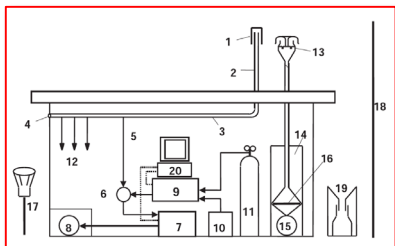


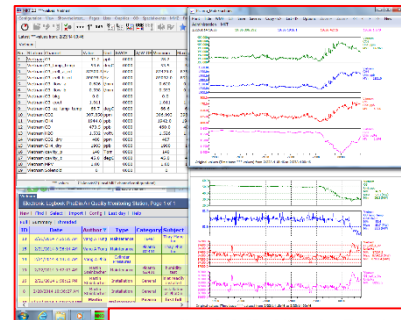
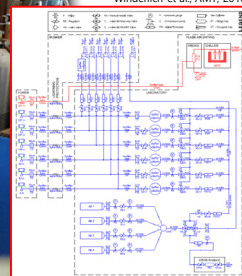
The Importance of Quality Assurance and Quality Control for long-term in-situ atmospheric composition observations



design & station setup



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

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 Jungfrauoch
 - Manager of WMO/GAW Quality Assurance/Science Activity Centre Switzerland
 - Chair of the Atmospheric Monitoring Station Assembly of the Integrated Carbon Observation System

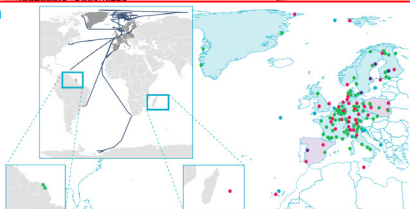


support of observations in data sparse regions



ICOS Station Network

- Site type
- Urban, roadside
 - Urban
 - Suburban



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



supported by



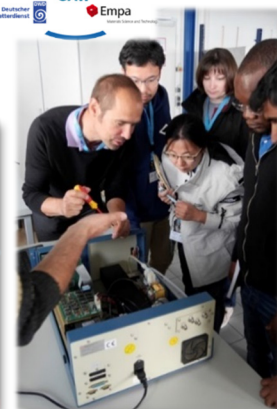
Schweizerische Eidgenossenschaft
Confédération suisse
Confederazione Svizzera
Confederaziun svizra

Federal Office of Meteorology
and Climatology MeteoSwiss

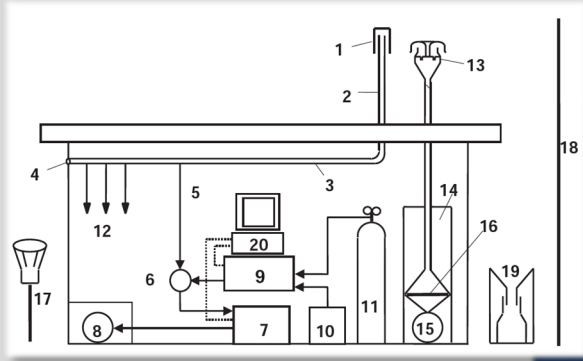


Global Atmosphere Watch
QA / SAC Switzerland

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

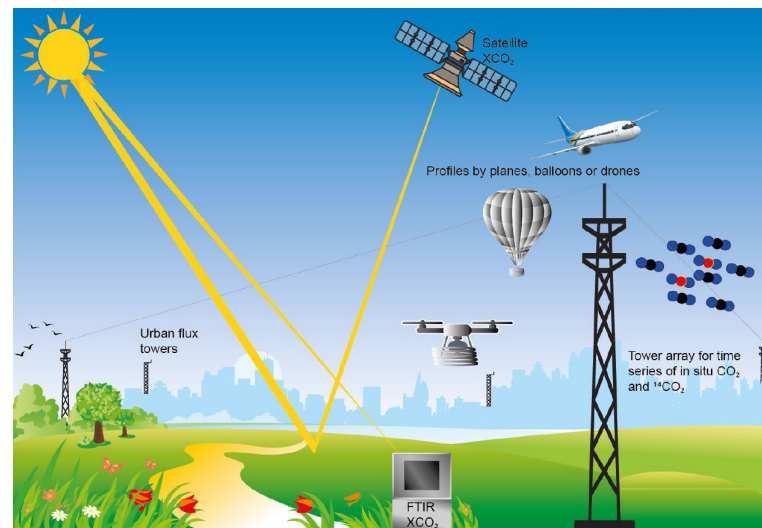


Design & setup



Fundamental questions

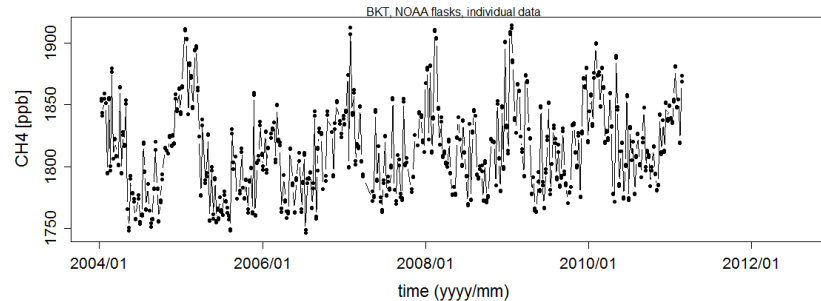
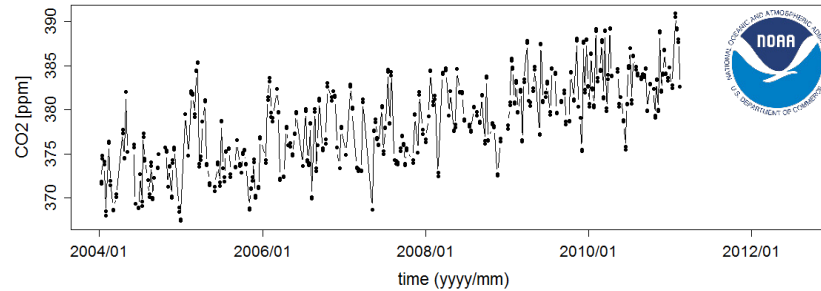
- Why do I want/need to measure?
- Which compounds are of interest?
(gaseous compounds, particulates, deposition, meteorological parameters)
- Where are measurements reasonable?
(e.g., representativeness of the sample, avoid influence of undesirable sources)
- What kind of data series are needed?
(continuous,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



© ICOS ERIC, 2020

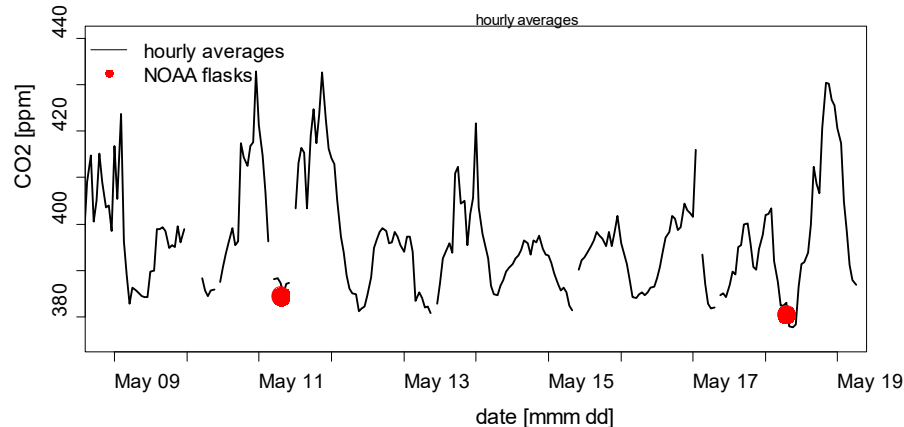
Discrete (flasks) vs. continuous observations

greenhouse gas observations
through flask sampling and in-situ monitoring



Discrete (flasks) vs. continuous observations

greenhouse gas observations
through flask sampling and in-situ monitoring

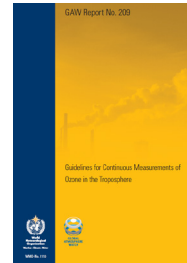


- long-term flask observations suitable for trend estimates
- continuous measurements allow gaining insight into local to regional processes

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 CO₂ 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
- ...



