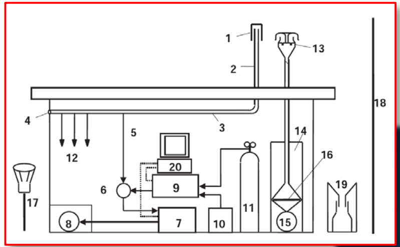
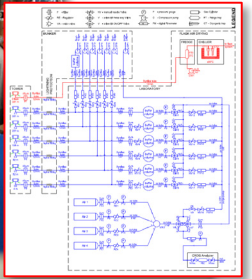
The Importance of Quality Assurance and Quality Control for long-term in-situ atmospheric composition observations

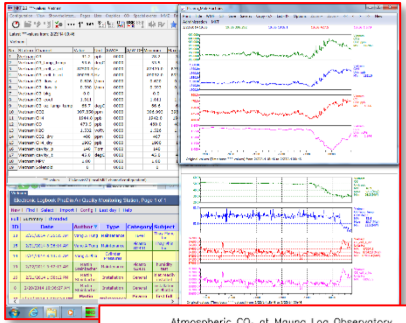


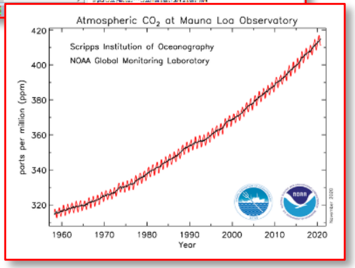
design & station setup

Winderlich et al., AMT; 2010



instrumentation & operation





data management & data processing

Martin Steinbacher

Empa, Laboratory for Air Pollution / Environmental Technology &
WMO/GAW Quality Assurance / Science Activity Centre Switzerland

GAWTEC webinar, 07 December 2020

GAW
Global Atmosphere Watch
QA / SAC Switzerland

Empa
Materials Science and Technology

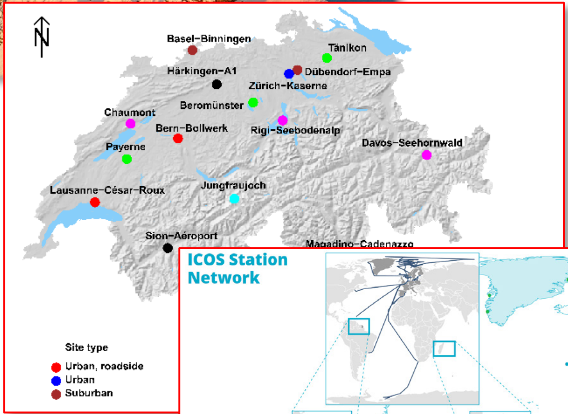
About me

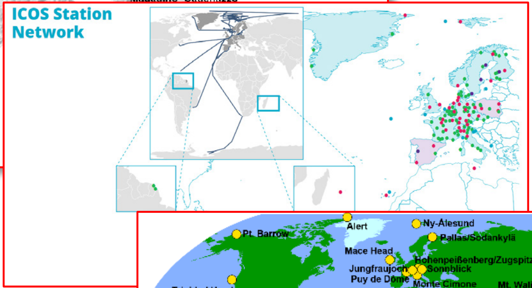
- meteorologist (University of Frankfurt, Germany)
- 2001 – 2004 PhD Fellow at the Laboratory of Atmospheric Chemistry, Paul Scherrer Institute, Villigen, Switzerland
- 2004: PhD in Atmospheric Chemistry at ETH in Zurich
- since 2004: Scientist at Laboratory for Air Pollution / Environmental Technology, Empa, Duebendorf, Switzerland
    - Principal operator of the air quality observations within the Swiss National Air Pollution Monitoring Network at the GAW site Jungfraujoch
    - Manager of WMO/GAW Quality Assurance/Science Activity Centre Switzerland
    - Chair of the Atmospheric Monitoring Station Assembly of the Integrated Carbon Observation System

WMO OMM

GAW

Global Atmosphere Watch
QA / SAC Switzerland





observations in Switzerland as part of national, European and global programmes

support of observations in data sparse regions

supported by

Schweizerische Eidgenossenschaft
Confédération suisse
Confederazione Svizzera
Confederaziun svizra

Federal Office of Meteorology and Climatology MeteoSwiss

WMO OMM

GAW
Global Atmosphere Watch
QA / SAC Switzerland

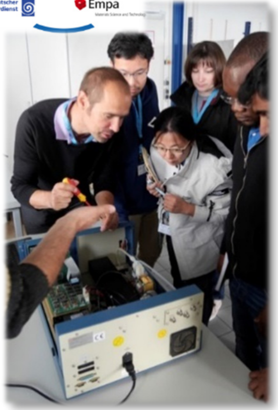


training & capacity building is an integral part of QA/SAC CH

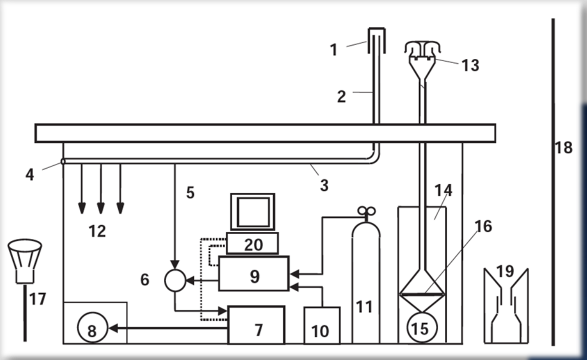


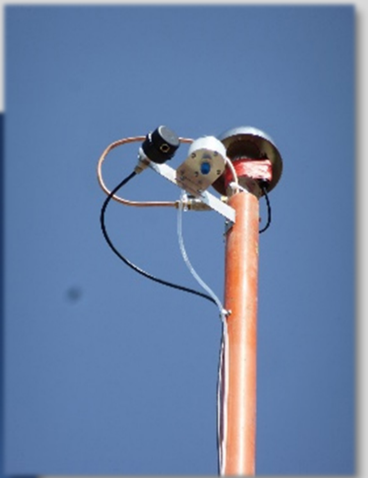
Umwelt Bundesamt
GAW Training & Education Centre
GAW
Deutscher Wetterdienst
Empa



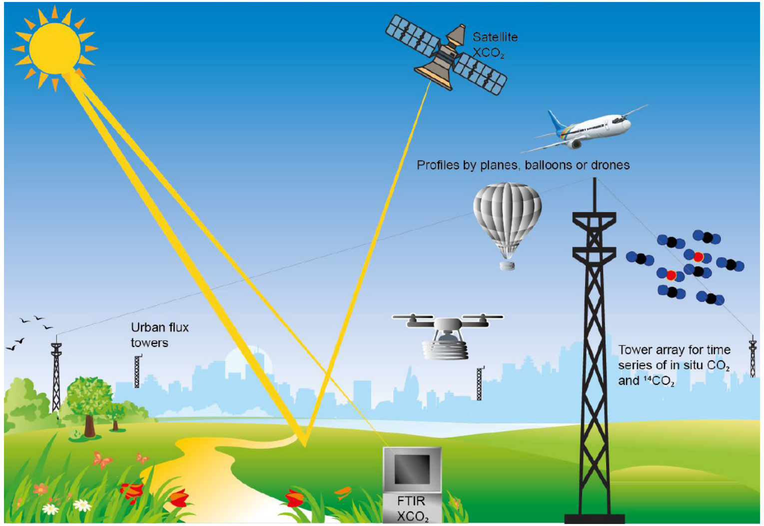
Design & setup





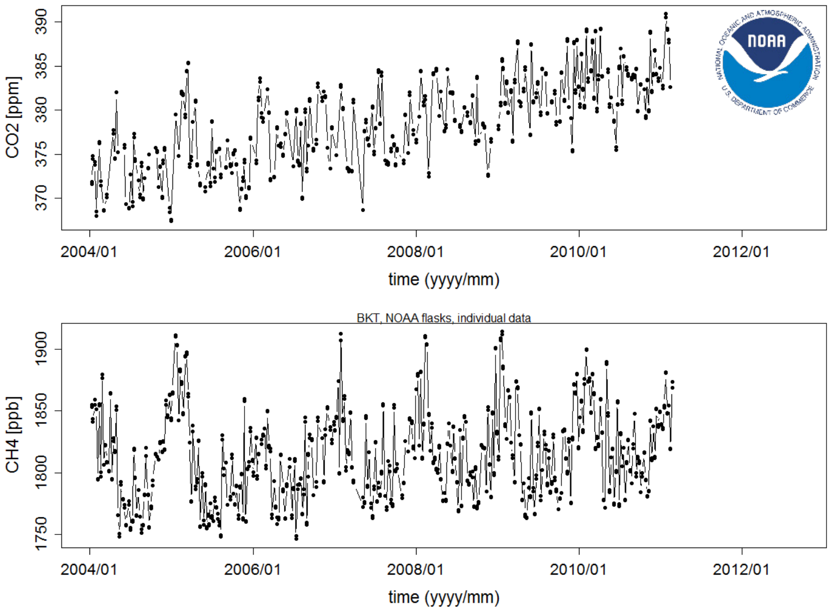
Fundamental questions

- Why do I want/need to measure?
- Which compounds are of interest?
  (gaseous compounds, particulates, deposition, meteorological parameters)
- Where are measurements reasonable?
  (e.g., representativeness of the sample, avoid influence of undesirable sources)
- What kind of data series are needed?
  (continuous, discrete, time resolution, concentration range, spatial resolution, stationary vs. mobile, etc.)



