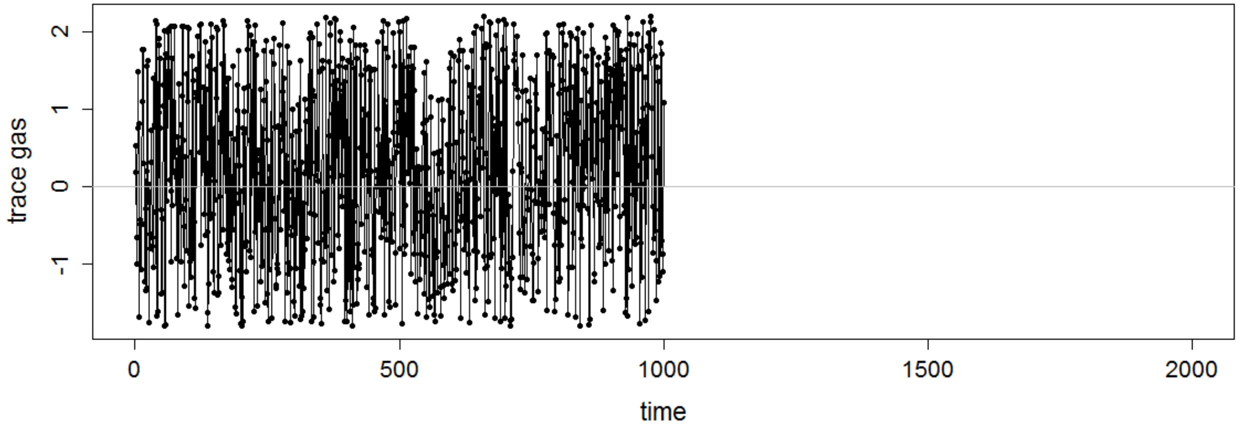
Tarasick et al., 2019, Elemanta

Practical examples

Do not delete negative values

Negative mixing ratios are impossible by definition but are still likely to be recorded by analyzer when the atmospheric levels are lower than the instrumental noise. However, do not delete these numbers as a removal will change the calculated averages.

Low concentrations, noisy analyzer



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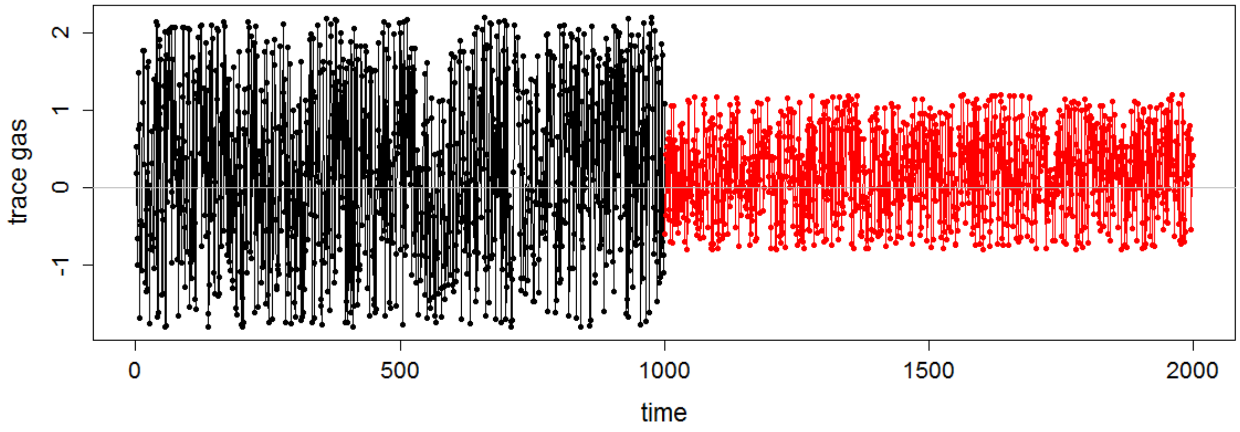
Low concentrations, less noisy analyzer



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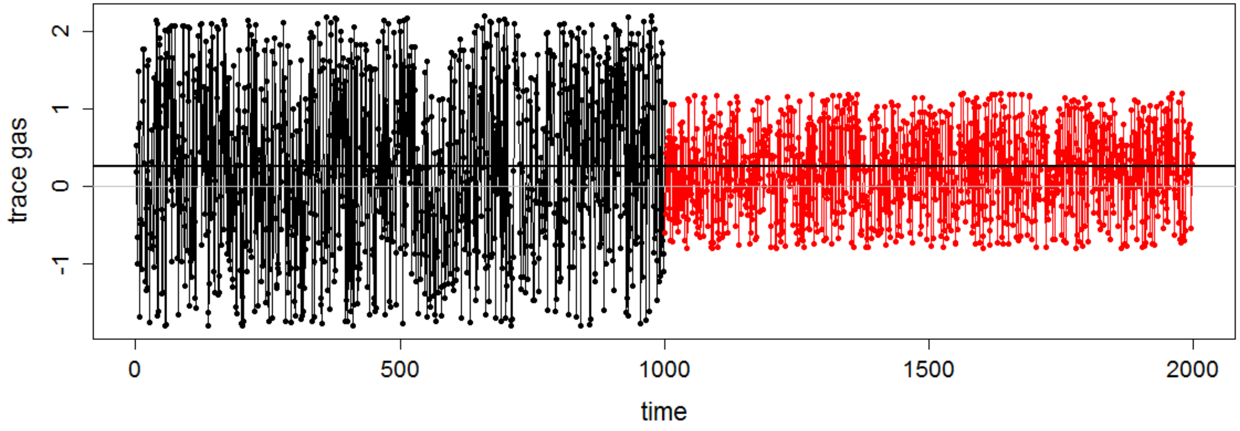

average

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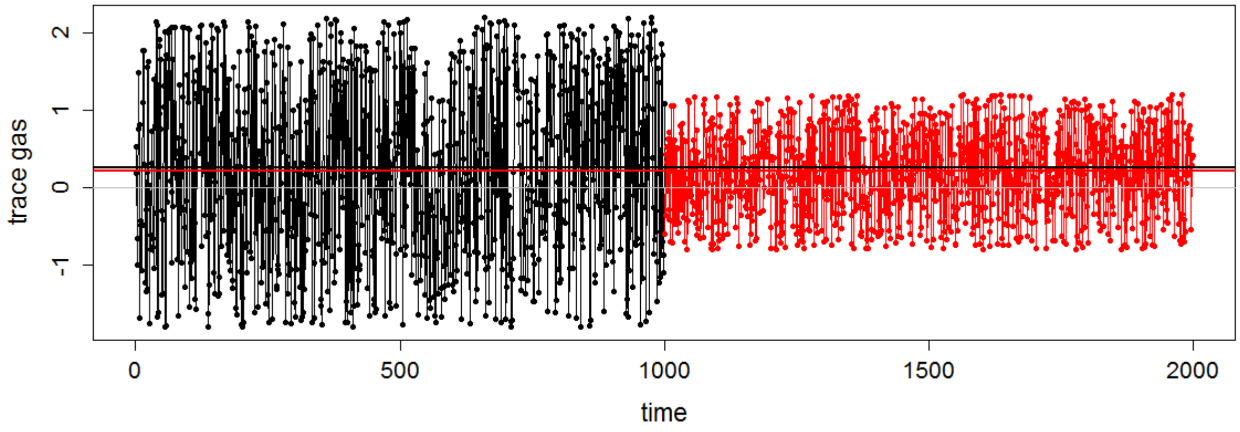