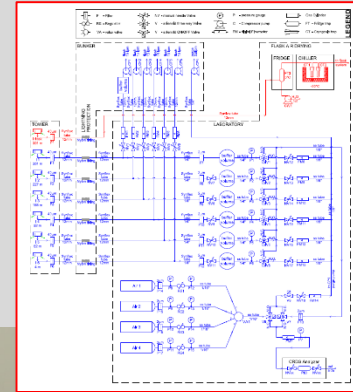
Instrument(s) and periphery

- 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

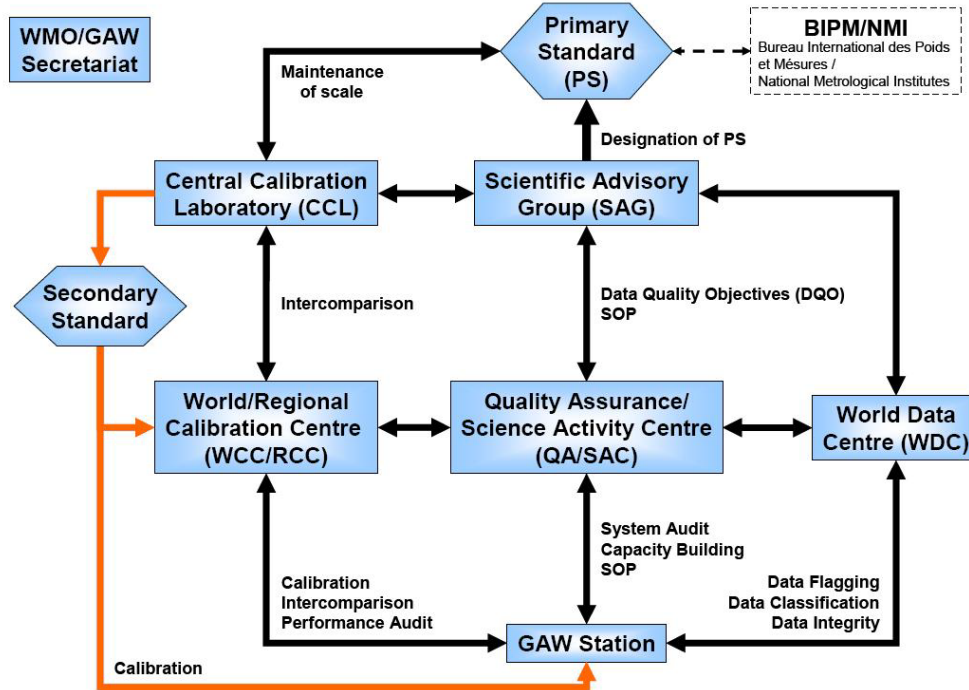


Winderlich et al., AMT; 2010



GAW Quality Management Framework

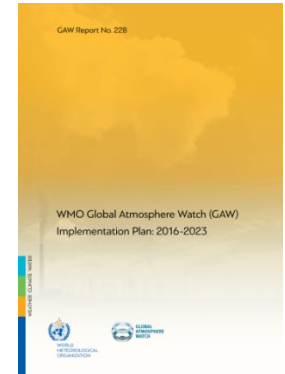
Elements of the Quality Assurance system,
QA activities and workflow in GAW



map of GAW stations



<https://gawsis.meteoswiss.ch>

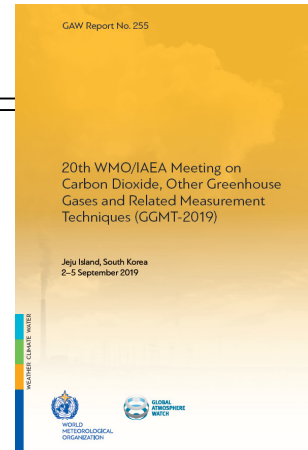


GAW Implementation Plan 2016-2023,
GAW Report Nr. 228, 2017

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 ₂ O	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
δ ¹³ C-CO ₂	0.01‰	0.1‰	-9.5 to -7.5‰ (VPDB)	
δ ¹⁸ O-CO ₂	0.05‰	0.1‰	-2 to +2‰ (VPDB-CO ₂)	
δ ¹³ C-CH ₄	0.02‰	0.2‰	-51 to -46‰ (VPDB)	
δ ² H-CH ₄	1‰	5‰	-120 to -63‰ (VSMOW)	
Δ ¹⁴ C-CO ₂	0.5‰	3‰	-80 to 20‰	
Δ ¹⁴ C-CH ₄	0.5‰		50-350‰	
Δ ¹⁴ C-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

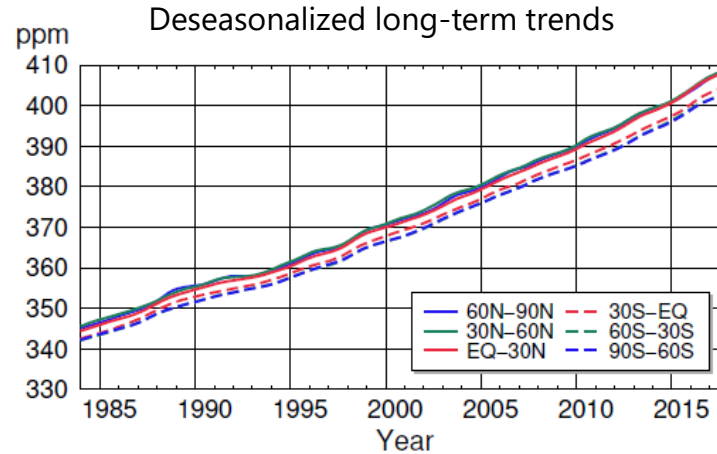
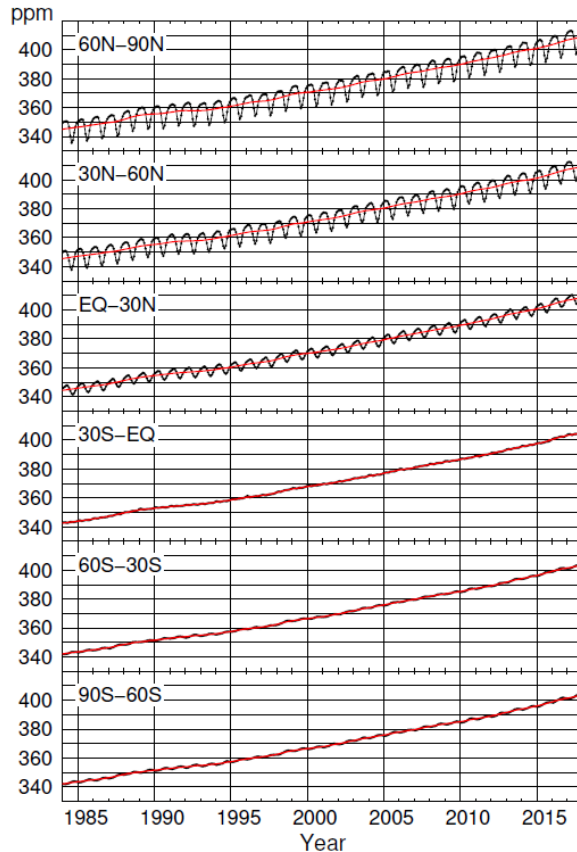
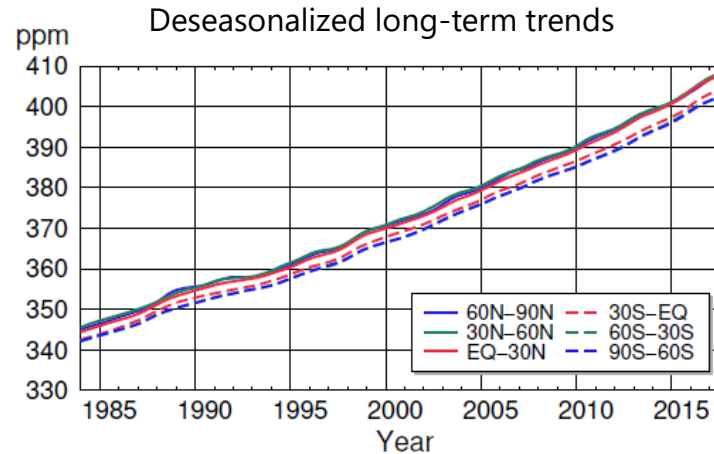
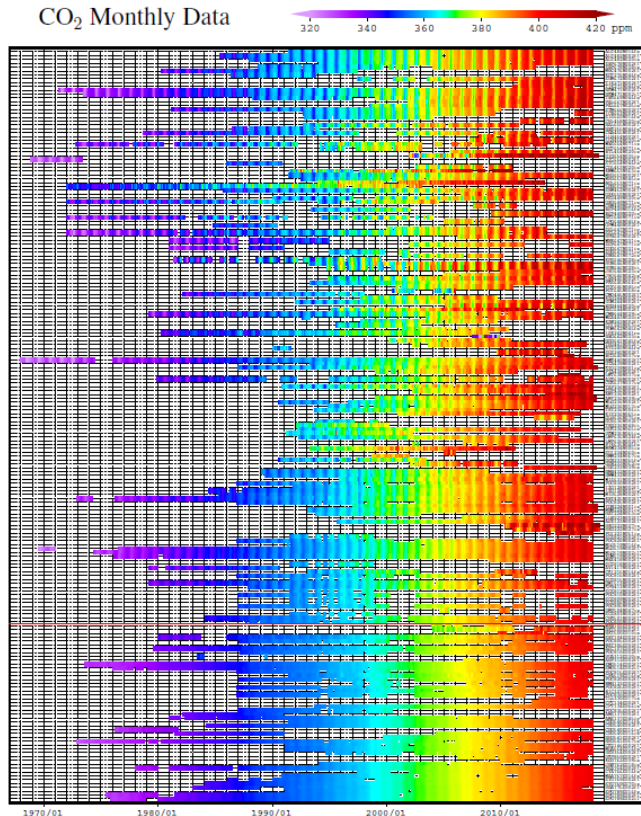


Fig. 1.3 Monthly mean mole fractions of CO₂ from 1984 to 2017 averaged over each 30° latitudinal zone (black) and their deseasonalized long-term trends (red).