Discrete (flasks) vs. continuous observations

greenhouse gas observations
through flask sampling and in-situ monitoring



Discrete (flasks) vs. continuous observations

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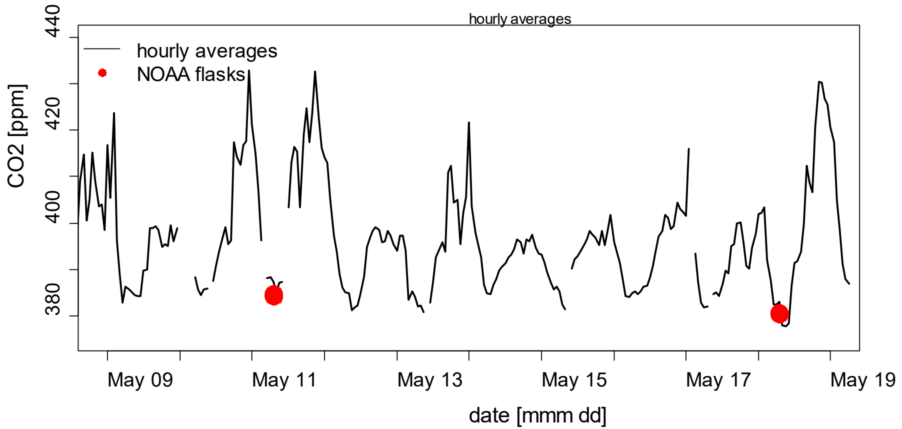
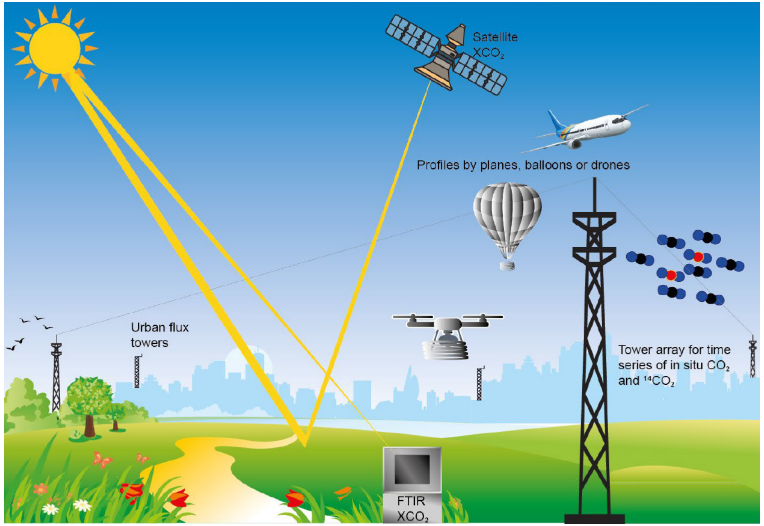


- long-term flask observations suitable for trend estimates
- continuous measurements allow gaining insight into local to regional processes

Fundamental questions

- Why do I want/need to measure?
- Which compounds are of interest?
  (gaseous compounds, particulates, deposition, meteorological parameters)
- Where are measurements reasonable?
  (e.g., representativeness of the sample, avoid influence of undesirable sources)
- What kind of data series are needed?
  (continuous, discrete, time resolution, concentration range, spatial resolution, stationary vs. mobile, etc.)
- When is the right time to measure?
  (e.g., annual or diurnal cycles of compounds, during special weather conditions, …)

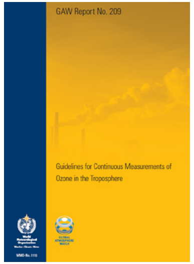


here: focus on ground-based in-situ observations

Infrastructure Requirements

Measurement site infrastructure

- shelter
- reliable power supply
- air conditioning
- internet access
- mast for free exposure of the inlet



O3 measurement guidelines, GAW Report Nr. 209, 2013

"The laboratory building and inlet location on site should be set upwind of any other buildings, garages, parking lots, generators, other emission sources – any nearby areas where fossil fuels or biomass may be combusted and where intensive agriculture is undertaken."

Special attention also needs to be paid when performing measurements in heavily vegetated environments (due to influence of biospheric uptake and respiration on the CO_2 levels)

Infrastructure Requirements

Measurement site infrastructure

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

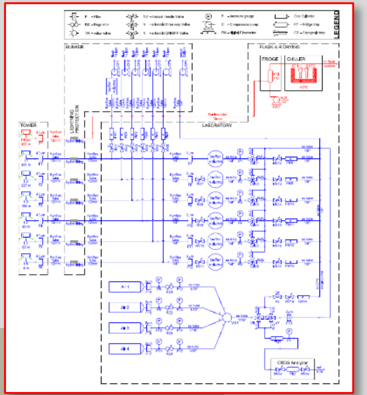
Instrument(s) and periphery

- adequate 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, …

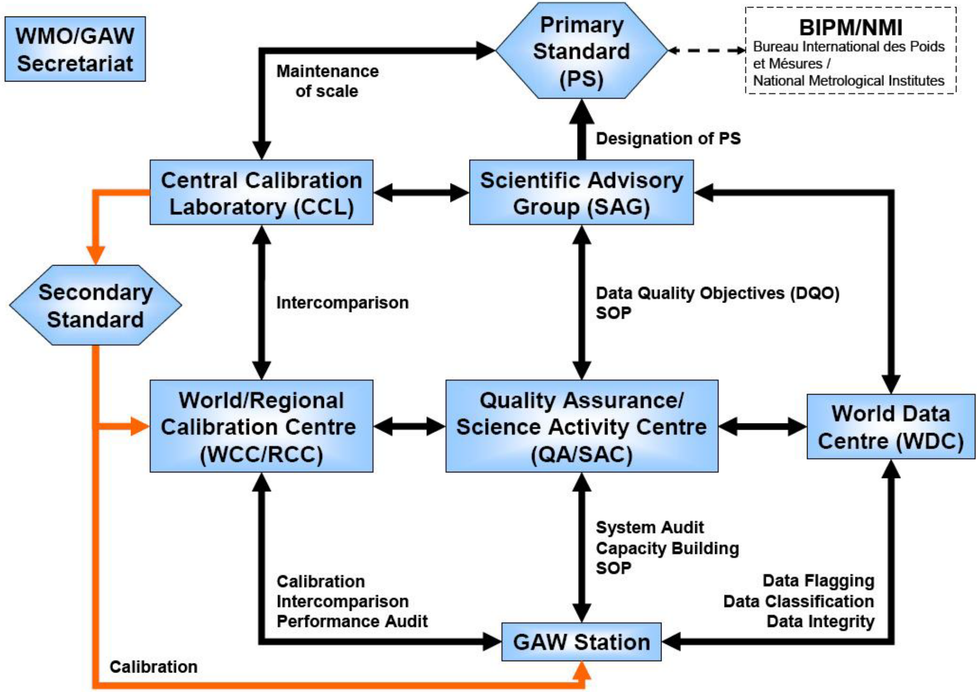
Instrumentation & operation

Winderlich et al., AMT; 2010



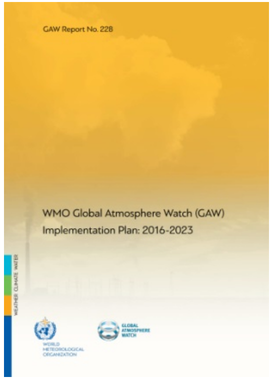
GAW Quality Management Framework

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



map of GAW stations

https://gawsis.meteoswiss.ch

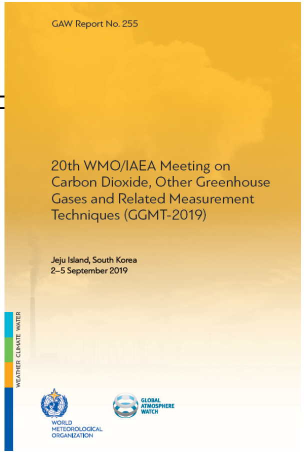


GAW Implementation Plan 2016-2023,
GAW Report Nr. 228, 2017

Instrumentation – required quality, example CO2

Table 1. Recommended network compatibility of measurements within the scope of WMO/GAW

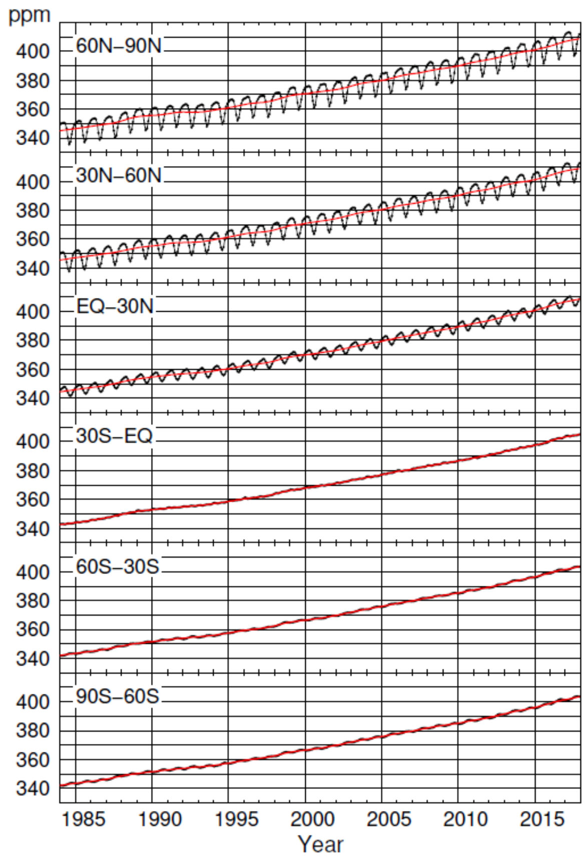
Component	*Network compatibility goal*[1]	*Extended network compatibility goal*[2]	*Range in unpolluted troposphere (approx. range for 2019)*	*Range covered by the WMO scale*
CO_2	0.1 ppm (NH) 0.05 ppm (SH)	0.2 ppm	380 - 450 ppm	250 – 520[3] ppm
CH_4	2 ppb	5 ppb	1750 – 2100 ppb	300 – 5900 ppb
CO	2 ppb	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	9 – 11 ppt	2.0 – 20 ppt
H_2	2 ppb	5 ppb	400 – 600 ppb	140 –1200 ppb
$\delta^{13}C\text{-}CO_2$	0.01‰	0.1‰	-9.5 to -7.5‰ (VPDB)	
$\delta\,^{18}O\text{-}CO_2$	0.05‰	0.1‰	-2 to +2‰ (VPDB-CO_2)	
$\delta\,^{13}C\text{-}CH_4$	0.02‰	0.2‰	-51 to -46‰ (VPDB)	
$\delta\,^{2}H\text{-}CH_4$	1‰	5‰	-120 to -63‰ (VSMOW)	
$\Delta^{14}C\text{-}CO_2$	0.5‰	3‰	-80 to 20‰	
$\Delta\,^{14}C\text{-}CH_4$	0.5‰		50-350‰	
$\Delta\,^{14}C\text{-}CO$	2 molecules cm^{-3}		0-25 molecules cm^{-3}	
O_2/N_2	2 per meg	10 per meg	-900 to -400 per meg (vs. SIO scale)	



GGMT-2019 Report,
GAW Report Nr. 255, 2020

"… The WMO/GAW network compatibility are the scientifically-determined maximum bias among monitoring programmes that can be included without significantly influencing fluxes inferred from observations with models. …"

Instrumentation – required quality, example CO2



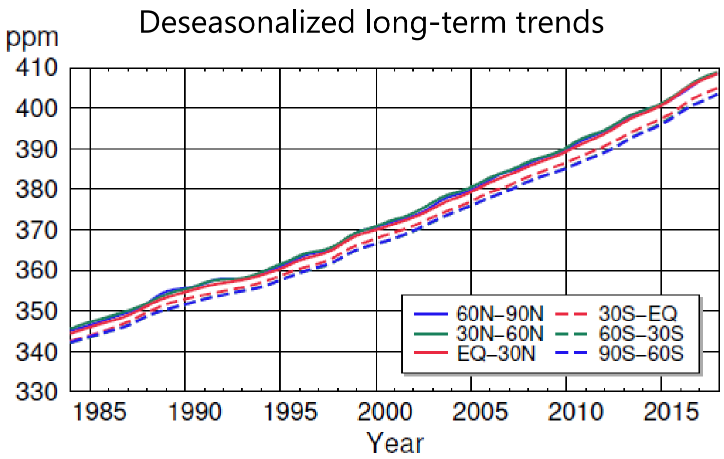
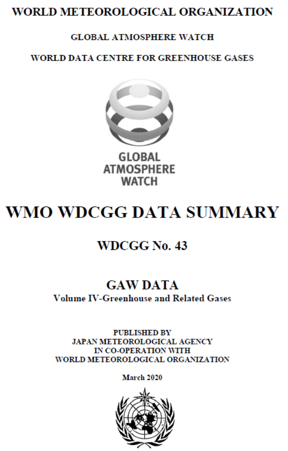


Fig. 1.3 Monthly mean mole fractions of CO_2 from 1984 to 2017 averaged over each 30° latitudinal zone (black) and their deseasonalized long-term trends (red).