average

average

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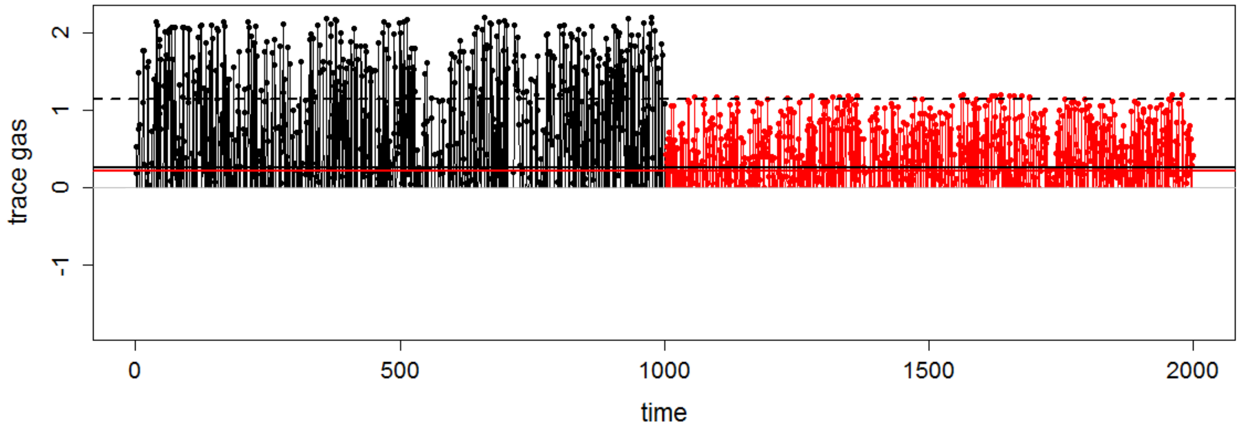

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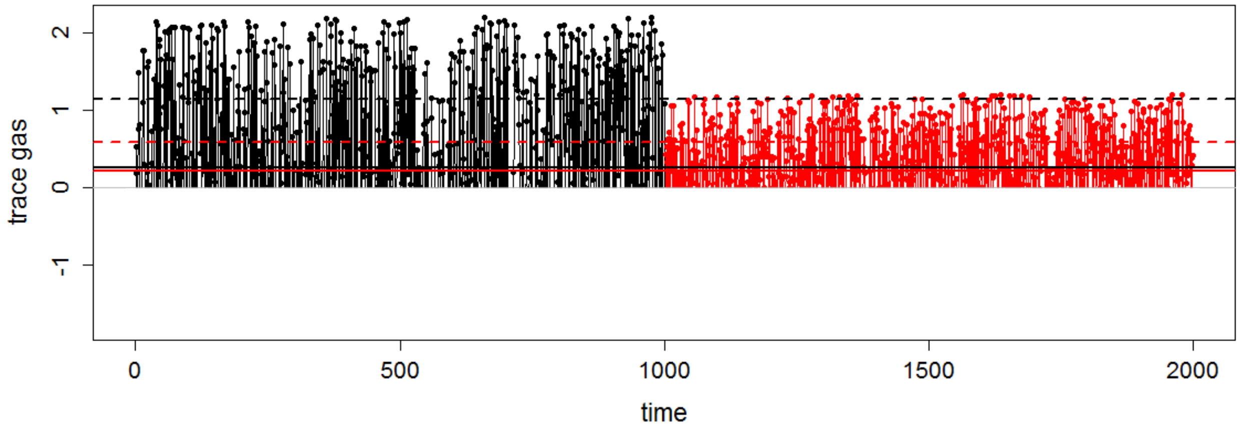


average, > 0 only

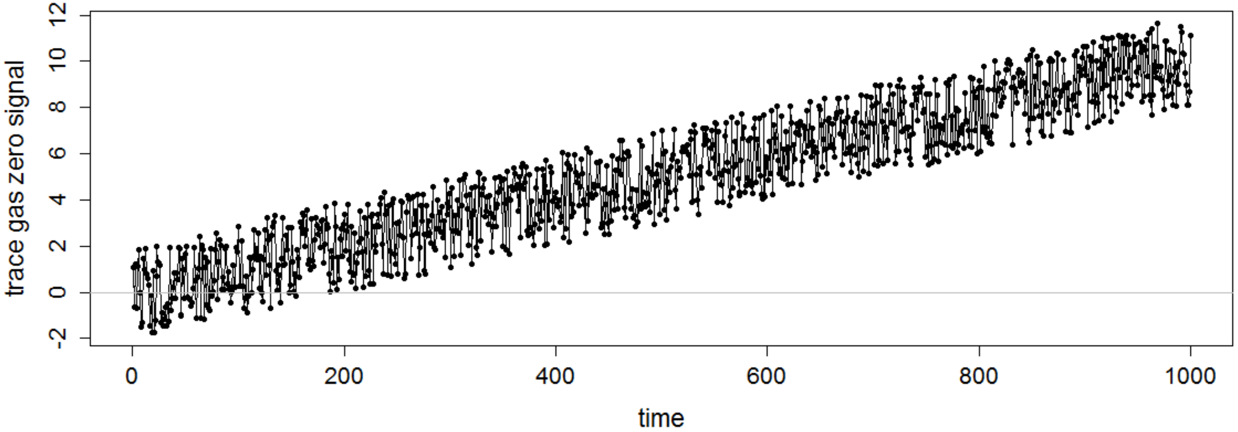
average, > 0 only

average

average

Do not change instrument parameters to often

Assumption: instrument with a changing background signal, determined by analysis of trace gas-free air



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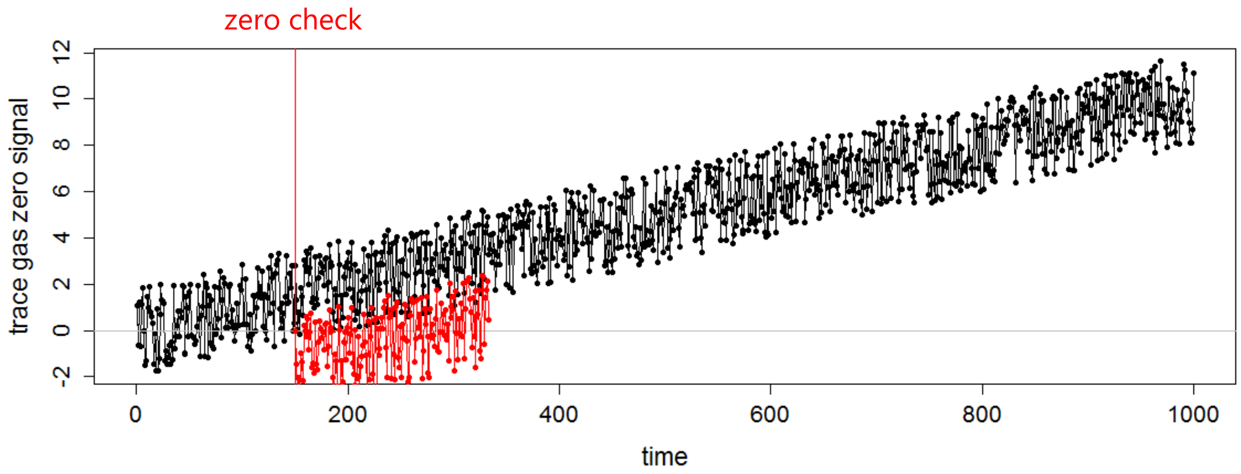