Instrumentation – required quality, example CO₂



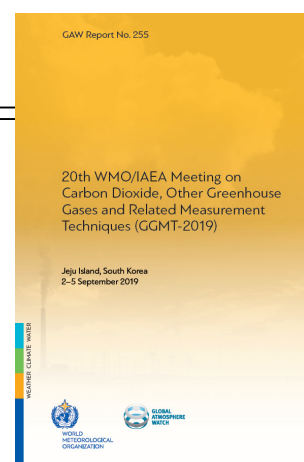
- compatibility goals mainly motivated by small spatial gradients

Plate 1.1 Monthly mean CO₂ mole fractions that have been reported to the WDCGG.



Instrumentation – required quality, example CO2

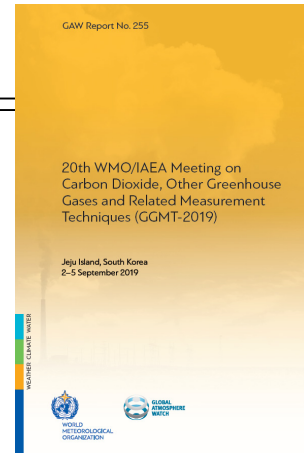
“... To achieve the required levels of network compatibility (see Table 1) it is important to understand and carefully consider the design of the whole analysis system including instrument, gas handling, calibration and data management. No single instrument type is recommended. Many can be used with 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 CO2

“... 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 $\sim 1 \text{ nmol mol}^{-1}$. 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 $\sim 25\%$ of the globe (<i>TOAR-Surface ozone database</i>). Sites with long-term records are very important.
Air quality model validation	Moderate accuracy and precision, preferably 3–5% level. Need vertical resolution of $\sim 0.2 \text{ km}$ 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/10.18160/9K39-3188>

Last revision: 22 September 2020

Global Monitoring Laboratory
Earth System Research Laboratories

Home About People Research Observing Networks Data Products Information

Carbon Cycle Greenhouse Gases > Measuring CO₂ CCGG Menu

How we measure background CO₂ 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 measurements at Mauna Loa is [available here](#).

Summary

We have confidence that the CO₂ 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 CO₂ 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 CO₂ (abbreviated as ppm) means that in every million molecules of (dry) air there are on average 413 CO₂ molecules. The table below gives approximate values of gases in the atmosphere for 413 ppm of CO₂ in dry air (this is roughly the average amount of CO₂ 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)

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)

Page 1



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 —

Performance Standards for Continuous Ambient Air Quality Monitoring Systems

Environment Agency
Version 10
June 2016



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., 5, 657–685, 2012
www.atmos-meas-tech.net/5/657/2012/
doi:10.5194/amt-5-657-2012
© Author(s) 2012. CC Attribution 3.0 License.



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. Wiedensohler¹, W. Birmili¹, A. Novak¹, A. Sonntag¹, K. Weinhold¹, M. Merkel¹, B. Wehner¹, T. Tuch¹, S. Pfeifer¹, M. Fiebig², A. M. Fjåraa³, E. Asimi⁴, K. Sellegri⁵, R. Dupuy⁴, H. Venzac⁶, P. Villani⁶, P. Laj⁶, P. Aalto⁷, J. A. Ogren⁷, E. Swietlicki⁸, P. Williams⁹, P. Roldin⁹, P. Quincey¹⁰, C. Hügel¹¹, R. Fierz-Schmidhauser¹², M. Gysel¹², E. Weingartner¹², F. Riccobono¹², S. Santos¹², C. Grünig¹³, K. Faloon¹⁴, D. Beecher¹⁵, C. Monahan¹⁵, S. G. Jennings¹⁵, C. D. O'Dowd¹⁵, A. Marinoni¹⁶, H.-G. Horn¹⁷, P. H. McMurry¹⁸, Z. Deng¹⁹, C. S. Zhao²⁰, M. Moerman²⁰, B. Henzing²¹, G. de Leeuw²², S. Bastian²²

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

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

Christoph Zellweger¹, Rainer Steinbrecher², Olivier Laurent³, Haeyoung Lee⁴, Sunin Kim⁴, Lukas Emmenegger¹, Martin Steinbacher¹, and Brigitte Buchmann¹

ELEMENTA
Science of the Atmosphere

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/10.15125/elementa.376

REVIEW

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

David Tarasick¹, Ian E. Galbally^{1,2}, Owen R. Cooper^{3,4}, Martin G. Schultz⁵, Gerard Ancellet⁶, Thierry Leblanc⁷, Timothy J. Wallington⁸, Jerry Ziemke⁹, Xiong Liu¹⁰, Martin Steinbacher¹¹, Johannes Staehelin¹², Corinne Vigouroux¹³, James W. Hannigan¹⁴, Omaira Garcia¹⁵, Gilles Foret¹⁶, Prodrôm Zanis¹⁷, Elizabeth Weatherhead¹⁸, Irina Petropavlovskikh¹⁹, Helen Worden²⁰, Mohammed Osman^{21,22,23,24}, Jane Liu^{25,26,27}, Kai-Lan Chang²⁸, Audrey Gaudel²⁹, Meiyun Lin^{30,31,32,33}, Maria Granados-Muñoz^{34,35}, Anne M. Thompson³⁶, Samuel J. Oltmans^{37,38}, Juan Cuesta³⁹, Gaëlle Dufour⁴⁰, Valerie Thouret^{41,42}, Birgit Hassler^{43,44}, Thomas Trickl^{45,46} and Jessica L. Neu⁴⁷

Atmos. Meas. Tech., 9, 4719–4736, 2016
www.atmos-meas-tech.net/9/4719/2016/
doi:10.5194/amt-9-4719-2016
© Author(s) 2016. CC Attribution 3.0 License.

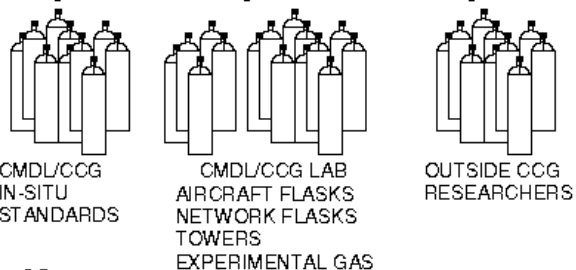
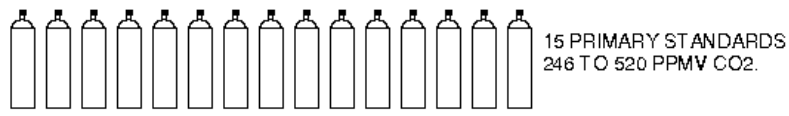


Atmospheric
Measurement
Techniques
EGU

Automatic processing of atmospheric CO₂ and CH₄ mole fractions at the ICOS Atmosphere Thematic Centre

Lynn Hazan, Jérôme Tarniewicz, Michel Ramonet, Olivier Laurent, and Amara Abbaris
Laboratoire des Sciences du Climat et de l'Environnement (LSE/IPSL), UMR CEA-CNRS-UVSQ, Gif-sur-Yvette, France

Instrumentation – traceability and calibration

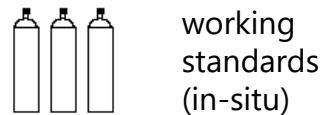
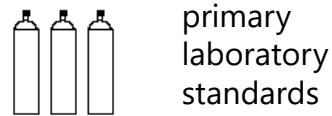


For CO₂:
 CALIBRATION PRECISION; 0.014 $\mu\text{mol/mol}$ [1 sd of calibrations < 6 months apart].
 precision for < 325 approx. 0.1
 precision for > 425 approx. 0.25

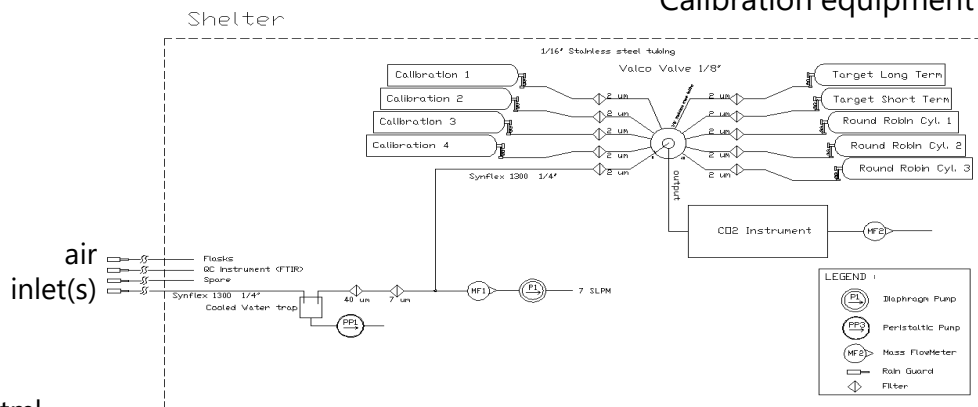
Absolute Uncertainty; 0.1 $\mu\text{mol/mol}$
 Internal consistency [325-425 $\mu\text{mol/mol}$]; 0.04 $\mu\text{mol/mol}$ [2 sigma] [< 2 years]

