

Long-term observations of atmospheric trace gases: challenges, implementation and operation



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BMKG webinar, 12 November 2020

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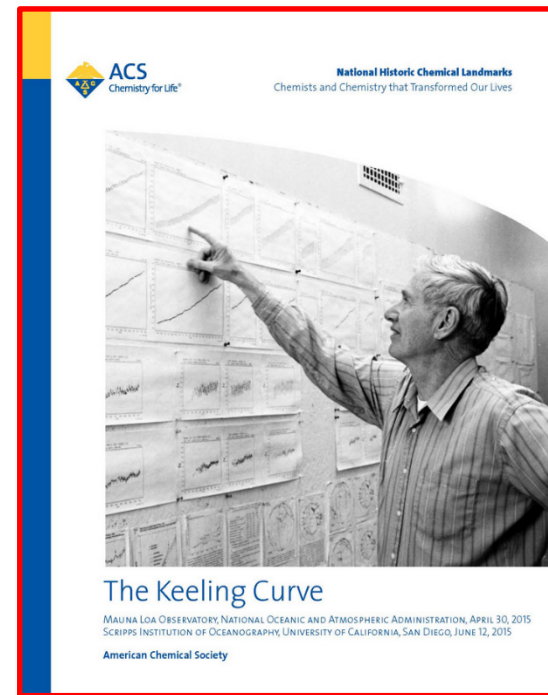
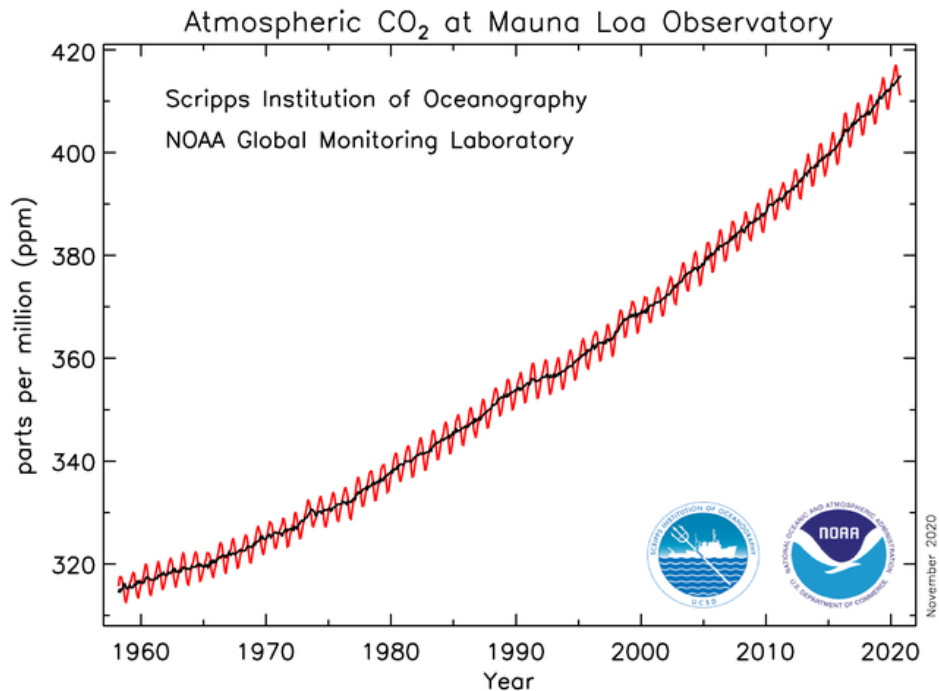
BMKG webinar, 12 November 2020

Key considerations – why ?

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

An iconic example – carbon dioxide (CO₂) at Mauna Loa

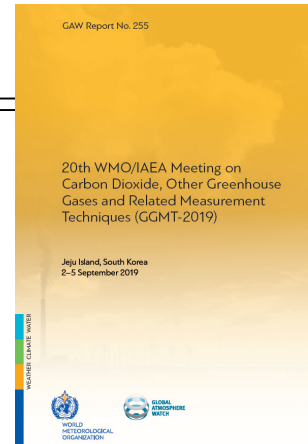
Most likely the best known atmospheric record



Example – targeted compatibility for 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. ..."