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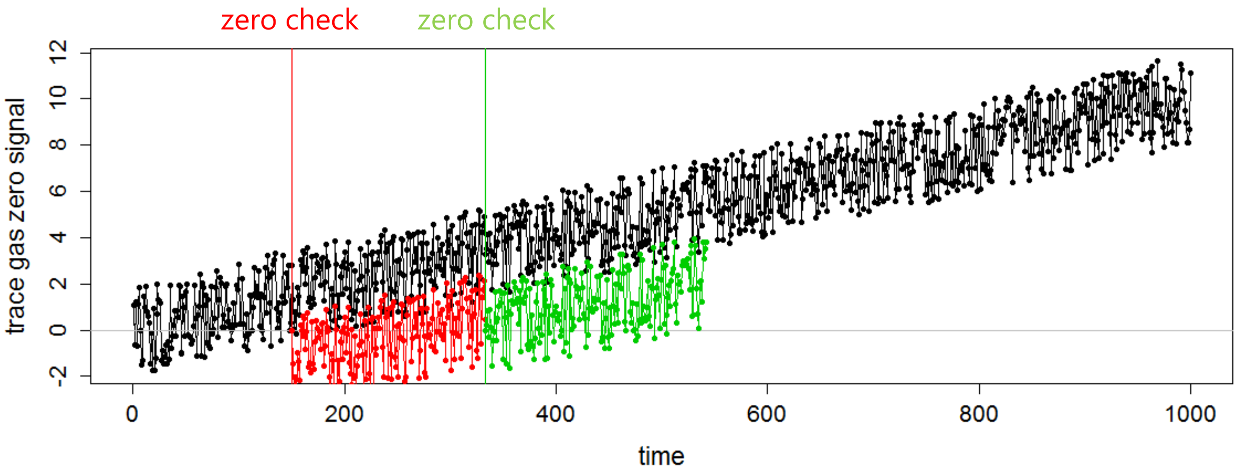

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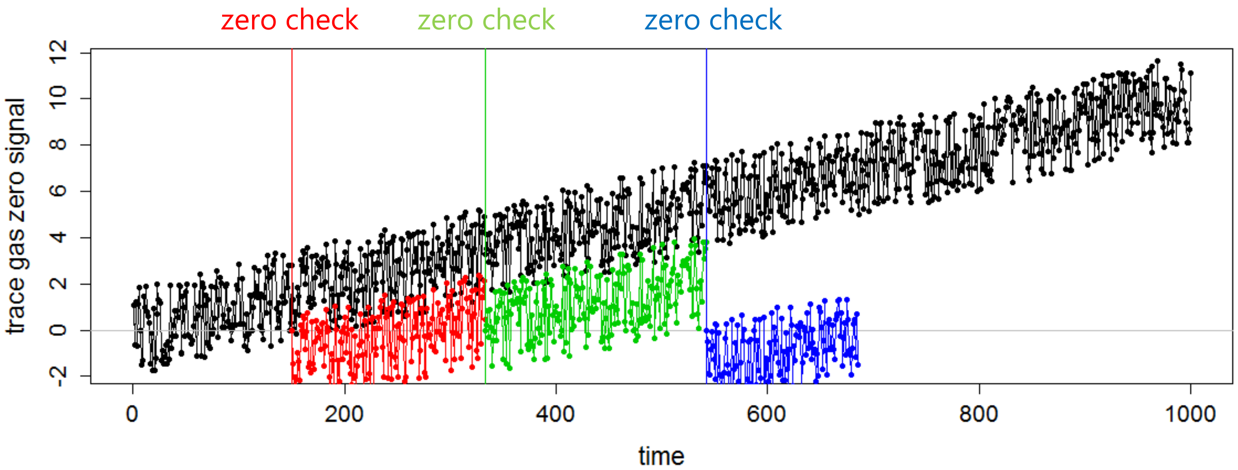

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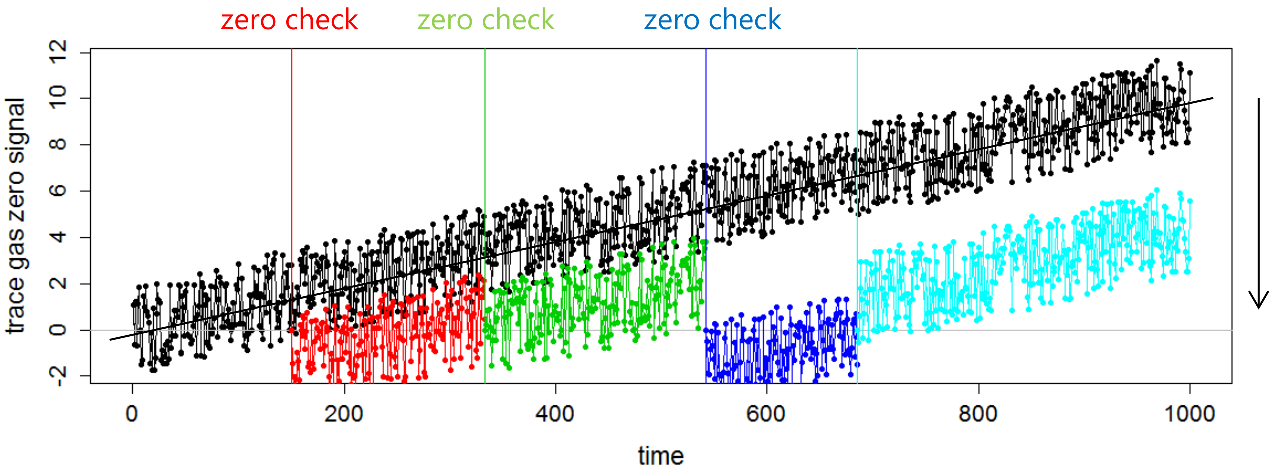


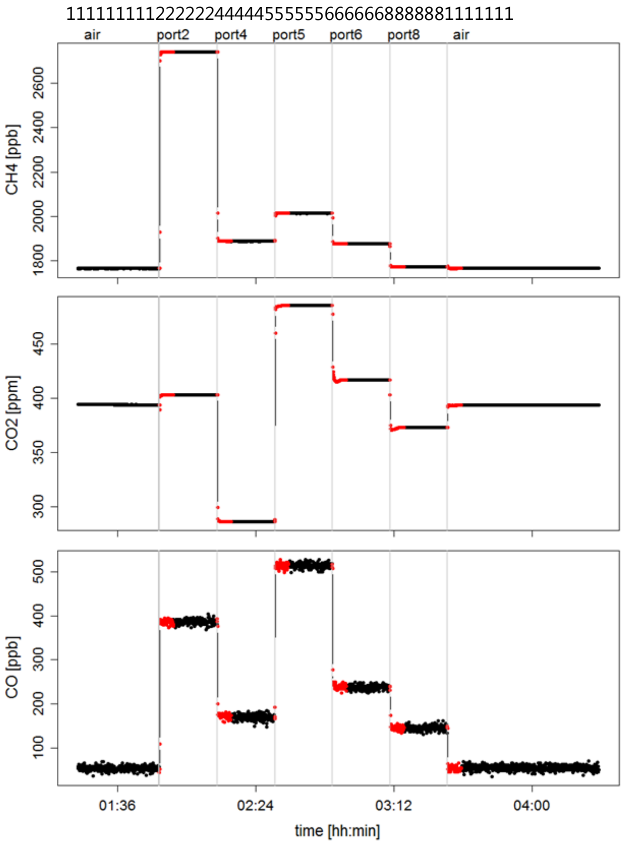
If instrumental parameters will be changed after each calibration, additional noise my be introduced and a reprocessing of the data will become more tedious. Moreover, careful documentation is required.