WORLD METEOROLOGICAL ORGANIZATION

GLOBAL ATMOSPHERE WATCH

WORLD DATA CENTRE FOR GREENHOUSE GASES

GLOBAL ATMOSPHERE WATCH

WMO WDCGG DATA SUMMARY

WDCGG No. 43

GAW DATA

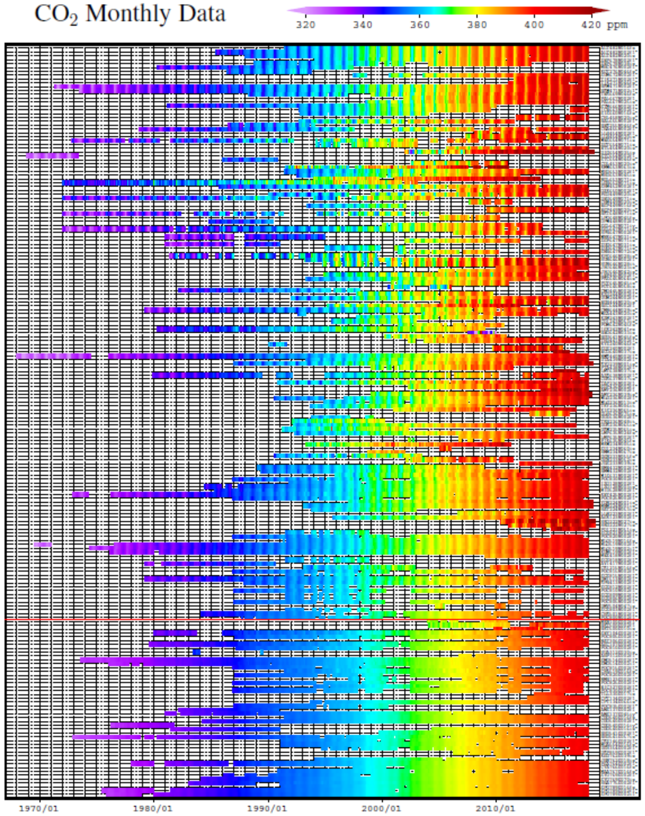
Volume IV-Greenhouse and Related Gases

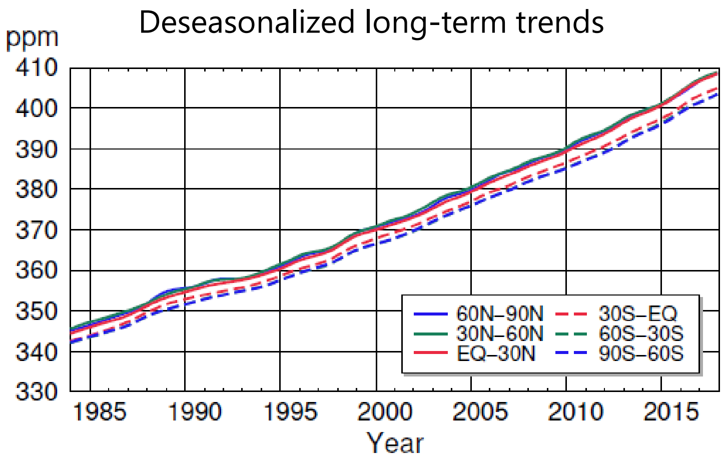
PUBLISHED BY
JAPAN METEOROLOGICAL AGENCY
IN CO-OPERATION WITH
WORLD METEOROLOGICAL ORGANIZATION

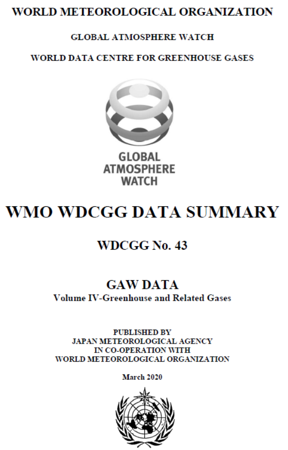
March 2020

WDCGG Data Summary
Report #43, 2020

Instrumentation – required quality, example CO2






WORLD METEOROLOGICAL ORGANIZATION

GLOBAL ATMOSPHERE WATCH

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WMO WDCGG DATA SUMMARY

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JAPAN METEOROLOGICAL AGENCY
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March 2020

WDCGG Data Summary
Report #43, 2020

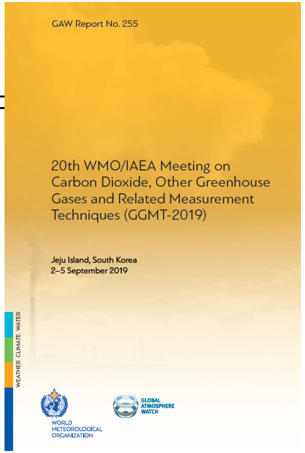
- compatibility goals mainly motivated by small spatial gradients

Plate 1.1 Monthly mean CO_2 mole fractions that have been reported to the WDCGG.

Empa
Materials Science and Technology

Instrumentation – required quality, example CO_2

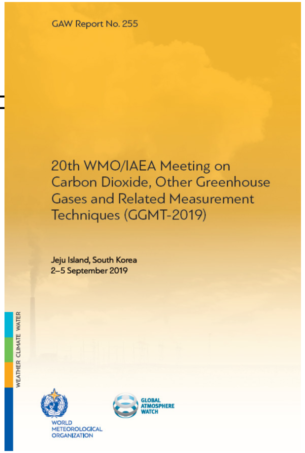
"… To achieve the required levels of network compatibility (see Table 1) it is important to understand and carefully consider the design of the whole analysis system including instrument, gas handling, calibration and data management. No single instrument type is recommended. Many can be used with equal success and none are fool proof when poor choices are made with gas handling or data management. A trade-off in instrument stability and complexity versus cost must often be balanced according to the needs, resources and challenges of the measurement programme. …"



GGMT-2019 Report,
GAW Report Nr. 255, 2020

Instrumentation – required quality, example CO_2

"… To achieve the required levels of network compatibility (see Table 1) it is important to understand and carefully consider the design of the whole analysis system including instrument, gas handling, calibration and data management. No single instrument type is recommended. Many can be used with equal success and none are fool proof when poor choices are made with gas handling or data management. A trade-off in instrument stability and complexity versus cost must often be balanced according to the needs, resources and challenges of the measurement programme. …"



GGMT-2019 Report, GAW Report Nr. 255, 2020

Instrumentation – required quality, example tropospheric O3

Table 12: Scientific tasks, goals, and requirements for future tropospheric ozone monitoring. DOI: https://doi.org/10.1525/elementa.376.t12

Scientific task or question	Goals and Requirements	Station location	Comment
Long-term tropospheric ozone monitoring	Detection of long-term ozone distribution changes, ozone transport changes. Need decadal stability of ~1 nmol mol^{-1}. Vertical profiling important.	Multiple sites in different regions and land use classifications. Choice of sites should be guided by objectively quantified station spatial representativeness.	Current global network is unevenly distributed and covers only ~25% of the globe (*TOAR-Surface ozone database*). Sites with long-term records are very important.
Air quality model validation	Moderate accuracy and precision, preferably 3–5% level. Need vertical resolution of ~0.2 km or better. Need hourly time resolution, at least for short (campaign) periods. Flux measurements.	Multiple sites in different regions. Choice of sites should be guided by objectively quantified station spatial representativeness. Collocated profile measurements of other species desirable. Sites with multi-year data records are of value for background climatology.	Measurement campaigns at multiple sites are desirable. Measurements of surface deposition fluxes for different environments are needed (Hardacre et al., 2015; Bariteau et al., 2010; Luhar et al. 2017, 2018).
Chemical data assimilation	Moderate accuracy and precision, preferable 3–5% level. Vertically-resolved measurements desirable. Daily or better time resolution.	Many sites in different regions. Choice of sites should be guided by objectively quantified site spatial representativeness. Satellite, surface monitor, aircraft data.	Can we increase the impact of sparse measurements? Aircraft, lidar, ozonesondes have small measurement errors, relative to model error. Data impact should therefore be significant.
Satellite ozone data validation	High accuracy and high precision, preferably 2–3% level. Profile (free tropospheric) information required.	Location should represent different observational conditions (latitude, ozone profiles, etc.) and preferably have related measurements (surface O_3, total O_3, aerosol)	Data quality of prime importance; periodic re-evaluation needed.
How do ozone levels in the free troposphere affect levels in the planetary boundary layer (PBL)?	Measurement campaigns with vertical sounding at a resolution down to a few hours – lidar, satellite, sonde and other met measurements, possibly at multiple sites.	Sites in different latitude bands. Sites with multi-year measurement records are of value for background climatology. More sites at lower latitudes.	Important to interpreting satellite measurements, which are primarily sensitive to ozone above the PBL (Crawford and Pickering, 2014; Martins et al. 2015).

Tarasick et al., 2019

Instrumentation – useful resources

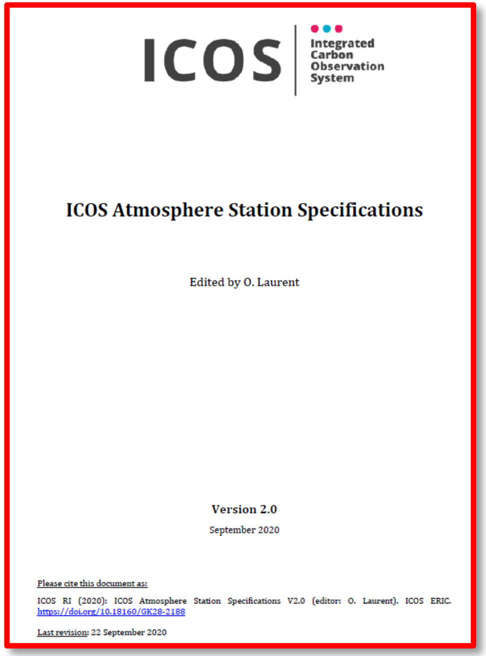
Useful resources:

- WMO/GAW reports
- measurement guidelines

Instrumentation – useful resources

Useful resources:

- WMO/GAW reports
- measurement guidelines
- project reports, webpages



ICOS Integrated Carbon Observation System

ICOS Atmosphere Station Specifications

Edited by O. Laurent

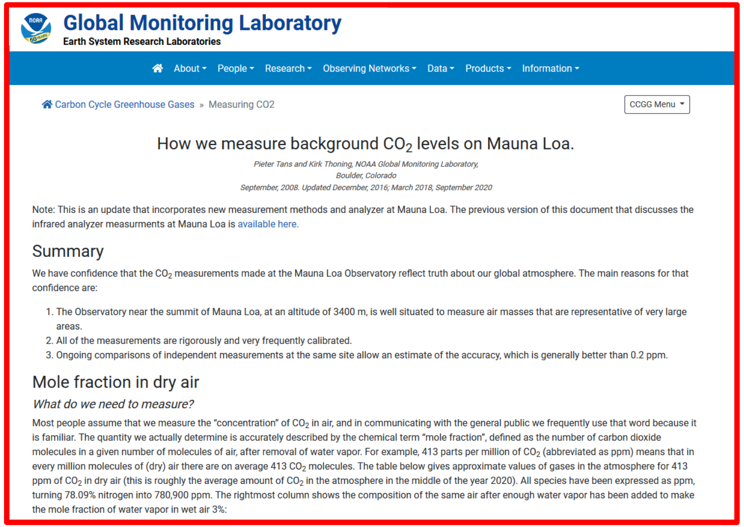
Version 2.0

September 2020

Please cite this document as:

ICOS RI (2020): ICOS Atmosphere Station Specifications V2.0 (editor: O. Laurent). ICOS ERIC. https://doi.org/10.18160/GK28-2188

Last revision: 22 September 2020



Global Monitoring Laboratory

Earth System Research Laboratories

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Carbon Cycle Greenhouse Gases » Measuring CO2 CCGG Menu ▾

How we measure background CO_2 levels on Mauna Loa.