Example – targeted compatibility for CO₂

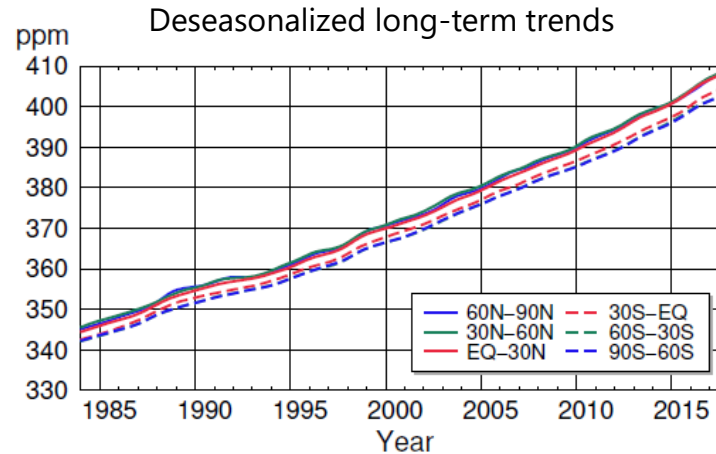
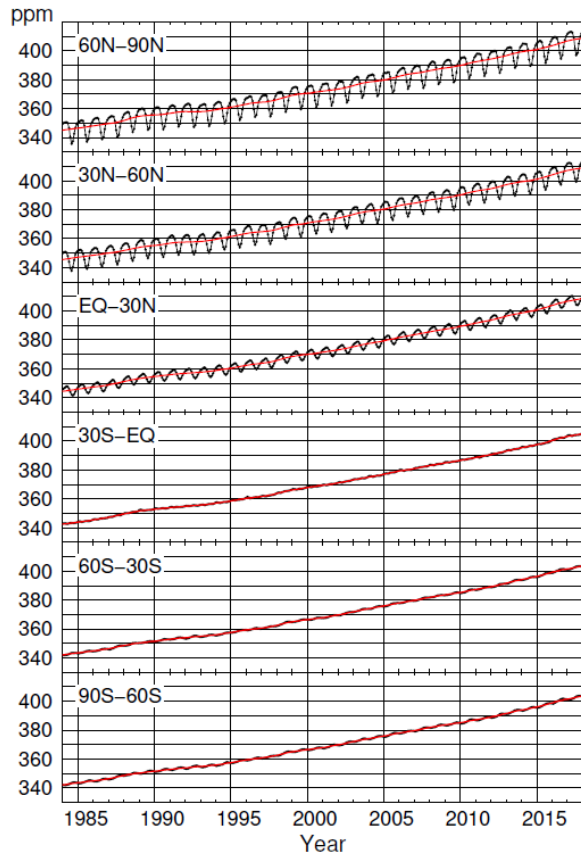
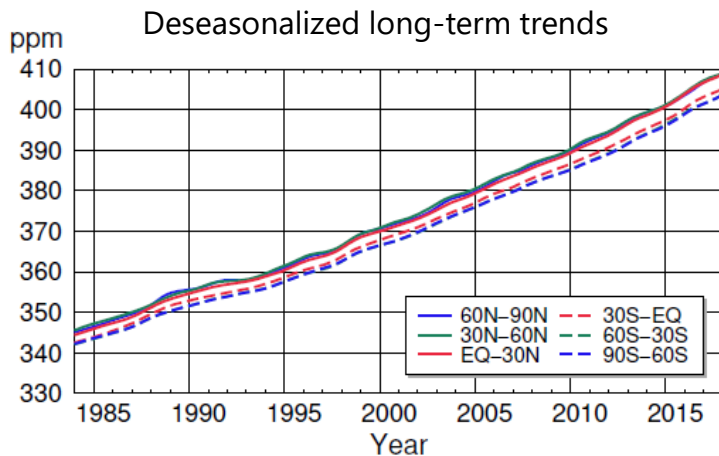
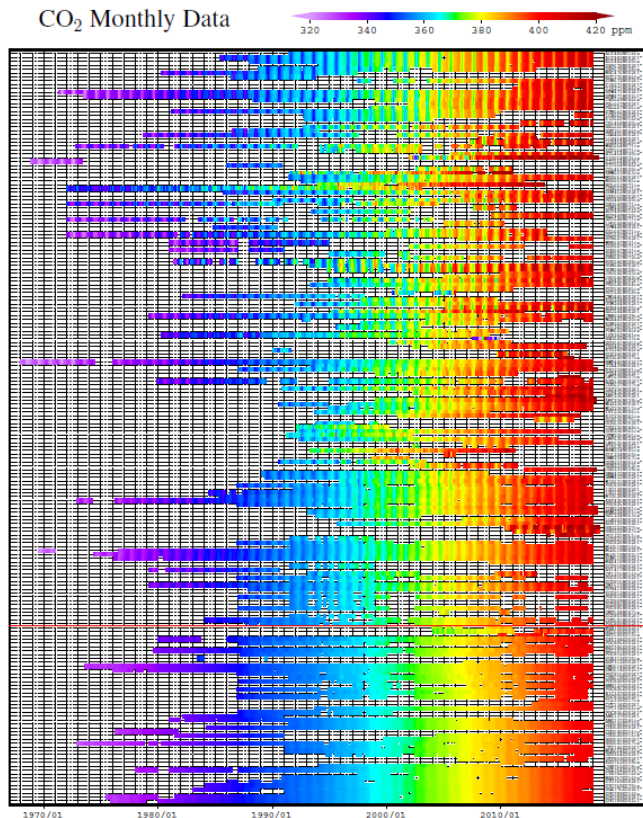