Alternatively an offline correction may be applied

Flag data after changing the sample type

When changing from ambient air to calibration gas, or from one calibration gas to another, do exclude the first data after the change to account for the transition time until a stable signal is reached.

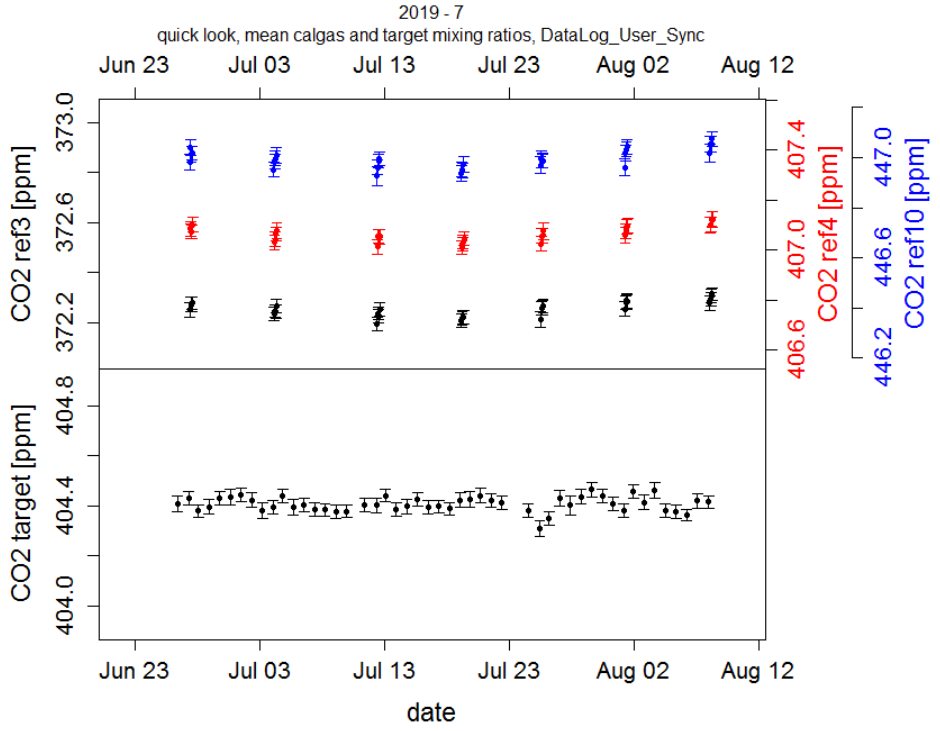
valve position



Use target references

Target reference is a known sample which is considered to be unknown and is treated like an ambient air sample.
Target references do not need to be of the highermost hierarchy, thus, are usually less expensive and can be used up faster. Therefore, more frequent analysis is possible, which will in turn allow fast detection of instrumental artefacts.

Your processing software needs to be able to distinguish individual calibrations (which do all have the same valve position (flag)).



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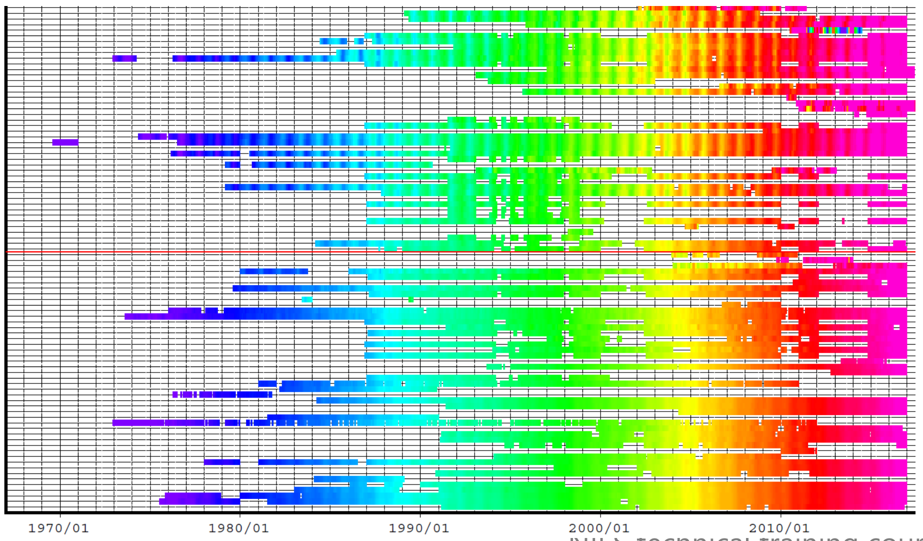
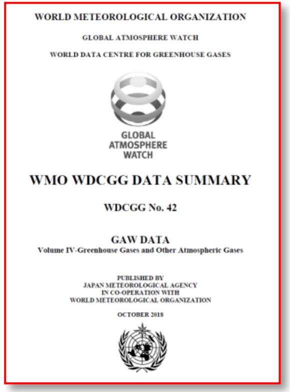
Useful tools for data interpretation

Comparison with other measurements

Additional quality control

- participation in comparison (e.g. round robin) exercises
- comparison of data with data from «similar» stations

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WMO WDCGG DATA SUMMARY

WDCGG No. 42

GAW DATA

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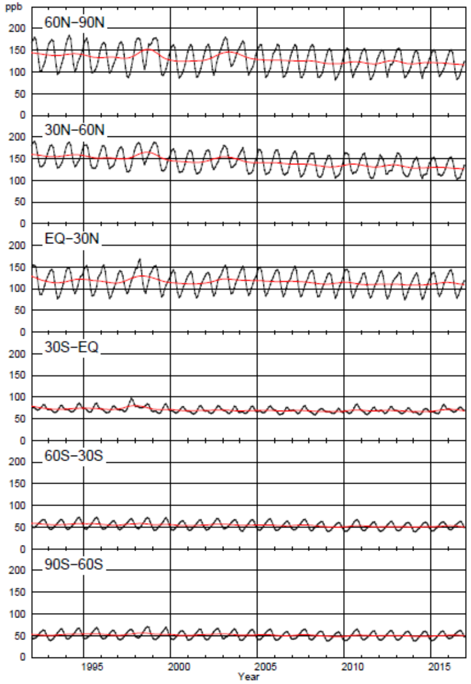


Fig. 7.2 Monthly mean mole fractions of CO from 1992 to 2016 for each 30° latitudinal zone (dots) and their deseasonalized long-term trends (red lines).