Pieter Tans and Kirk Thoning, NOAA Global Monitoring Laboratory, Boulder, Colorado

September, 2008. Updated December, 2016; March 2018, September 2020

Note: This is an update that incorporates new measurement methods and analyzer at Mauna Loa. The previous version of this document that discusses the infrared analyzer measurments at Mauna Loa is available here.

Summary

We have confidence that the CO_2 measurements made at the Mauna Loa Observatory reflect truth about our global atmosphere. The main reasons for that confidence are:

1. The Observatory near the summit of Mauna Loa, at an altitude of 3400 m, is well situated to measure air masses that are representative of very large areas.
2. All of the measurements are rigorously and very frequently calibrated.
3. Ongoing comparisons of independent measurements at the same site allow an estimate of the accuracy, which is generally better than 0.2 ppm.

Mole fraction in dry air

What do we need to measure?

Most people assume that we measure the "concentration" of CO_2 in air, and in communicating with the general public we frequently use that word because it is familiar. The quantity we actually determine is accurately described by the chemical term "mole fraction", defined as the number of carbon dioxide molecules in a given number of molecules of air, after removal of water vapor. For example, 413 parts per million of CO_2 (abbreviated as ppm) means that in every million molecules of (dry) air there are on average 413 CO_2 molecules. The table below gives approximate values of gases in the atmosphere for 413 ppm of CO_2 in dry air (this is roughly the average amount of CO_2 in the atmosphere in the middle of the year 2020). All species have been expressed as ppm, turning 78.09% nitrogen into 780,900 ppm. The rightmost column shows the composition of the same air after enough water vapor has been added to make the mole fraction of water vapor in wet air 3%:

Instrumentation – useful resources

Useful resources:

- WMO/GAW reports
- measurement guidelines
- project reports, webpages
- Environment Agencies, European Committee for Standardization (CEN)

List of Designated Reference and Equivalent Methods, June 15, 2020 — Page 1

EPA United States Environmental Protection Agency

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
CENTER FOR ENVIRONMENTAL MEASUREMENTS & MODELING
AIR METHODS & CHARACTERIZATION DIVISION (MD-D205-03)
Research Triangle Park, NC 27711

Office of
Research and Development

LIST OF DESIGNATED REFERENCE AND EQUIVALENT METHODS

***Issue Date*: June 15, 2020**
(www.epa.gov/ttn/amtic/criteria.html)

Environment Agency

Performance Standards for Continuous Ambient Air Quality Monitoring Systems

Environment Agency
Version 10
June 2016

mCERTS
THE ENVIRONMENT AGENCY'S MONITORING CERTIFICATION SCHEME

prEN 14211:2009 (E)

CEN/TC 264 N 1362

CEN/TC 264

Date: 2009-02

prEN 14211

CEN/TC 264

Secretariat: DIN

Ambient air quality — Standard method for the measurement of the concentration of nitrogen dioxide and nitrogen monoxide by chemiluminescence —

Instrumentation – useful resources

Useful resources:

- WMO/GAW reports
- measurement guidelines
- project reports, webpages
- Environment Agencies, European Committee for Standardization (CEN)
- publications
- consultation of peers
- don't forget the periphery

Atmos. Meas. Tech., 12, 5863–5878, 2019
https://doi.org/10.5194/amt-12-5863-2019

Atmospheric Measurement Techniques

Recent advances in measurement techniques for atmospheric carbon monoxide and nitrous oxide observations

Christoph Zellweger[1], Rainer Steinbrecher[2], Olivier Laurent[3], Haeyoung Lee[4], Sumin Kim[4], Lukas Emmenegger[1], Martin Steinbacher[1], and Brigitte Buchmann[5]

Atmos. Meas. Tech., 5, 657–685, 2012
www.atmos-meas-tech.net/5/657/2012/
doi:10.5194/amt-5-657-2012

Mobility particle size spectrometers: harmonization of technical standards and data structure to facilitate high quality long-term observations of atmospheric particle number size distributions

A. Wiedensohler[1], W. Birmili[1], A. Nowak[1], A. Sonntag[1], K. Weinhold[1], M. Merkel[1], B. Wehner[1], T. Tuch[1], S. Pfeifer[1], M. Fiebig[2], A. M. Fjäraa[2], E. Asmi[3], K. Sellegri[4], R. Depuy[4], H. Venzac[4], P. Villani[4], P. Laj[5], P. Aalto[6], J. A. Ogren[7], E. Swietlicki[8], P. Williams[9], P. Roldin[8], P. Quincey[10], C. Hüglin[11], R. Fierz-Schmidhauser[12], M. Gysel[12], E. Weingartner[12], F. Riccobono[12], S. Santos[13], C. Grüning[13], K. Faloon[14], D. Bed…, C. Monahan[15], S. G. Jennings[15], C. D. O'Dowd[15], A. Marinoni[16], H.-G. Horn[17], … P. H. McMurry[19], Z. Deng[20], C. S. Zhao[20], M. Moerman[20], B. Henzing[21], G. de L…, S. Bastian[22]

Tarasick, D, et al. 2019. Tropospheric Ozone Assessment Report: Tropospheric ozone from 1877 to 2016, observed levels, trends and uncertainties. *Elem Sci Anth*, 7: 39. DOI: https://doi.org/10.1525/elementa.376
ELEMENTA Science of the Anthropocene

REVIEW

Tropospheric Ozone Assessment Report: Tropospheric ozone from 1877 to 2016, observed levels, trends and uncertainties

David Tarasick*, Ian E. Galbally†,‡, Owen R. Cooper§,‖, Martin G. Schultz¶, Gerard Ancellet**, Thierry Leblanc††, Timothy J. Wallington‡‡, Jerry Ziemke§§, Xiong Liu‖‖, Martin Steinbacher¶¶, Johannes Staehelin***, Corinne Vigouroux†††, James W. Hannigan‡‡‡, Omaira García§§§, Gilles Foret‖‖‖, Prodromos Zanis¶¶¶, Elizabeth Weatherhead§,‖, Irina Petropavlovskikh§,‖, Helen Worden‡‡‡, Mohammed Osman****,††††,‡‡‡‡, Jane Liu§§§§,‖‖‖‖, Kai-Lan Chang§,‖, Audrey Gaudel§,‖, Meiyun Lin¶¶¶¶,*****, Maria Granados-Muñoz†††††, Anne M. Thompson§§, Samuel J. Oltmans‡‡‡‡‡, Juan Cuesta‖‖‖, Gaelle Dufour‖‖‖, Valerie Thouret§§§§§, Birgit Hassler‖‖‖‖‖, Thomas Trickl¶¶¶¶¶ and Jessica L. Neu******

Atmos. Meas. Tech., 9, 4719–4736, 2016
www.atmos-meas-tech.net/9/4719/2016/
doi:10.5194/amt-9-4719-2016

Atmospheric Measurement Techniques

Automatic processing of atmospheric CO_2 and CH_4 mole fractions at the ICOS Atmosphere Thematic Centre

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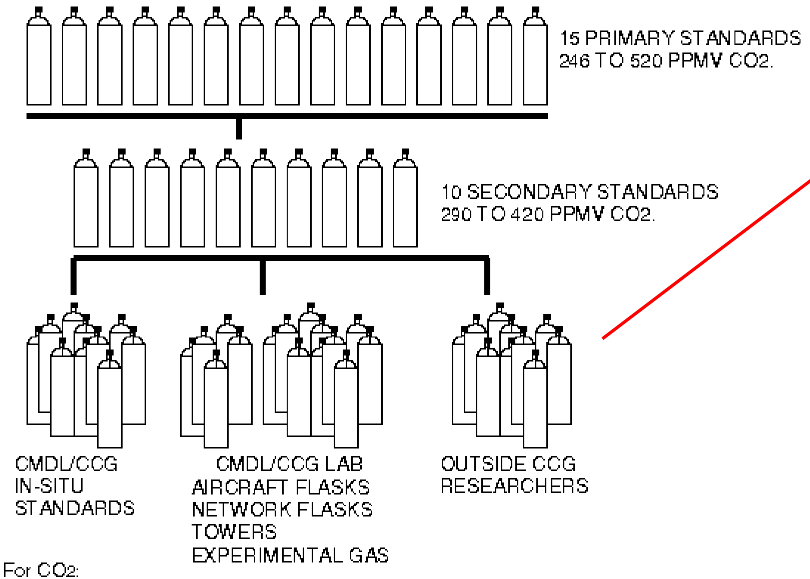
Instrumentation – traceability and calibration

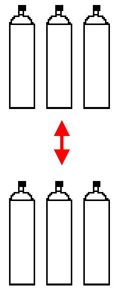


For CO_2:
CALIBRATION PRECISION; 0.014 µmol/mol [1 sd of calibrations < 6 months apart].
precision for < 325 approx. 0.1
precision for > 425 approx. 0.25

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

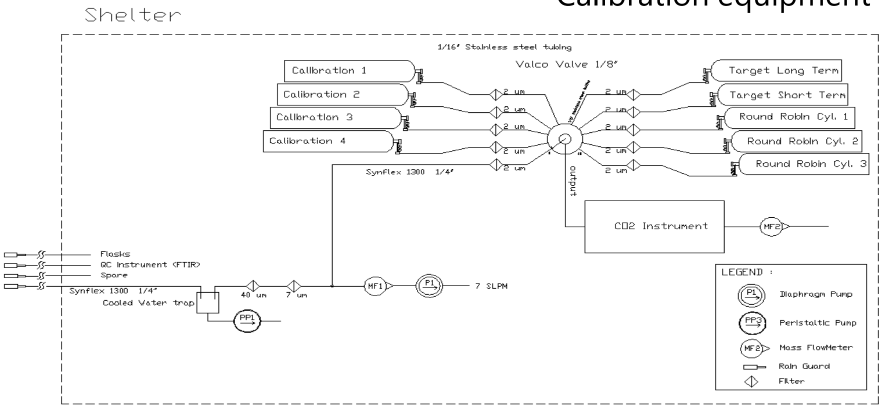
station operators



primary laboratory standards

working standards (in-situ)