Fig. 1.3 Monthly mean mole fractions of CO₂ from 1984 to 2017 averaged over each 30° latitudinal zone (black) and their deseasonalized long-term trends (red).



Example – targeted compatibility for CO₂



- compatibility goals mainly motivated by small spatial gradients

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



Example – ozone: different goals for different tasks

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

Key consideration – which technique to be used ?

Useful resources:

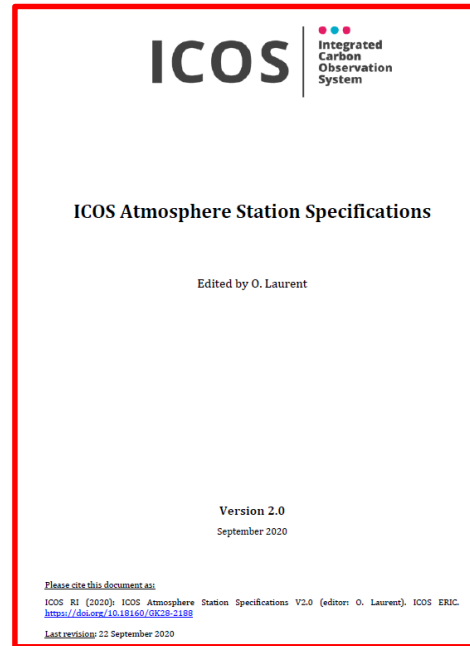
- WMO/GAW reports
- measurement guidelines



Key consideration – which technique to be used ?