source: WDCGG Data Summary 42, 2018
https://gaw.kishou.go.jp/

Comparison with other measurements

Additional quality control

- participation in comparison (e.g. round robin) exercises
- comparison of data with data from «similar» stations

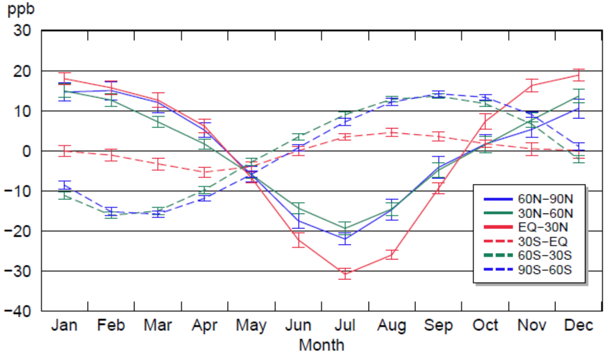
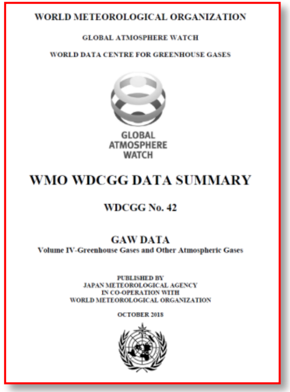


Fig. 4.4 Average seasonal cycles of CH_4 mole fractions for each 30° latitudinal zone obtained by subtracting long-term trends from the zonal mean time series. Vertical error bars represent the range of ±1σ calculated for each month (period 1984 to 2016).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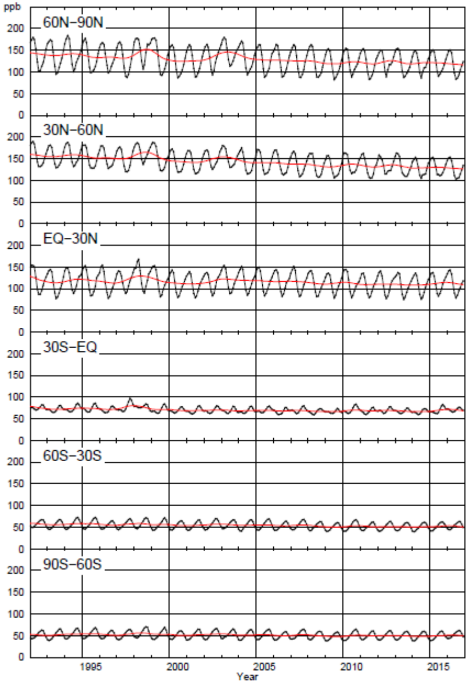

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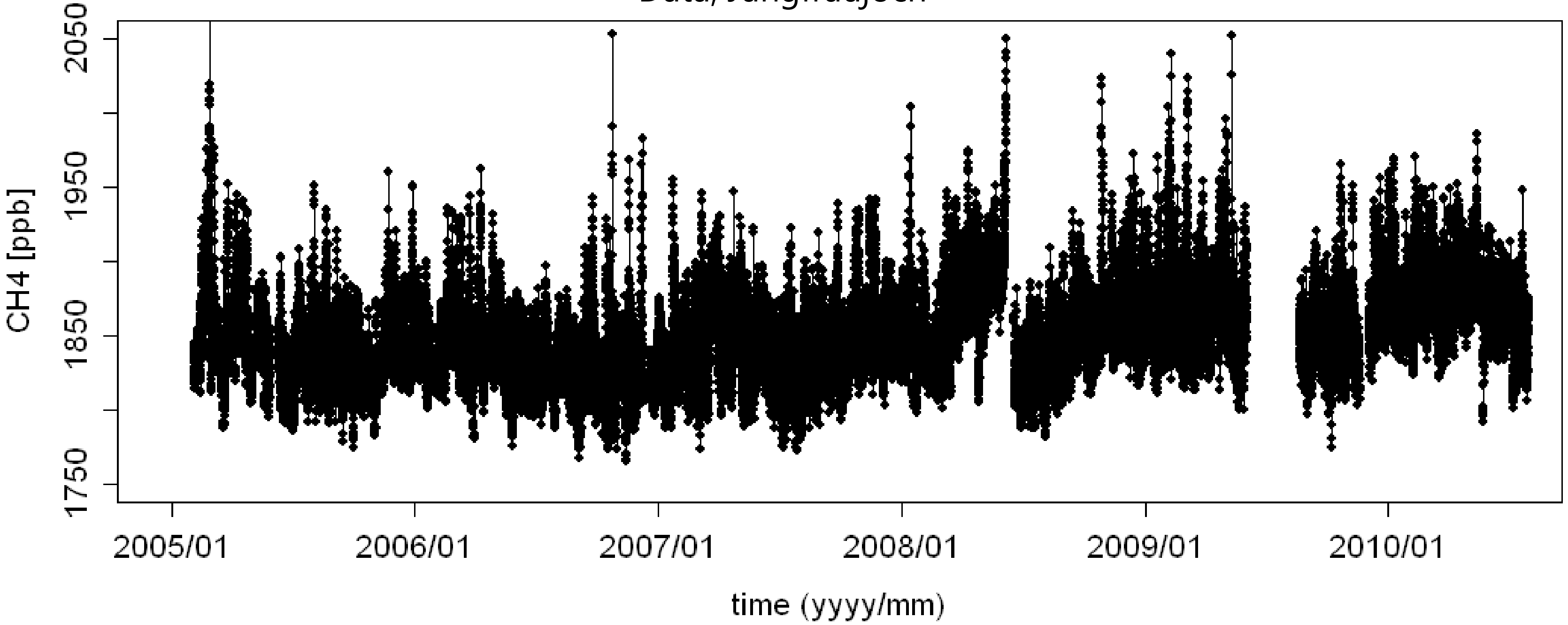
Comparison with other measurements