Calibration equipment



ICOS RI, 2020

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Instrumentation – traceability and calibration

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

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/

CO2 _

File	Contact	Observation	Ref

Search by a keyword: (start typing)

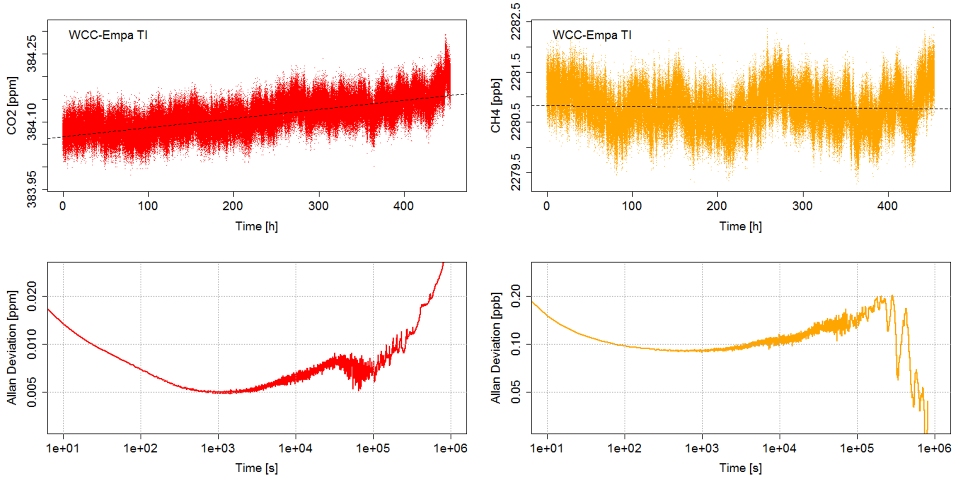
Collaborator(s)	NO: 23; Acronym: Empa; Name: Swiss Federal Laboratories for Materials Science and Technology
Aim of Observation	Background observation
Data Time zone	UTC
Unit	ppm
Calibration Scale	9999-12-31 00:00:00 - 9999-12-31 23:59:59: WMO CO2 X2007
Instruments(s)	9999-12-31 00:00:00 - 9999-12-31 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