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

station operators



Calibration equipment



ICOS RI, 2020

Instrumentation – traceability and calibration

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

Data header

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# 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
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# scale_1_code : 1
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# scale_1_start_date : 2013-05-01T00:00:00Z
# scale_1_end_date : 2015-12-30T00:00:00Z
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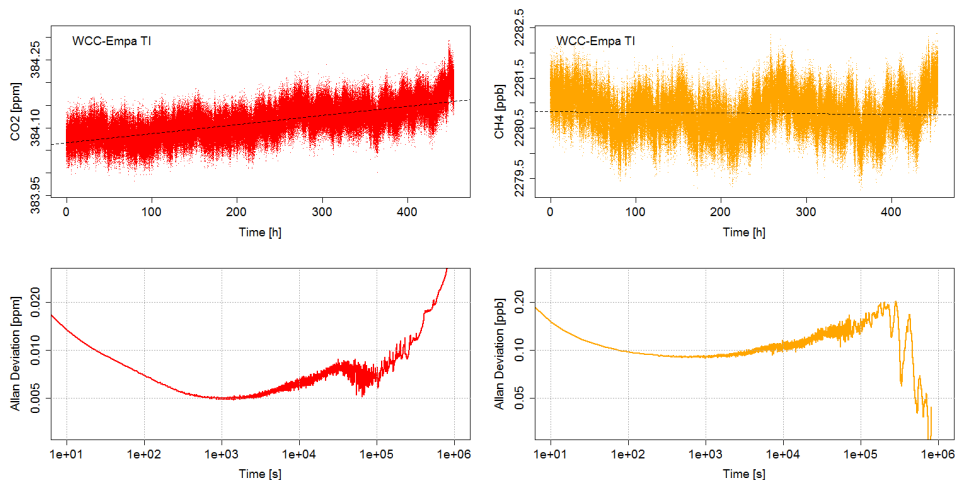
The screenshot displays a web-based interface for data management. At the top, there are tabs for 'File', 'Contact', 'Observation', 'Reference(s)', and 'Gallery'. Below these is a search bar with the text 'Search by a keyword: (start typing)'. The main content area is divided into two sections: 'Organization' and 'Observation'. The 'Organization' section shows details for 'DMC' (Direccion Meteorologica de Chile), including its address and website. The 'Observation' section shows details for a specific observation, including the instrument used (Picarro Inc., G2401, S/N CFKADS2031) and the calibration scale (WMO CO2 X2007). A red circle highlights the text 'WMO CO2 X2007' in the 'Calibration Scale' field. A red arrow points to the 'Data header' text on the left side of the slide.

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/

Observation							
Collaborator(s)	<table border="1"><tbody><tr><td>NO</td><td>23</td></tr><tr><td>Acronym</td><td>Empa</td></tr><tr><td>Name</td><td>Swiss Federal Laboratories for Materials Science and Technology</td></tr></tbody></table>	NO	23	Acronym	Empa	Name	Swiss Federal Laboratories for Materials Science and Technology
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 1 min 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						

Instrumentation – frequency of calibration and QA/QC

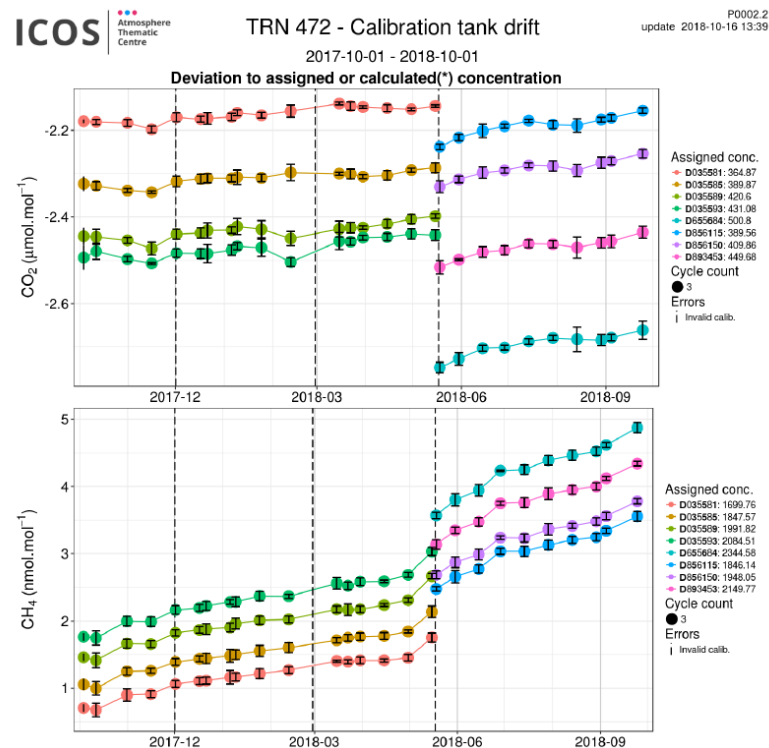
laboratory tests



Zellweger et al., 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. ..."

(long-term) field tests



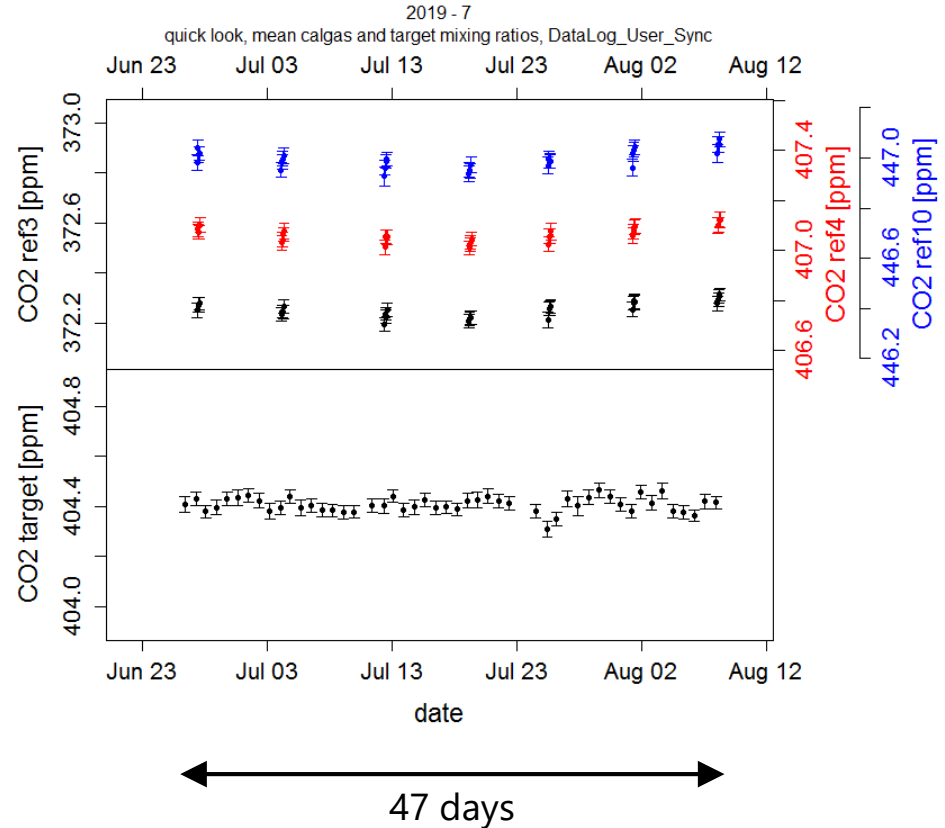
Yver-Kwok et al., 2020

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.

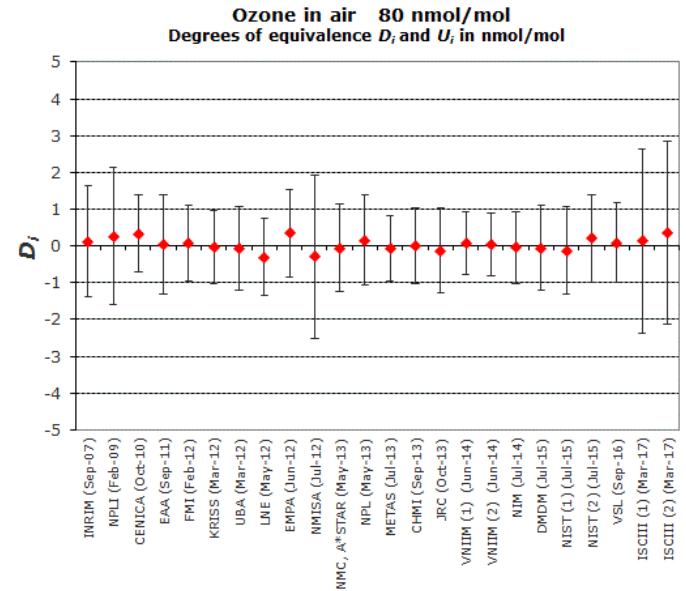
Target references do not need to be of the highest hierarchy, thus, are usually less expensive and can be used up faster. Therefore, more frequent analysis is possible, which will in turn allow fast detection of instrumental artefacts.