Data, Jungfraujoch



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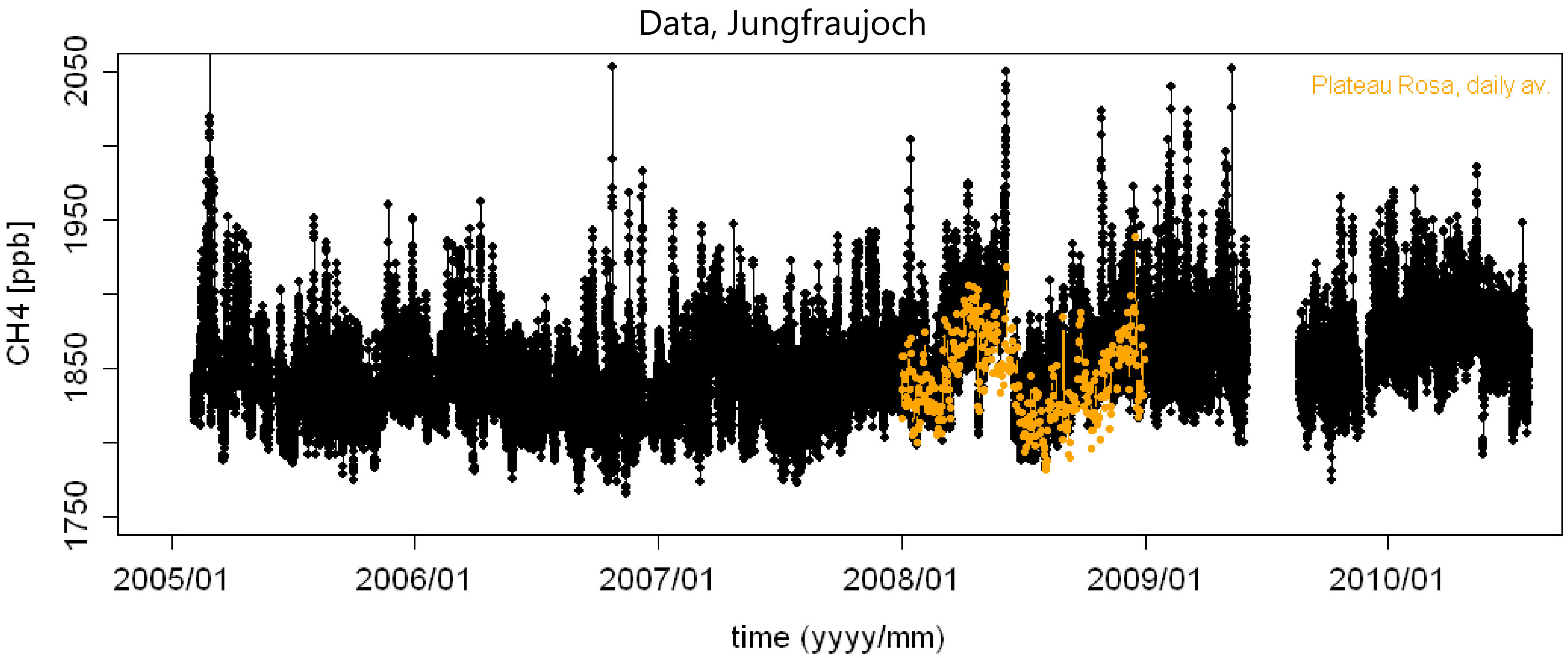
Materials Science and Technology

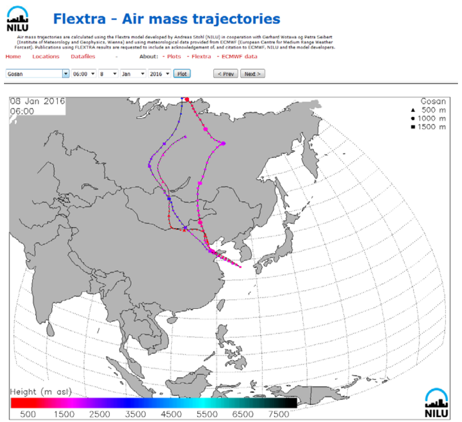
Comparison with other measurements



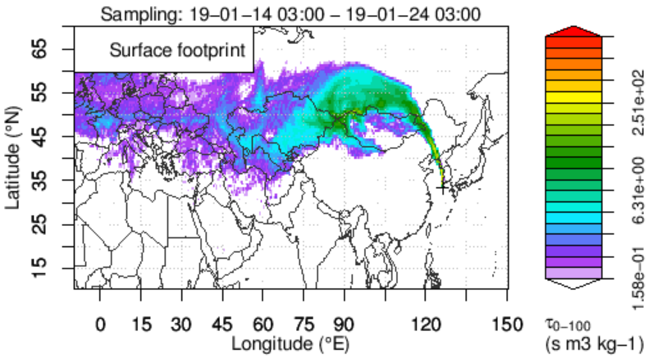
Data handling and analysis

Additional quality control

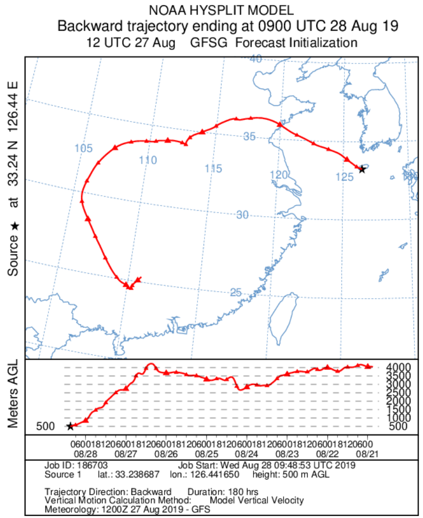
- participation in comparison (e.g. round robin) exercises
- comparison of data with data from «similar» stations
- use available online tools for trajectory calculations, e.g.