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
```

Instrumentation – frequency of calibration and QA/QC

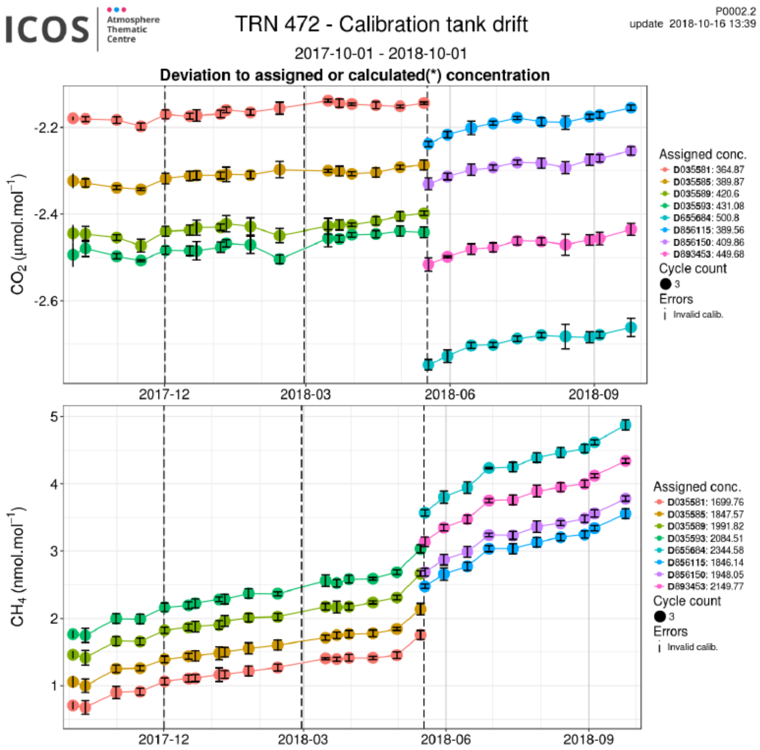
laboratory tests



Zellweger et al., 2016

"... A thorough analysis of the CO_2 and CH_4 stability of [this type of cavity enhanced laser spectrometer] indicates that the optimal calibration frequency is approximately 30 h. ..."

(long-term) field tests

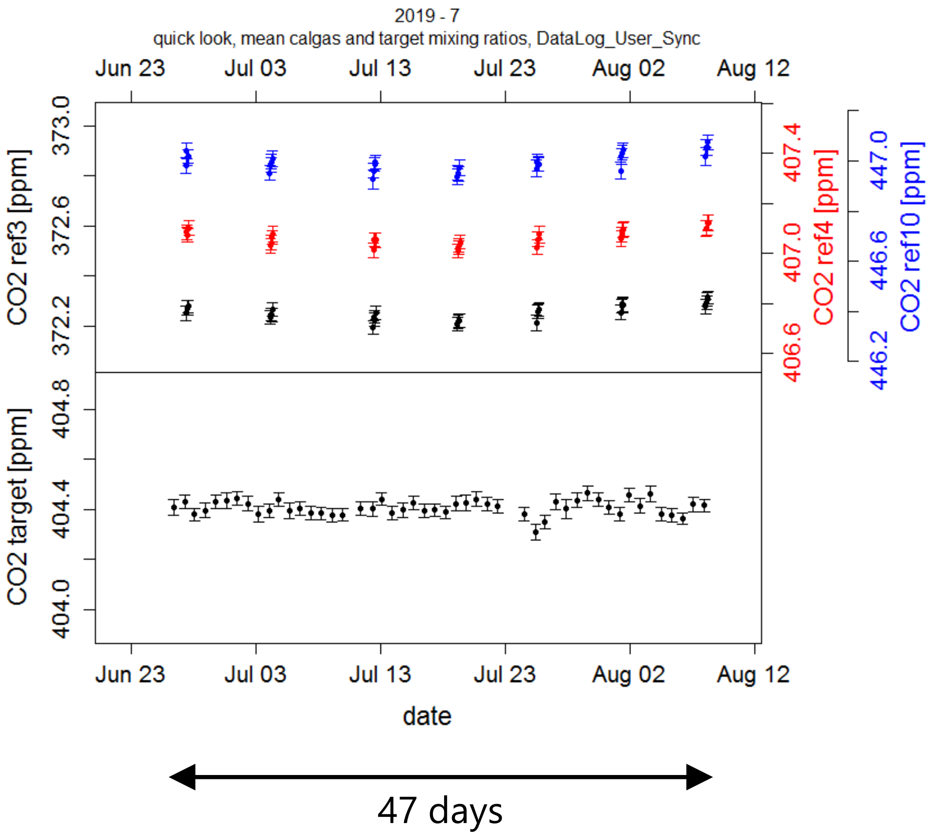


Yver-Kwok et al., 2020

Instrumentation – use target gases for QA/QC

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.

Appropriate processing software needs to be available.



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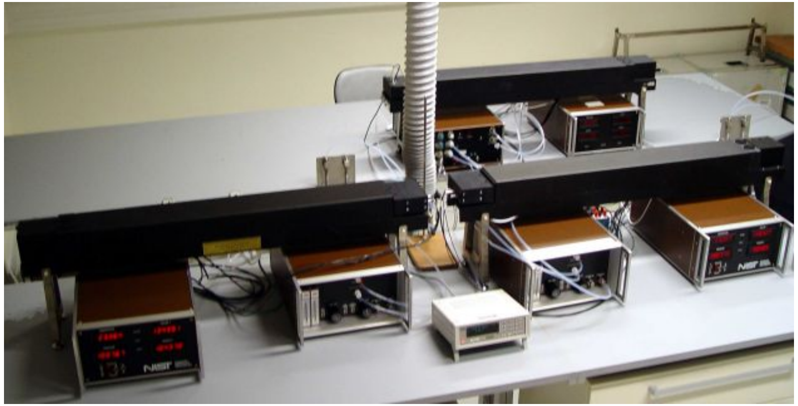
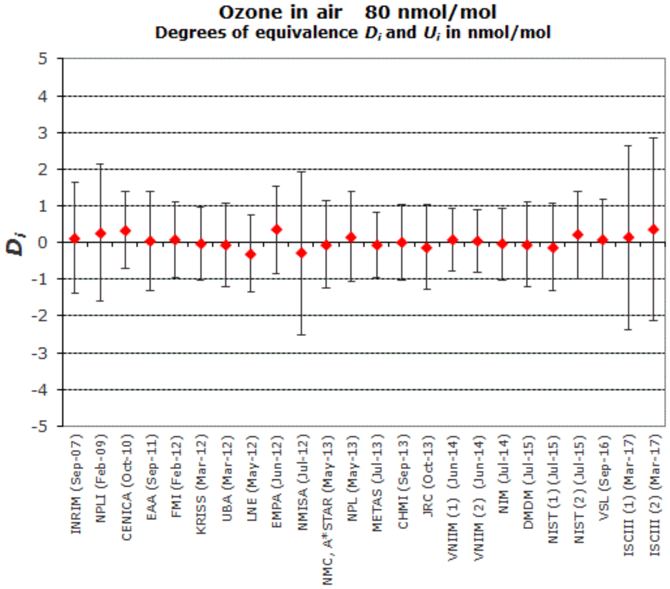
Traceability for surface ozone measurements

- 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)





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Calibration (and auditing) of surface O3 analyzers

Reference: Standard Reference Photometer (SRP)

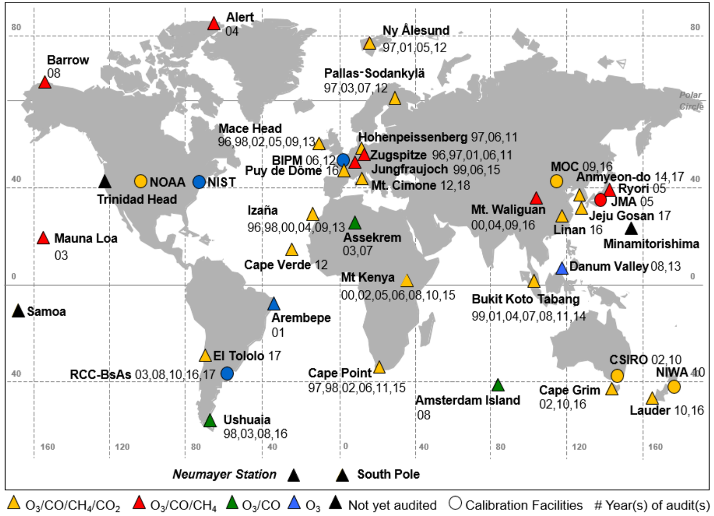
World reference: SRP #2 at National Institute for Standards and Technology

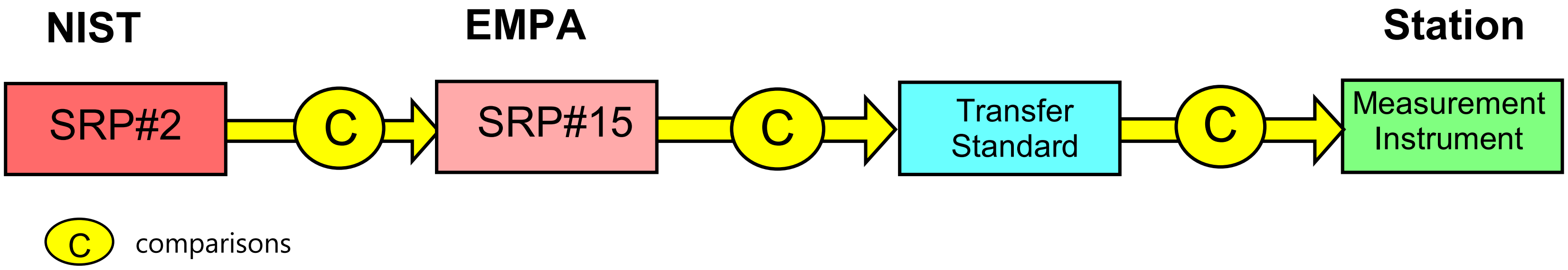
Currently: approx. 60 SRPs worldwide

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

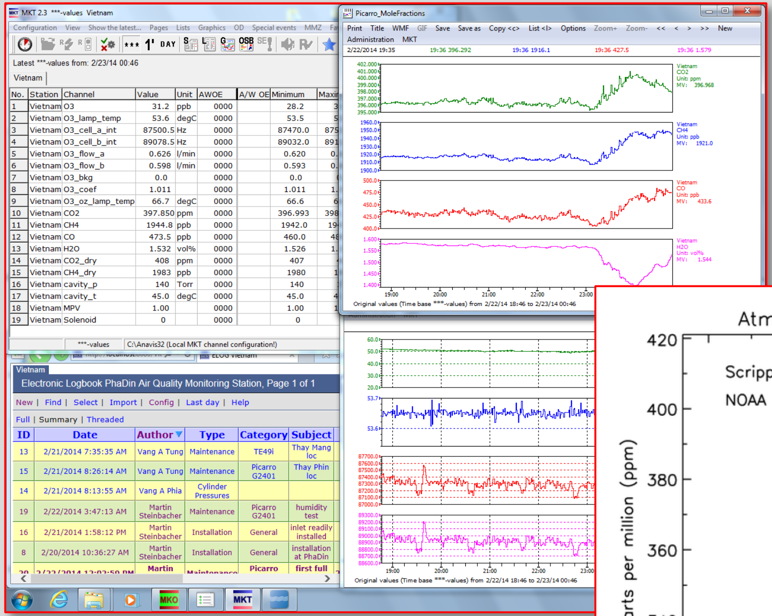
Traceability chain:

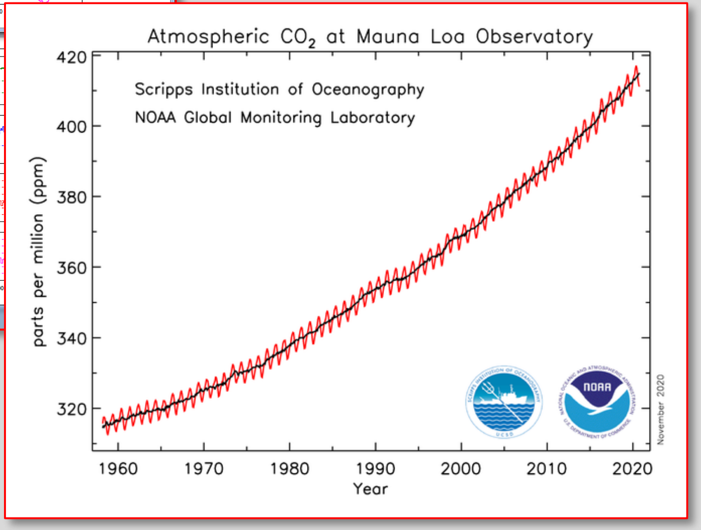
WCC-Empa Audits / Comparisons 1996 – 2018





Data management & data processing

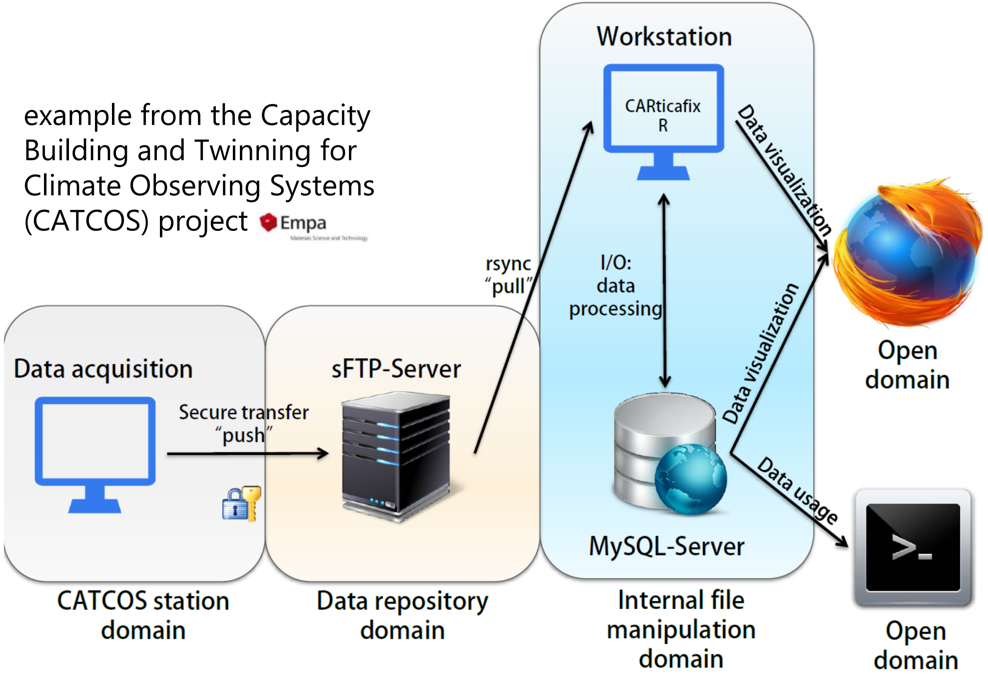




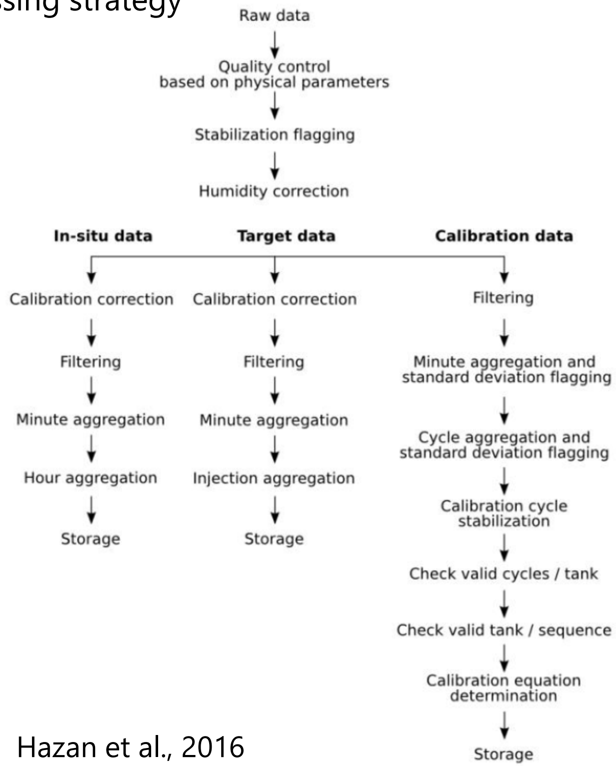
Data management

overall concept

example from the Capacity Building and Twinning for Climate Observing Systems (CATCOS) project



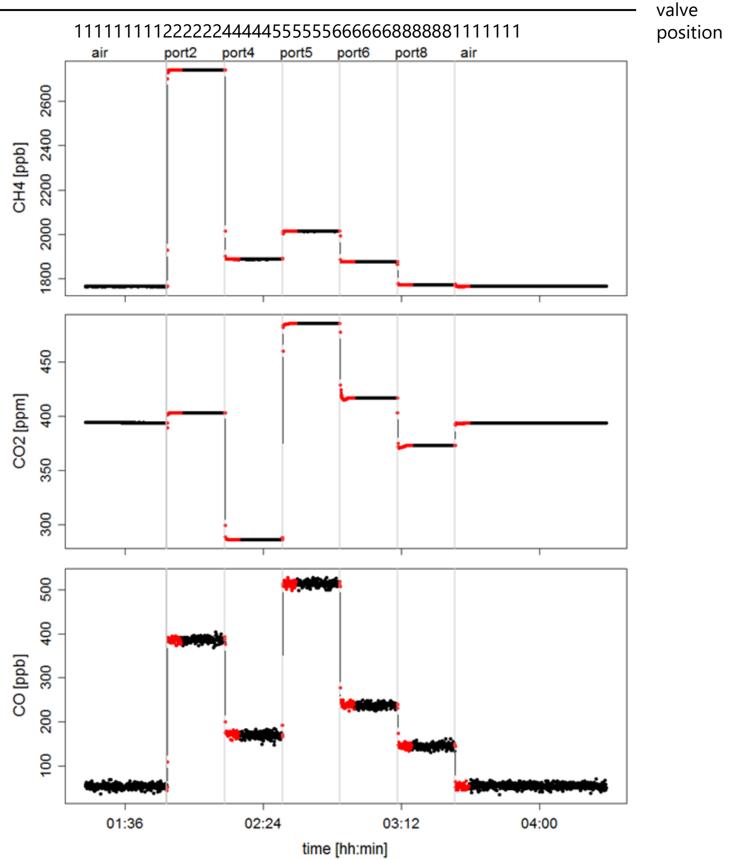
data processing strategy



Hazan et al., 2016

Data management

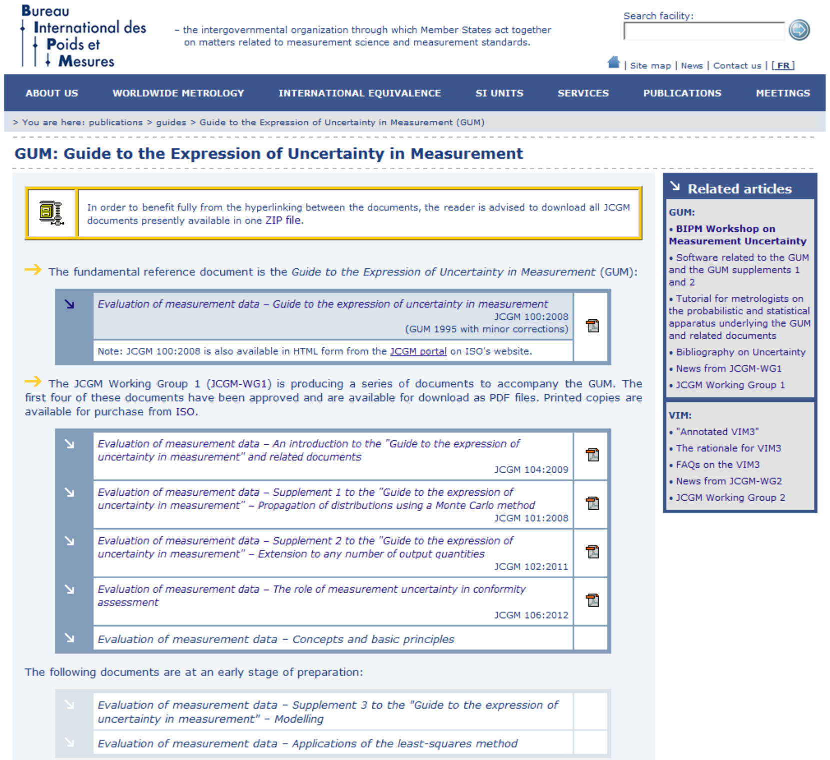
When changing from ambient air to calibration gas, or from one calibration gas to another, do exclude the first data after the change to account for the transition time until a stable signal is reached.



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

Data management – measurement uncertainty

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·*x*[*]
Repeatability	Instrument stability	Rectangular	0.0016·*x*
Span drift	Instrument stability	Rectangular	0.0040·*x*
Zero drift	Instrument stability	Rectangular	0.17
Pressure *P*	Pressure measurement	Rectangular	0.0002·*x*