Appropriate processing software needs to be available.



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)

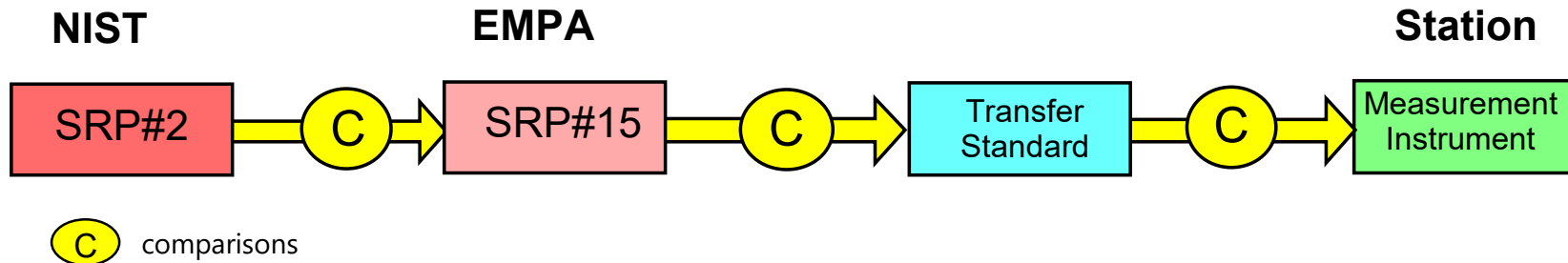
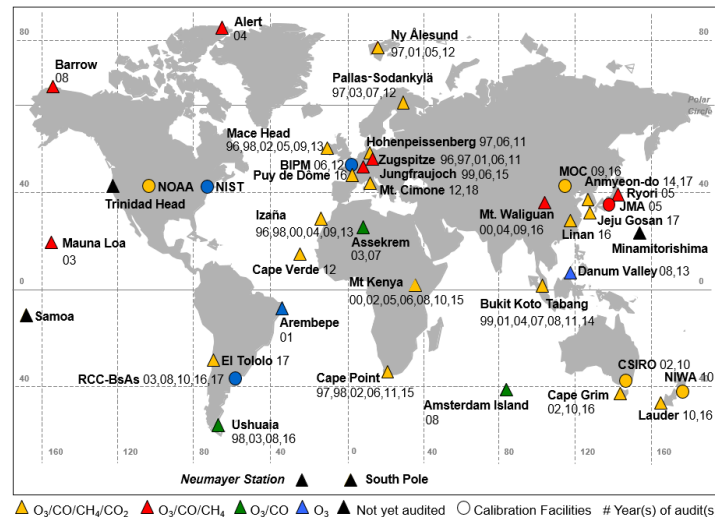
World reference: SRP #2 at National Institute for Standards and Technology

Currently: approx. 60 SRPs worldwide

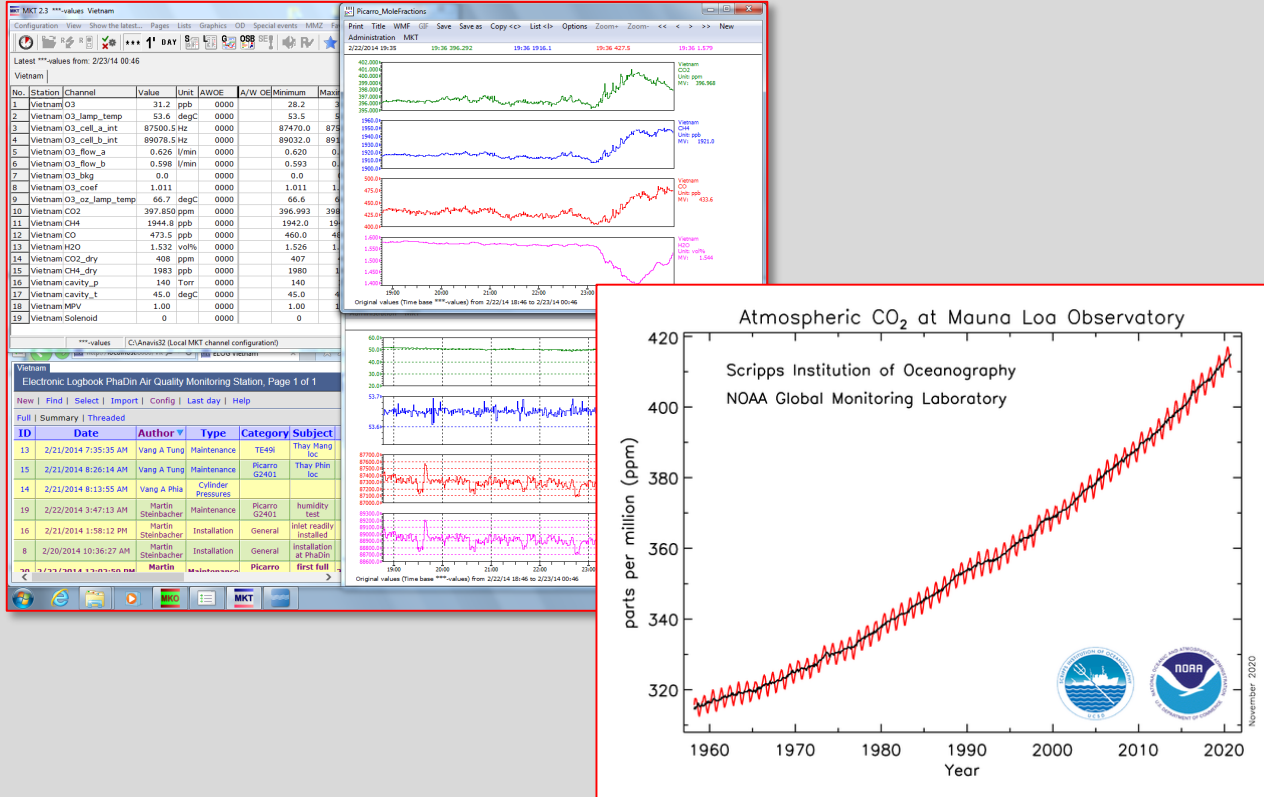
Transfer standard / calibrator is calibrated against a reference photometer and used for the calibration of ozone instruments

Traceability chain:

WCC-Empa Audits / Comparisons 1996 – 2018




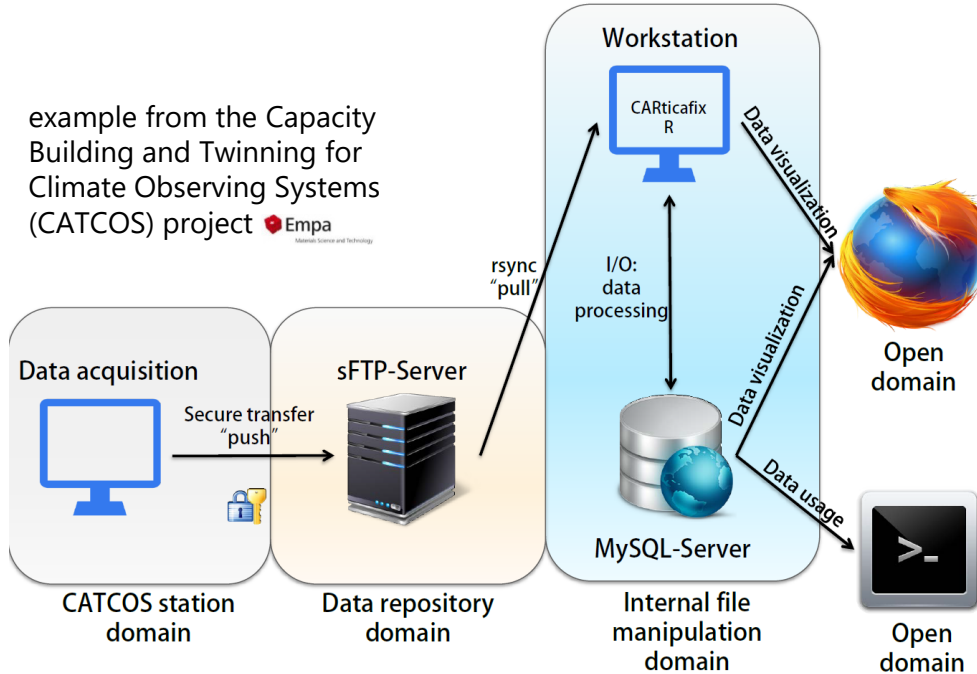
Data management & data processing



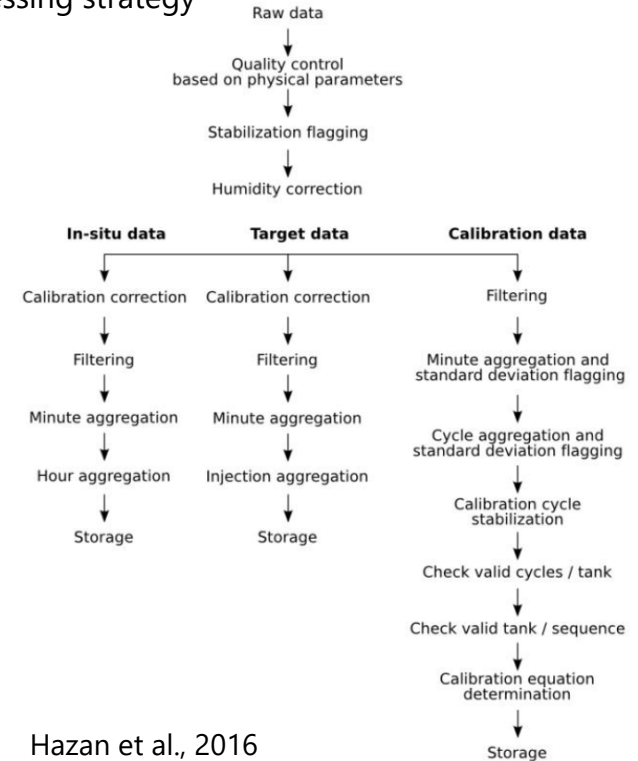
Data management

overall concept

example from the Capacity Building and Twinning for Climate Observing Systems (CATCOS) project  Empa
Materials Science and Technology



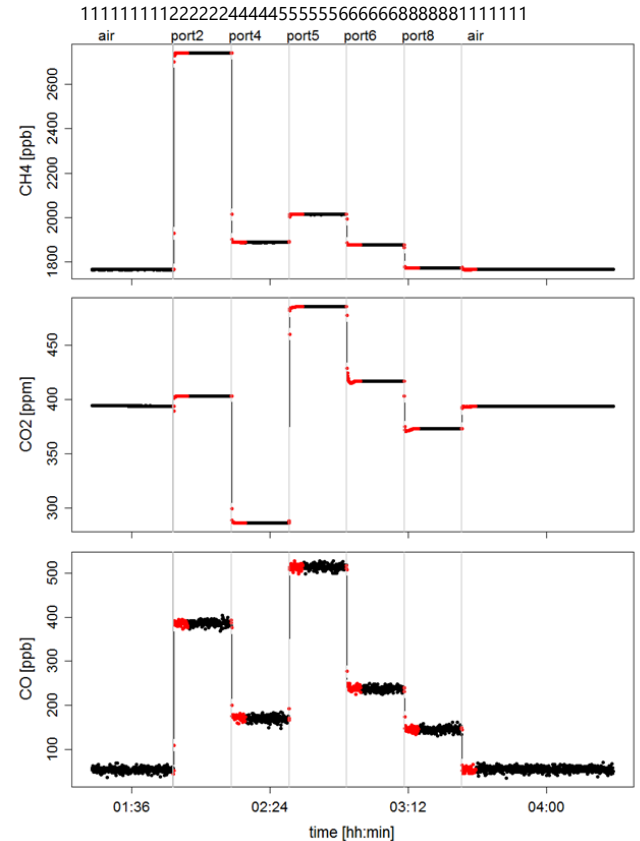
data processing strategy



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.



valve
position

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

Bureau International des Poids et Mesures – the intergovernmental organization through which Member States act together on matters related to measurement science and measurement standards.

Search facility:

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ABOUT US WORLDWIDE METROLOGY INTERNATIONAL EQUIVALENCE SI UNITS SERVICES PUBLICATIONS MEETINGS

> You are here: publications > guides > Guide to the Expression of Uncertainty in Measurement (GUM)

GUM: Guide to the Expression of Uncertainty in Measurement

In order to benefit fully from the hyperlinking between the documents, the reader is advised to download all JCGM documents presently available in one ZIP file.

→ The fundamental reference document is the *Guide to the Expression of Uncertainty in Measurement* (GUM):

↓	<i>Evaluation of measurement data – Guide to the expression of uncertainty in measurement</i> JCGM 100:2008 (GUM 1995 with minor corrections)	
Note: JCGM 100:2008 is also available in HTML form from the JCGM portal on ISO's website.		

→ The JCGM Working Group 1 (JCGM-WG1) is producing a series of documents to accompany the GUM. The first four of these documents have been approved and are available for download as PDF files. Printed copies are available for purchase from ISO.

↓	<i>Evaluation of measurement data – An introduction to the "Guide to the expression of uncertainty in measurement" and related documents</i> JCGM 104:2009	
↓	<i>Evaluation of measurement data – Supplement 1 to the "Guide to the expression of uncertainty in measurement" – Propagation of distributions using a Monte Carlo method</i> JCGM 101:2008	
↓	<i>Evaluation of measurement data – Supplement 2 to the "Guide to the expression of uncertainty in measurement" – Extension to any number of output quantities</i> JCGM 102:2011	
↓	<i>Evaluation of measurement data – The role of measurement uncertainty in conformity assessment</i> JCGM 106:2012	
↓	<i>Evaluation of measurement data – Concepts and basic principles</i>	

The following documents are at an early stage of preparation:

↓	<i>Evaluation of measurement data – Supplement 3 to the "Guide to the expression of uncertainty in measurement" – Modelling</i>	
↓	<i>Evaluation of measurement data – Applications of the least-squares method</i>	

Related articles

GUM:

- **BIPM Workshop on Measurement Uncertainty**
- Software related to the GUM and the GUM supplements 1 and 2
- Tutorial for metrologists on the probabilistic and statistical apparatus underlying the GUM and related documents
- Bibliography on Uncertainty
- News from JCGM-WG1
- JCGM Working Group 1

VIM:

- "Annotated VIM3"
- The rationale for VIM3
- FAQs on the VIM3
- News from JCGM-WG2
- JCGM Working Group 2

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

Data management – measurement uncertainty

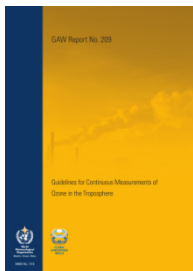
Table 1 - Example of an uncertainty budget of an ozone analyser

Component (y)	Source	Distribution	Contribution to $u(x)$
Imperfect calibration / linearity	Comparison between TS and OA	Rectangular	$0.0017 \cdot x'$
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 ₂ O 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

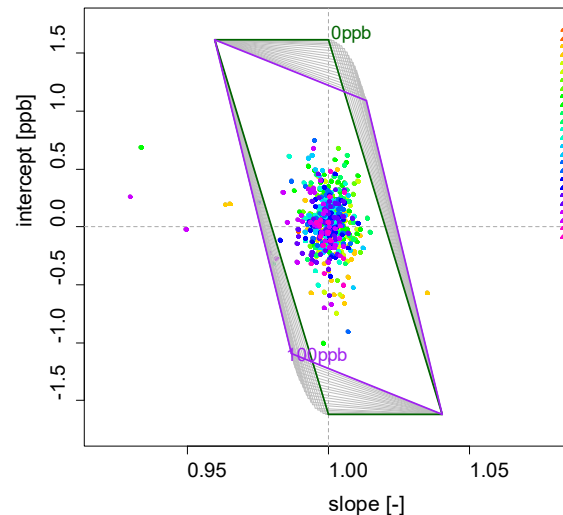
A conservative estimate of the total uncertainty can now be obtained by combing the uncertainties of the ozone analyser (13), the transfer standard (12) and the primary reference (11).