https://projects.nilu.no//ccc/

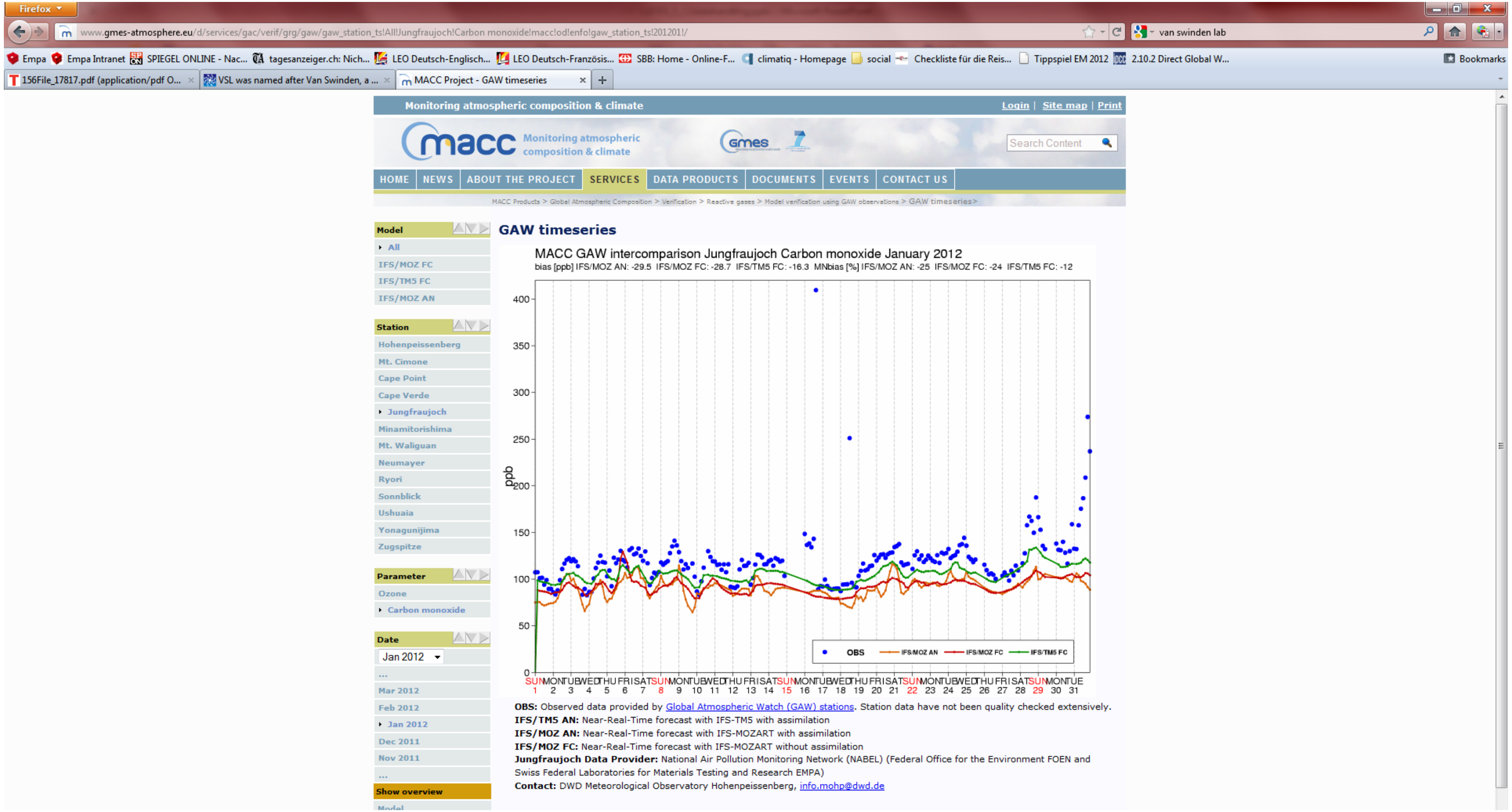


http://lagrange.empa.ch/



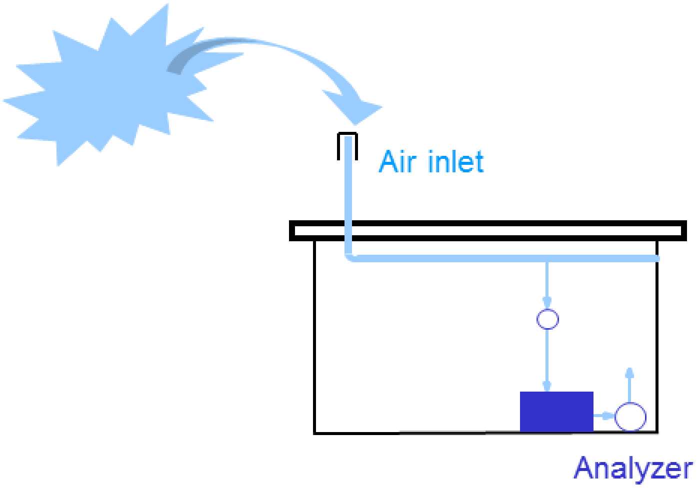
https://ready.arl.noaa.gov/hypub-bin/trajtype.pl

Comparison with and use of models

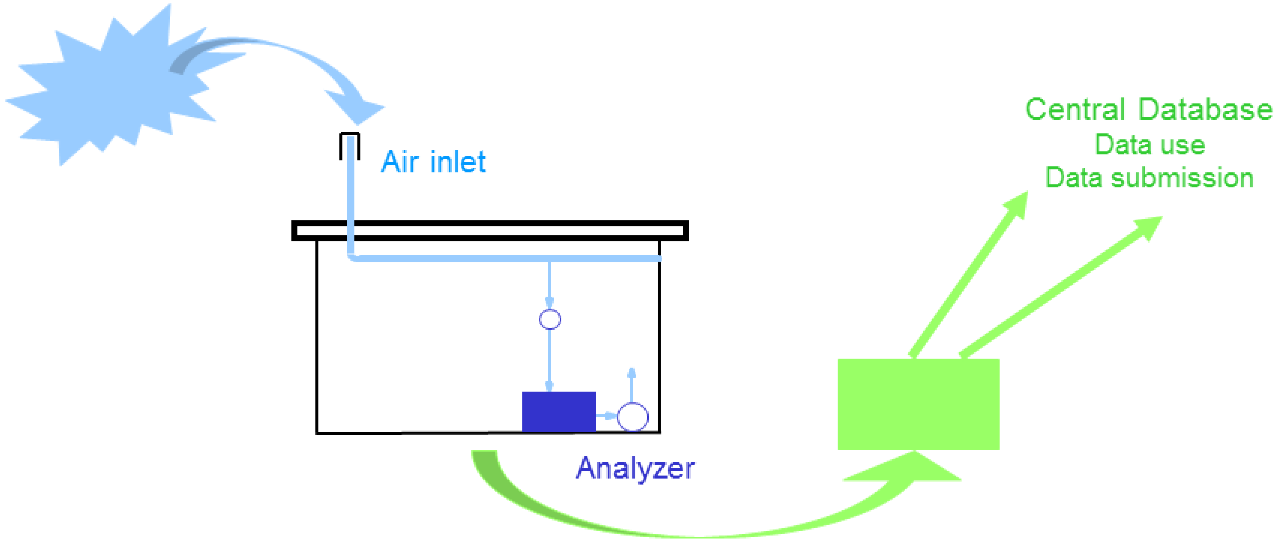


Wrap up

What do we need for in-situ GHG observations?



What do we need for in-situ GHG observations?



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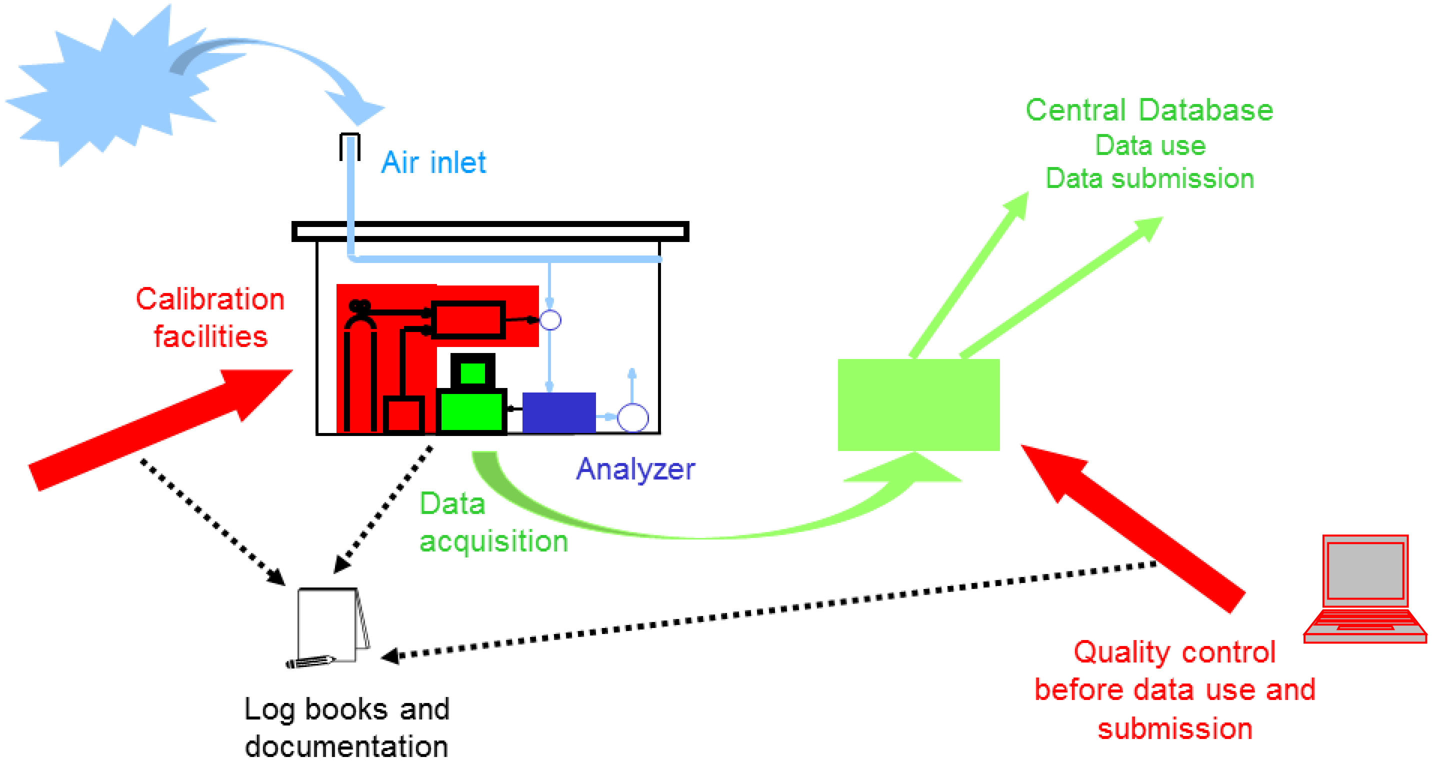