Temperature *T*	Temp. measurement	Rectangular	0.0005·*x*
H_2O interference	Interference in the UV		0.0060·*x*
Other interferences	Interference in the UV		0.6
Sampling loss (Inlet)	Inlet material, dirt	Rectangular	0.0014·*x*

[*] *where x refers to ozone mole fraction*

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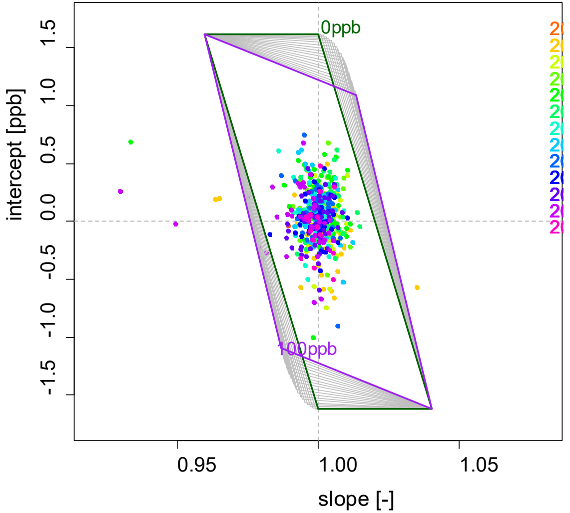
.

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).

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

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

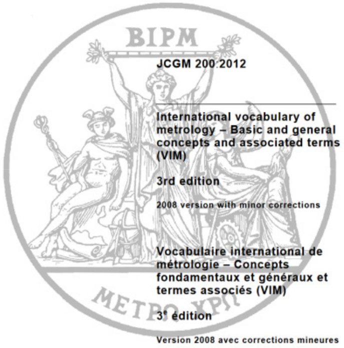


Tarasick et al., 2019, Elementa

O3 measurement guidelines, GAW Report Nr. 209, 2013

Data management – terminology

The GAW programme recommends adoption and use of internationally accepted methods and vocabulary to deal with measurement uncertainty as outlined in various ISO/BIPM publications



A selection of the most relevant terms can be found can be found at

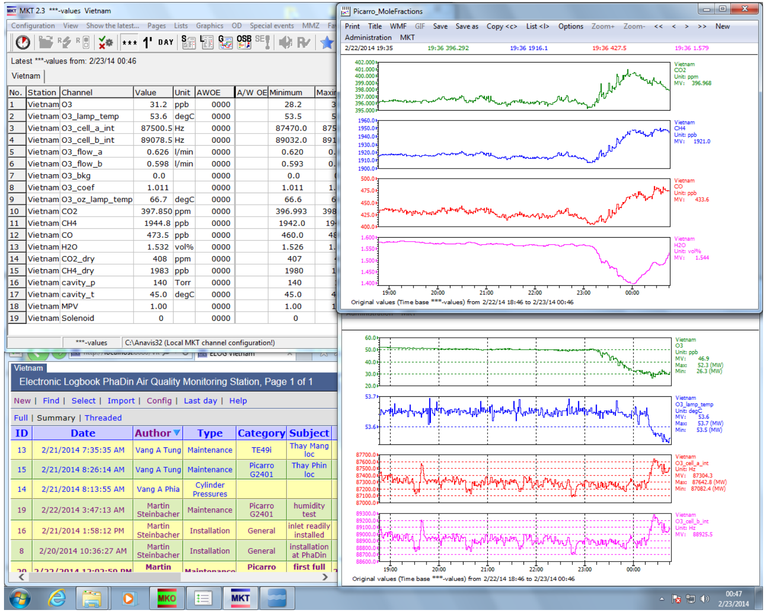
https://www.empa.ch/web/s503/gaw_glossary

Data management

IT (hardware and software) resources are needed

on-site

central data processing unit



log book (meta data management) !

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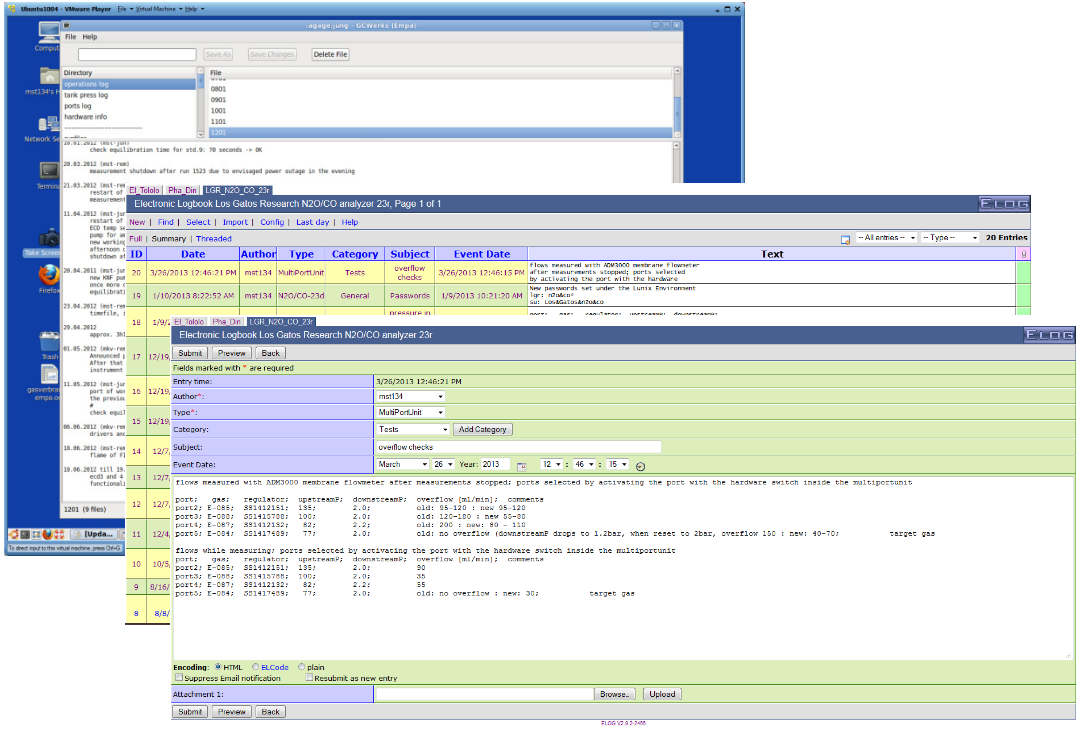
Metadata management

- documentation, log books



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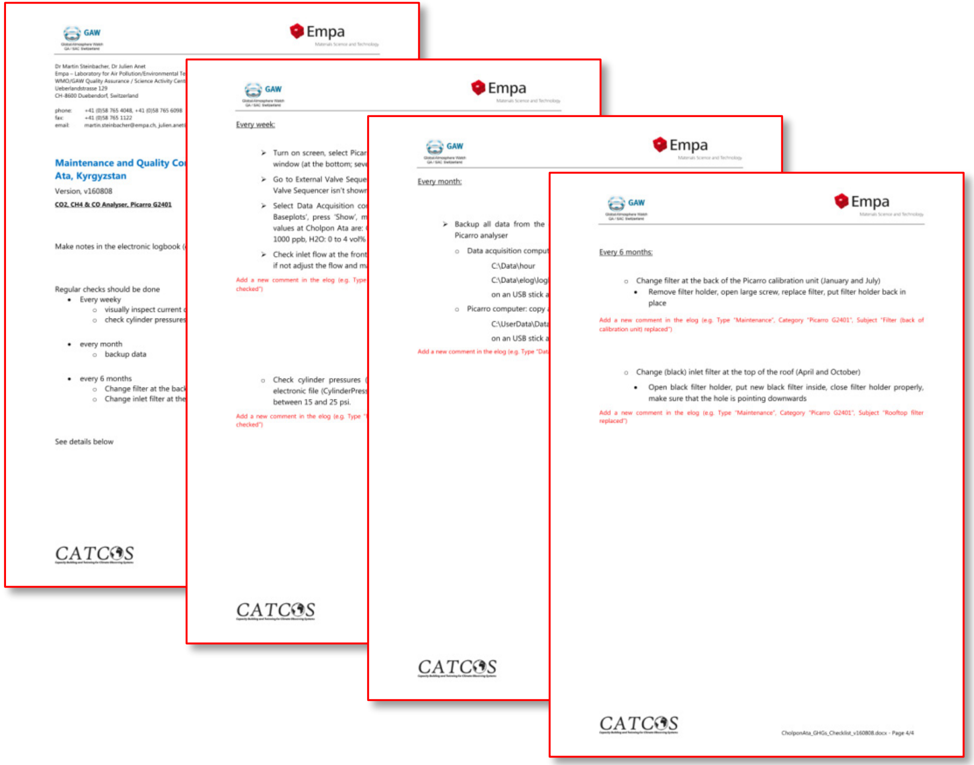
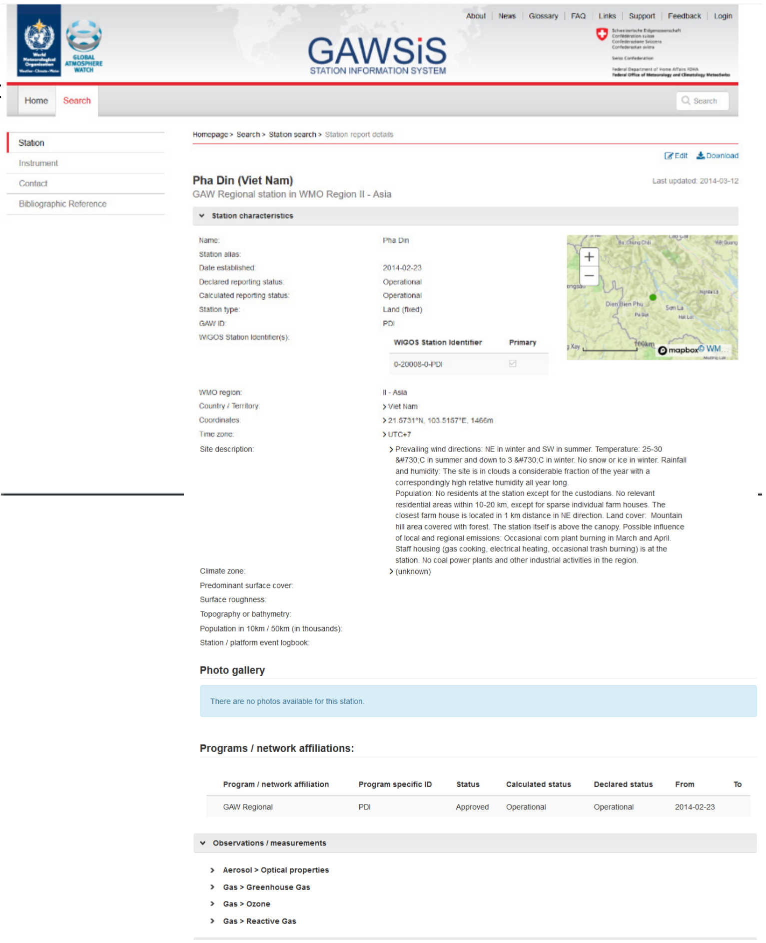
Metadata management

- documentation, log books
- checklists / standard operation procedures



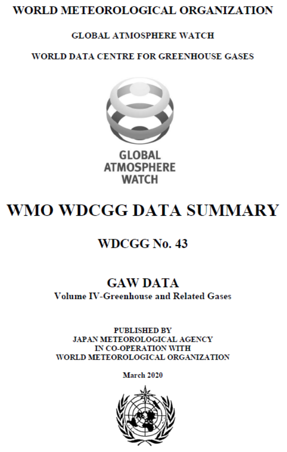
Metadata management

- documentation, log books
- checklists / standard operation procedures
- regular updates in GAWSIS https://gawsis.meteoswiss.ch



Additional quality control

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



WORLD METEOROLOGICAL ORGANIZATION

GLOBAL ATMOSPHERE WATCH

WORLD DATA CENTRE FOR GREENHOUSE GASES

GLOBAL ATMOSPHERE WATCH

WMO WDCGG DATA SUMMARY

WDCGG No. 43

GAW DATA
Volume IV-Greenhouse and Related Gases

PUBLISHED BY
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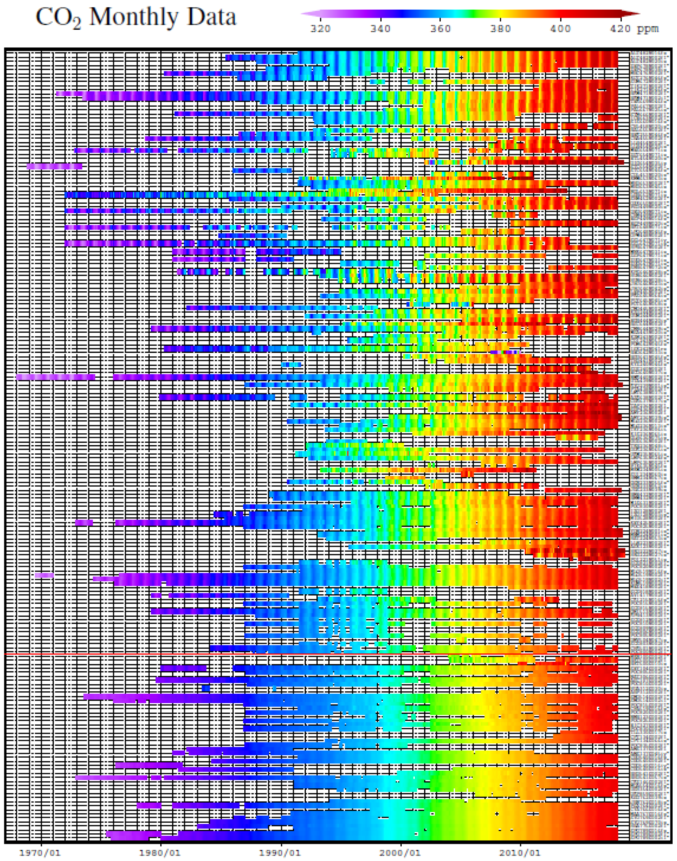
IN CO-OPERATION WITH
WORLD METEOROLOGICAL ORGANIZATION

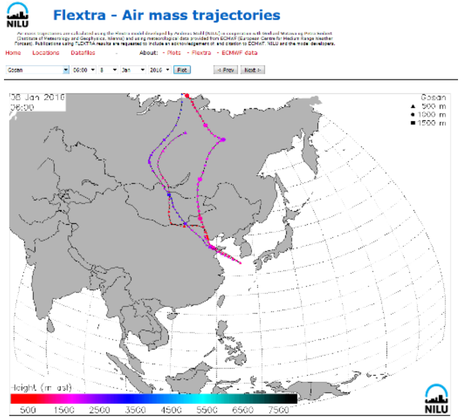
March 2020

WDCGG Data Summary
Report #43, 2020

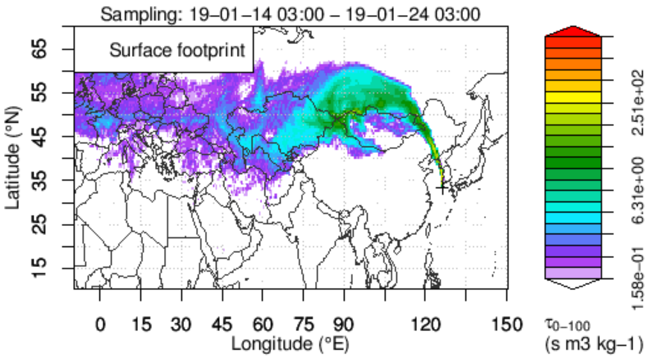


Additional quality control