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



O₃ measurement guidelines,
GAW Report Nr. 209, 2013

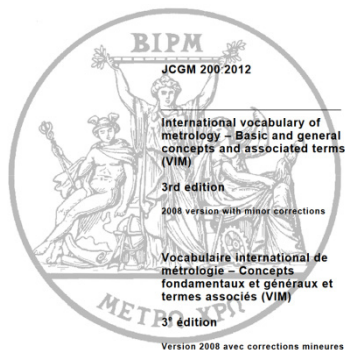
Intercept vs. slope plot for 559 calibrations of various ozone analysers with transfer standards within the Swiss National Air Pollution Monitoring Network between November 2005 and April 2017



Tarasick et al., 2019, Elemanta

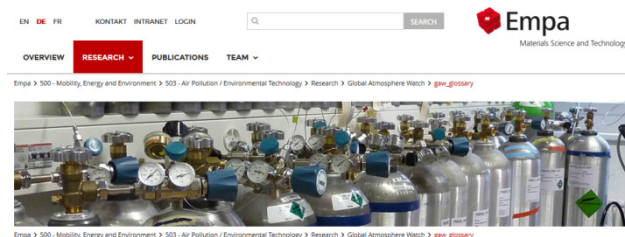
Data management – terminology

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



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

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Glossary

Alphabetical list of terms

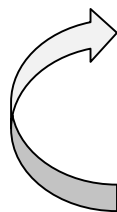
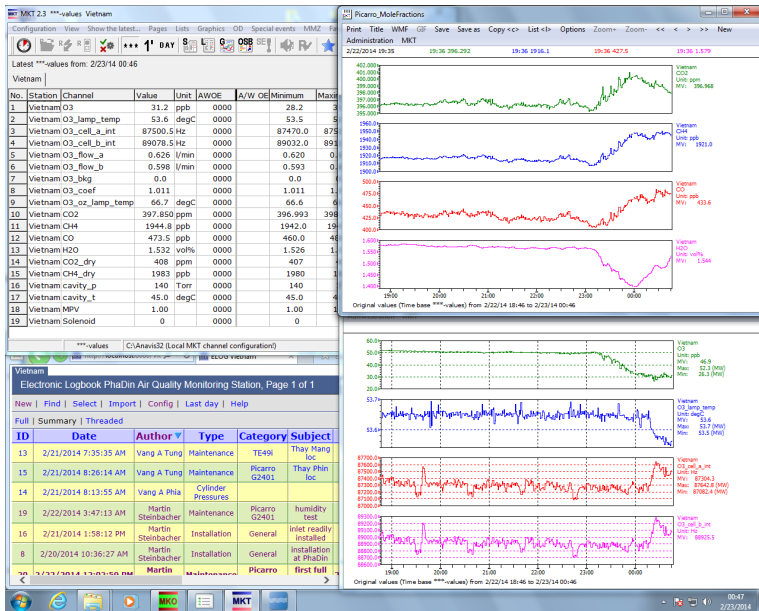
[accuracy](#) | [adjustment of a measuring system](#) | [audit](#) | [calibration](#) | [calibration curve](#) | [calibration hierarchy](#) | [Central Calibration Laboratory \(CCL\)](#) | [certified reference material](#) | [combined standard measurement uncertainty](#) | [concentration](#) | [conventional 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](#) | [mesurand](#) | [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](#)

Data management

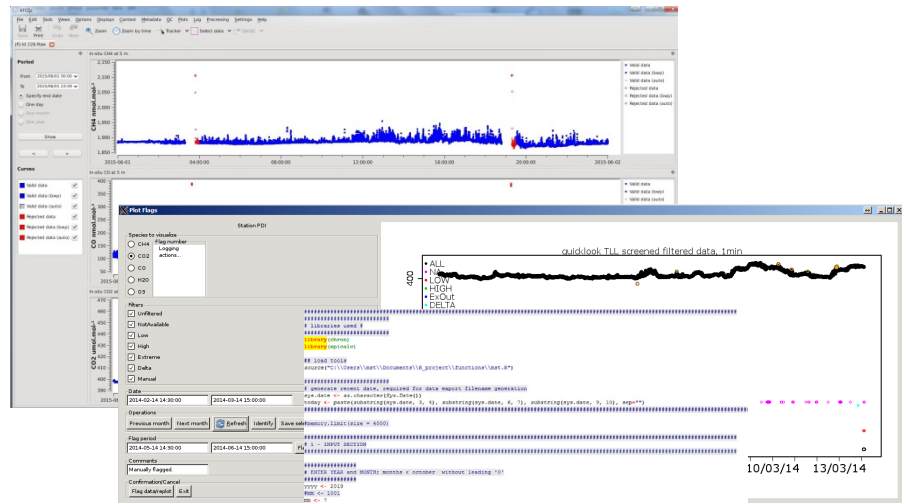
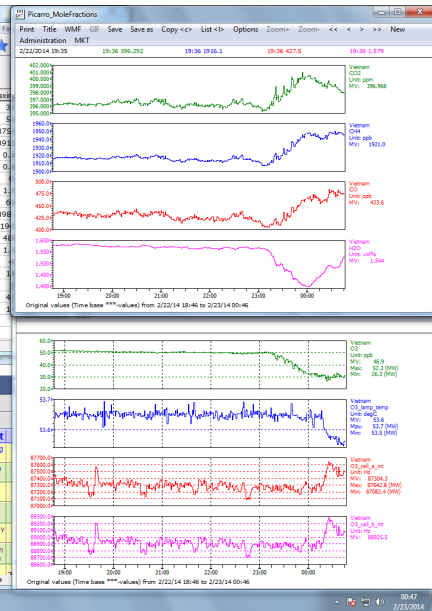
IT (hardware and software) resources are needed

on-site

central data processing unit



log book (meta data management) !



Metadata management

- documentation, log books

The screenshot displays a virtual machine environment. On the left, a file manager window shows a directory structure with files like 'logbook.log', 'ports log', and 'hardware info'. The main window is a logbook application titled 'Electronic Logbook Los Gatos Research NZO/CO analyzer 23r'. It features a table of log entries with columns for ID, Date, Author, Type, Category, Subject, and Event Date. The selected entry (ID 20) is shown in a detailed view, including fields for 'Entry time', 'Author', 'Type', 'Category', 'Subject', and 'Event Date'. The 'Text' field contains a detailed description of a measurement procedure involving a membrane flowmeter and a multiport unit.

ID	Date	Author	Type	Category	Subject	Event Date	Text
20	3/26/2013 12:46:21 PM	mt134	Multipoint	Tests	overflow checks	3/26/2013 12:46:15 PM	Flows measured with ADM3000 membrane flowmeter after measurements stopped; ports selected by activating the port with the hardware switch.
19	1/9/2013 8:22:52 AM	mt134	NZO/CO-23r	General	Passwords	1/9/2013 10:21:20 AM	New password set under the Unix Environment for: root@losgatos.com
18	1/9/2013 8:22:52 AM	mt134	NZO/CO-23r	General	Passwords	1/9/2013 10:21:20 AM	New password set under the Unix Environment for: root@losgatos.com

Metadata management

- documentation, log books
- checklists / standard operation procedures

The image displays four overlapping screenshots of a maintenance checklist for a Picamo analyser. The documents are from GAW (Graz University of Applied Sciences) and Empa (Materials Science and Technology). The checklist is titled 'Maintenance and Quality Control of the Picamo Analyser' and is for the 'Picamo G2M1' model. It includes contact information for Dr. Martin Steinbacher at Empa and CATGOS (Central Analytical Testing Group of Graz University of Applied Sciences).

Every week:

- Turn on screen, select Picamo window (at the bottom; save)
- Go to External Valve Sequence Value Sequencer isn't shown
- Select Data Acquisition on Baseplots', press 'Show', if values at Chelpon Ata are: 1200 gpb, H2O: 0 to 4 vol%
- Check inlet flow at the front if not adjust the flow and m

Add a new comment in the e-log (e.g. Type "checked")

Every month:

- Backup all data from the Picamo analyser
 - Data acquisition computer: C:\Data\hour
 - C:\Data\elog\log on an USB stick
 - Picamo computer: copy C:\UserData\Data on an USB stick

Add a new comment in the e-log (e.g. Type "Done")

Every 6 months:

- Change filter at the back of the Picamo calibration unit (January and July)
 - Remove filter holder, open large screw, replace filter, put filter holder back in place
- 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 e-log (e.g. Type "Maintenance", Category "Picamo G2M1", Subject "Filter (back of calibration unit) replaced")

Add a new comment in the e-log (e.g. Type "Maintenance", Category "Picamo G2M1", Subject "Roof-top filter replaced")

Metadata management

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

The screenshot displays the GAWSiS Station Information System interface. The top navigation bar includes links for Home, Search, and a search input field. The main content area is titled 'Pha Din (Viet Nam)' and provides detailed station characteristics. A sidebar on the left lists navigation options: Station, Instrument, Contact, and Bibliographic Reference. The main content is organized into sections: Station characteristics, WMO region, Climate zone, and Programs / network affiliations. A photo gallery section indicates that there are no photos available for this station. The Programs / network affiliations section includes a table with columns for Program / network affiliation, Program specific ID, Status, Calculated status, Declared status, and From. The table shows one entry for GAW Regional with a PDI ID, Approved status, Operational calculated status, Operational declared status, and a start date of 2014-02-23. Below the table, there is a section for Observations / measurements, which includes links for Aerosol > Optical properties, Gas > Greenhouse Gas, Gas > Ozone, and Gas > Reactive Gas. A map of the station location is also visible on the right side of the page.

Home Search

Station

Instrument

Contact

Bibliographic Reference

Homepage > Search > Station search > Station report details

Pha Din (Viet Nam)
GAW Regional station in WMO Region II - Asia

Station characteristics

Name: Pha Din

Station alias:

Date established: 2014-02-23

Declared reporting status: Operational

Calculated reporting status: Operational

Station type: Land (land)

GAW ID: PDI

WIGOS Station identifier(s):

WIGOS Station Identifier	Primary
0-20008-0-413	

WMO region: II - Asia

Country / Territory: Viet Nam

Coordinates: > 21 5731'N, 103 5167'E, 1466m

Time zone: > UTC+7

Site description:

Prevalving wind directions: NE in winter and SW in summer. Temperature: 25-30 ˚C in summer and down to 3 ˚C in winter. No snow or ice in winter. Rainfall and humidity: The site is in clouds a considerable fraction of the year with a correspondingly high relative humidity all year long.