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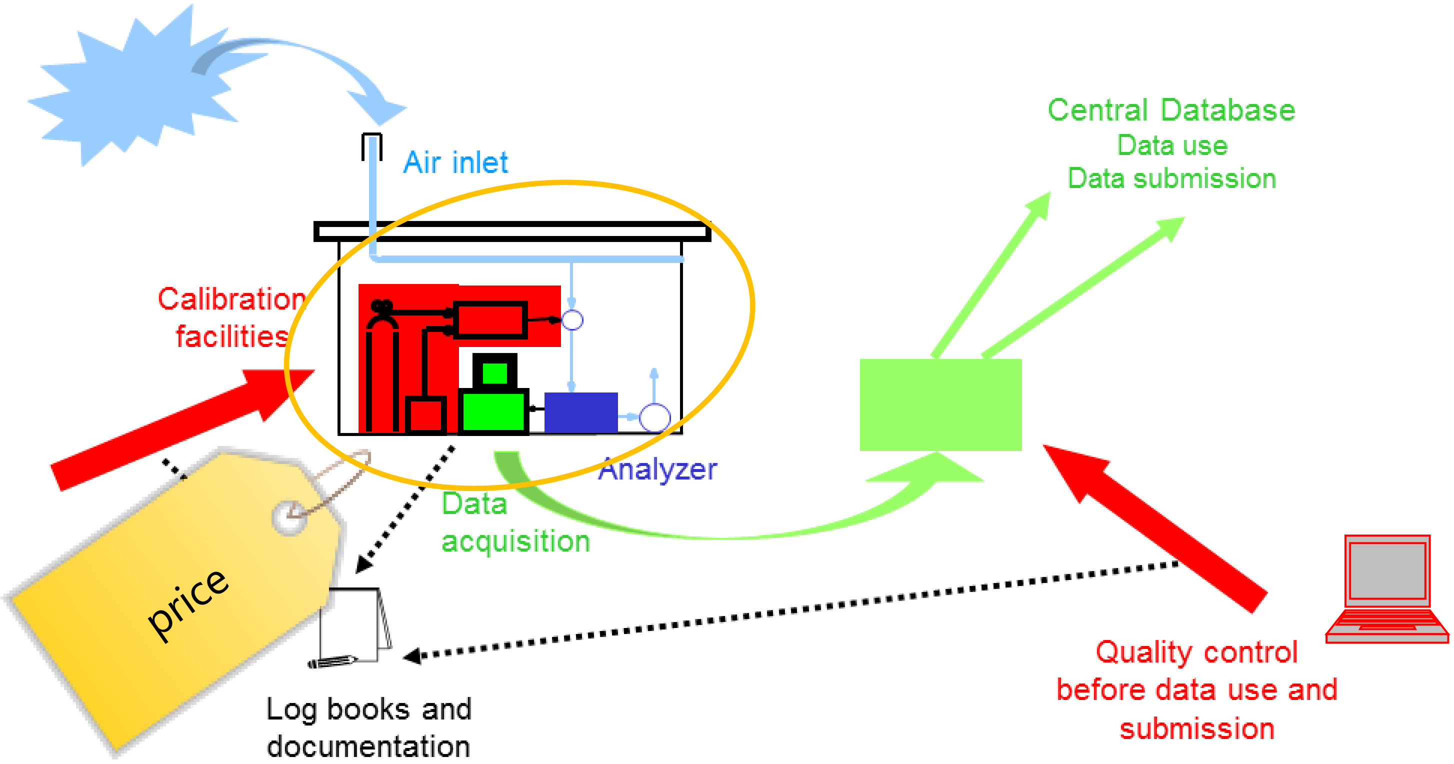

Obstacles


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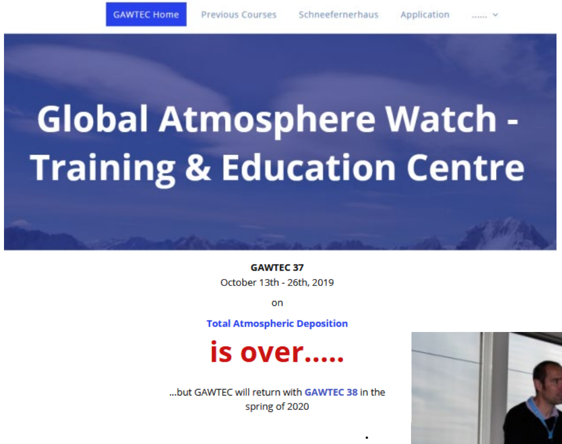
- lack of consumables
- lack of spare parts
- lack of budget, lack of financial authority
- hierarchy issues within the organisation
- (long-term) commitment of the partner
- insufficient know-how
- distance to the headquarters
- unclear responsibilities within an institution and among the partners
- fluctuation in staff
- language barriers
- ...

Conclusions & suggestions

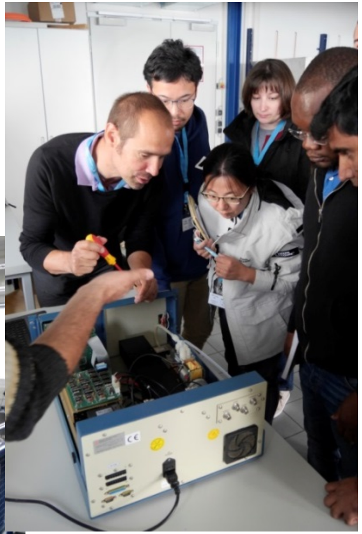
- data sparse regions still exist, new measurements are highly welcome
- a comprehensive quality management framework exists
- a wide range of data from observations and models are available online
  - make use of it !
  - profit from training opportunities and potential collaborations

Training Opportunities



https://www.gawtec.de/

two courses per year



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Conclusions & suggestions

- data sparse regions still exist, new measurements are highly welcome
- a comprehensive quality management framework exists
- a wide range of data from observations and models are available online
  - ➢ make use of it !
  - ➢ profit from training opportunities and potential collaborations
- need for more catchy information (like tick lists) is identified

You need:

✓ shelter	✓ instrument
✓ power	✓ cal gases
✓ A/C	✓ calibrator
✓ internet	✓ plumbing
✓ …	✓ …

- e.g., new CO_2 measurement guidelines are in preparation