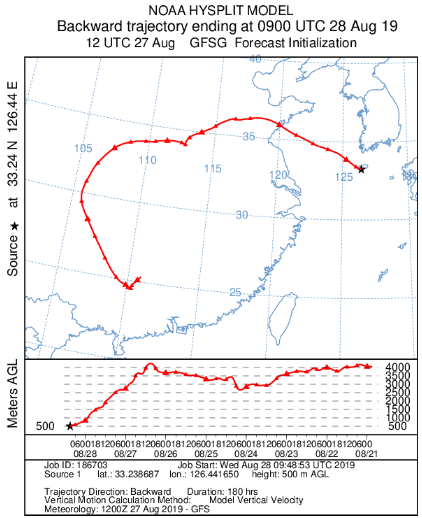
- participation in comparison (e.g. round robin) exercises
- comparison of data with data from «similar» stations
- use available online tools for trajectory calculations, e.g.



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



http://lagrange.empa.ch/

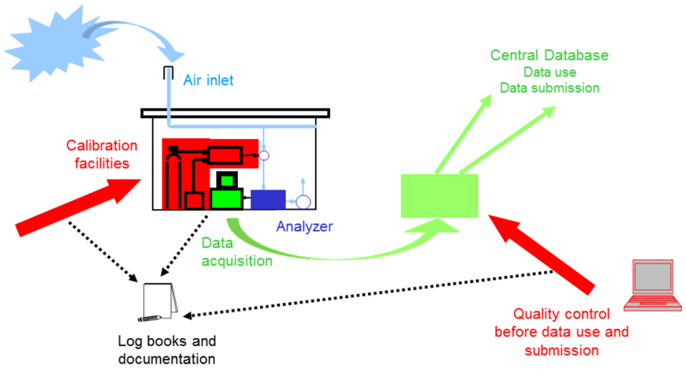


https://ready.arl.noaa.gov/hypub-bin/trajtype.pl

Conclusions

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
- …



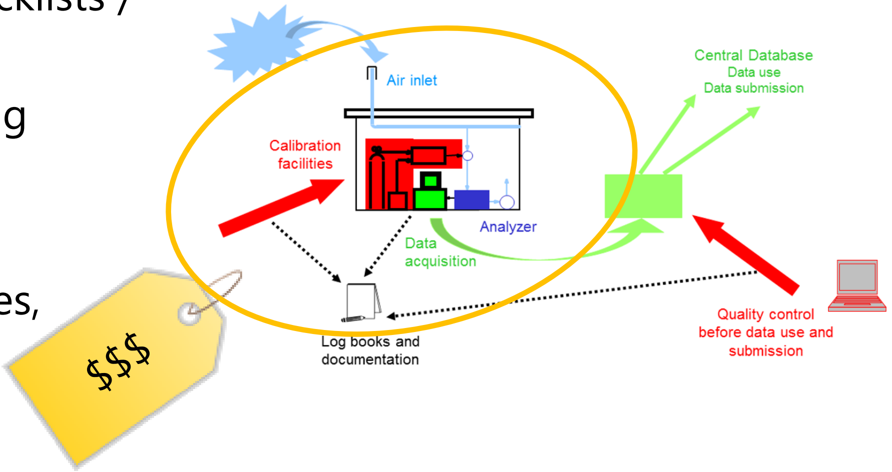
Instrument(s) and periphery

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

- consumables, spare parts, backup instruments, …

Conclusions, con’td

- clearly define the motivation / goals of your monitoring
  - identify data quality objectives
- select suitable instrumentation (and periphery)
- design operation and calibration strategy (and revise if needed)
- prepare Standard Operation Procedures / checklists / troubleshooting strategies
- implement robust data management (including documentation and meta data)
- draw up a sustainable budget (for consumables, wear parts, instrument replacements, ...)



Further reading

The Global Atmosphere Watch Programme: 25 Years of Global Coordinated Atmospheric Composition Observations and Analyses, https://library.wmo.int/doc_num.php?explnum_id=7886, 2014.

WMO/GAW reports can be found at https://community.wmo.int/gaw-reports

Hazan et al., Automatic processing of atmospheric CO2 and CH4 mole fractions at the ICOS Atmosphere Thematic Centre, Atmos. Meas. Tech., 9, 4719–4736, https://doi.org/10.5194/amt-9-4719-2016, 2016.

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Wiedensohler et al., Mobility particle size spectrometers: harmonization of technical standards and data structure to facilitate high quality long-term observations of atmospheric particle number size distributions, Atmos. Meas. Tech., 5, 657–685, https://doi.org/10.5194/amt-5-657-2012, 2012.

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Zellweger et al., Assessment of recent advances in measurement techniques for atmospheric carbon dioxide and methane observations, Atmos. Meas. Tech., 9, 4737-4757, doi:10.5194/amt-9-4737-2016, 2016.ICOS RI (2020): ICOS Atmosphere Station Specifications v2.0, ICOS ERIC, https://doi.org/10.18160/GK28-2188

https://www.esrl.noaa.gov/gmd/ccgg/about/co2_measurements.html

Thank you for your attention !