Population: No residents at the station except for the custodians. No relevant residential areas within 10-20 km, except for sparse individual farm houses. The closest farm house is located in 1 km distance in NE direction, and cover Mountain hill area covered with forest. The station itself is above the canopy. Possible influence of local and regional emissions: Occasional corn plant burning in March and April. Staff housing (gas cooking, electrical heating, occasional trash burning) is at the station. No coal power plants and other industrial activities in the region.

Climate zone: > (unknown)

Predominant surface cover:

Surface roughness:

Topography or bathymetry:

Population in 10km / 50km (in thousands):

Station / platform event logbook:

Photo gallery

There are no photos available for this station.

Programs / network affiliations:

Program / network affiliation	Program specific ID	Status	Calculated status	Declared status	From	To
GAW Regional	PDI	Approved	Operational	Operational	2014-02-23	

Observations / measurements

- > Aerosol > Optical properties
- > Gas > Greenhouse Gas
- > Gas > Ozone
- > Gas > Reactive Gas

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

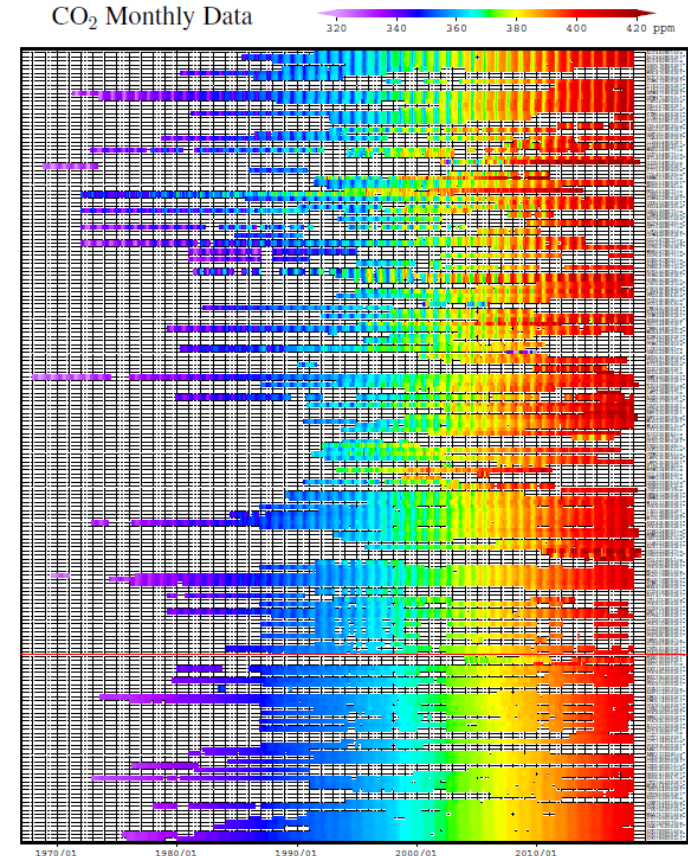
PUBLISHED BY
JAPAN METEOROLOGICAL AGENCY
IN CO-OPERATION WITH
WORLD METEOROLOGICAL ORGANIZATION

March 2020



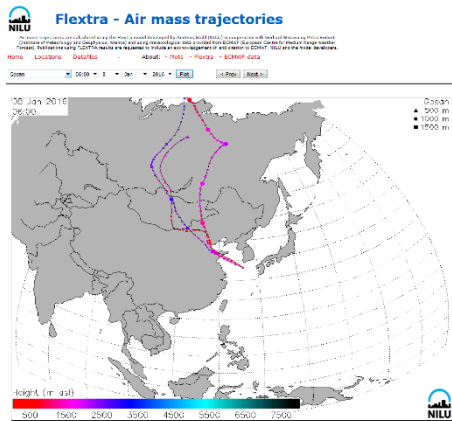
WDCGG Data Summary
Report #43, 2020

CO₂ Monthly Data

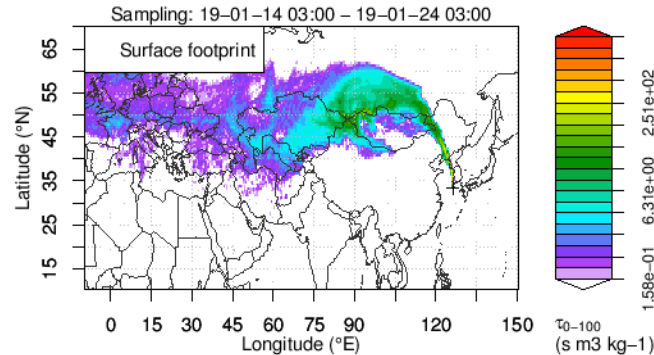


Additional quality control

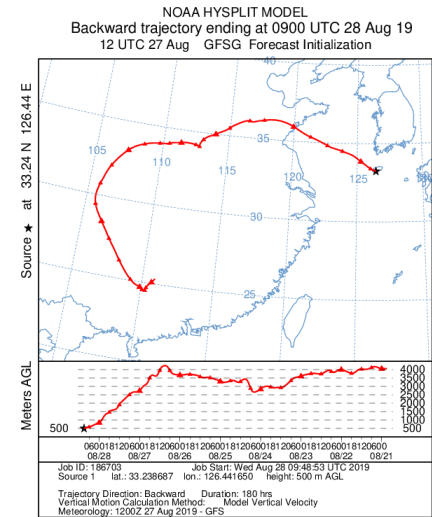
- participation in comparison (e.g. round robin) exercises
- comparison of data with data from «similar» stations
- use available online tools for trajectory calculations, e.g.



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



<http://lagrange.empa.ch/>



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

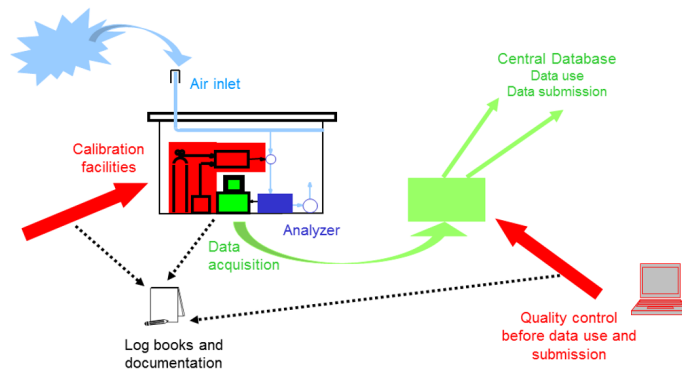
Conclusions

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
- ...

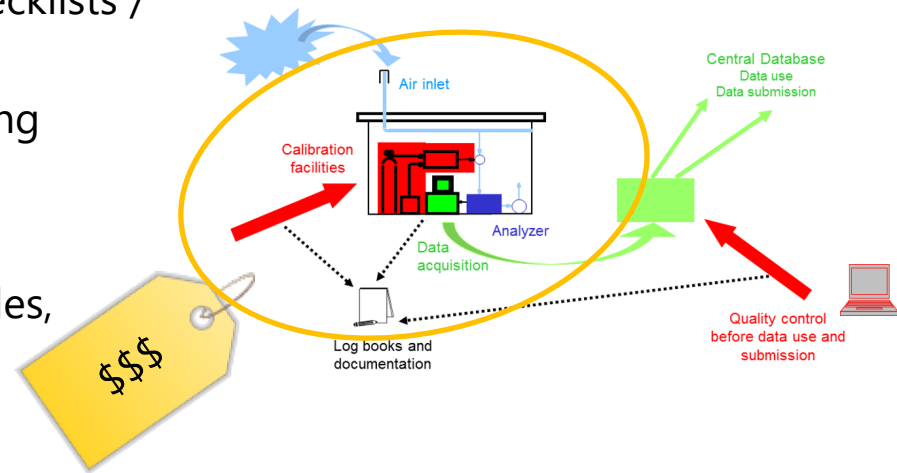
Instrument(s) and periphery

- 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.

Tarasick et al., Tropospheric Ozone Assessment Report: Tropospheric ozone from 1877 to 2016, observed levels, trends and uncertainties, Elementa, 7 (39), <https://doi.org/10.1525/elementa.376>, 2019.

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.

Yver-Kwok et al., Evaluation and optimization of ICOS atmospheric station data as part of the labeling process, Atmospheric Measurement Techniques Discussion, in review, <https://doi.org/10.5194/amt-2020-213>, 2020.

Zellweger et al., Recent advances in measurement techniques for atmospheric carbon monoxide and nitrous oxide observations, Atmos. Meas. Tech., 12, 5863–5878, <https://doi.org/10.5194/amt-12-5863-2019>, 2019.

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 !