Useful resources:

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

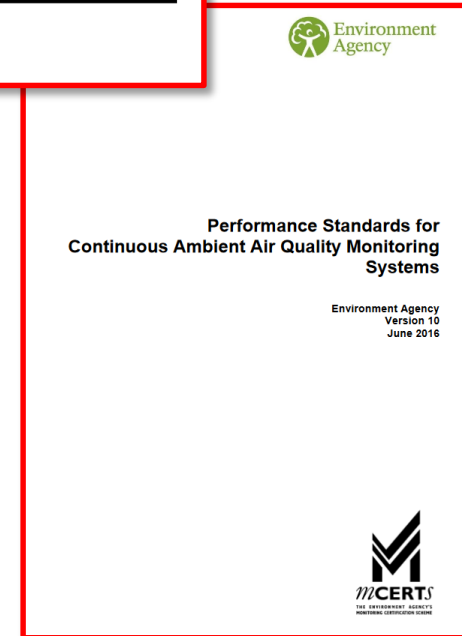
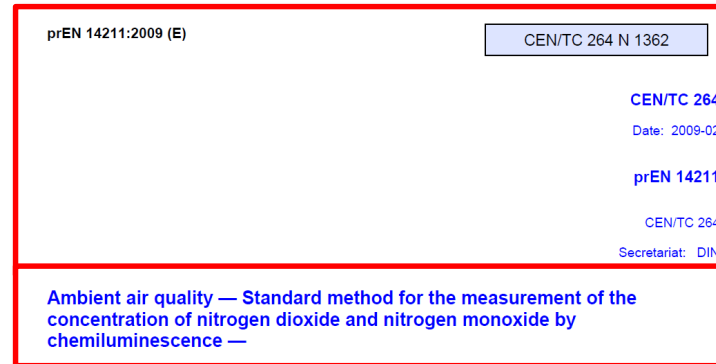
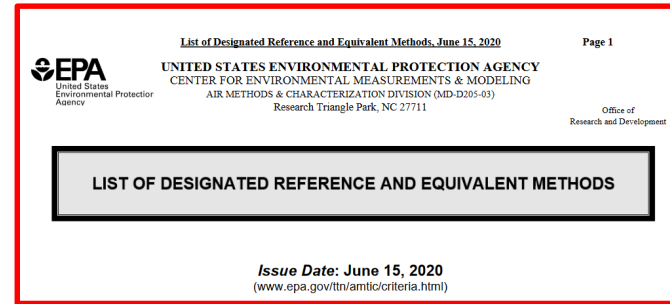


The image is a screenshot of a webpage from the Global Monitoring Laboratory (GML), part of Earth System Research Laboratories. The page title is 'How we measure background CO₂ levels on Mauna Loa'. It is authored by Pieter Tans and Kirk Thoning, NOAA Global Monitoring Laboratory, Boulder, Colorado. The page is dated September 2020. A note states: '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.' The 'Summary' section states: '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.' The section 'Mole fraction in dry air' includes a sub-section 'What do we need to measure?' and explains that the concentration of CO₂ in air is measured as a mole fraction, defined as the number of carbon dioxide molecules in a given number of molecules of air after removal of water vapor. It notes that 413 ppm of CO₂ in dry air means 413 molecules of CO₂ per million molecules of dry air. The page also mentions that 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%.

Key consideration – which technique to be used ?

Useful resources:

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



Key consideration – which technique to be used ?

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., 9, 4719–4736, 2016
www.atmos-meas-tech.net/9/4719/2016/
doi:10.5194/amt-9-4719-2016
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Automatic processing of atmospheric CO₂ and CH₄ mole fractions at the ICOS Atmosphere Thematic Centre

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Atmospheric
Measurement
Techniques
EGU

Atmos. Meas. Tech., 5, 657–685, 2012
www.atmos-meas-tech.net/5/657/2012/
doi:10.5194/amt-5-657-2012
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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. Fjåraa², E. Asimi², K. Sellegri³, R. Dupuy⁴, H. Venzac⁴, P. Villani⁴, P. Laj⁴, P. Aalto⁵, J. A. Ogren⁷, E. Swietlicki⁸, P. Williams⁹, P. Roldin⁹, P. Ounicev¹⁰, C. Hügel¹¹, R. Fierz-Schmidhauser¹², M. Gysel¹², E. Weingartner¹², F. Riccobono¹², S. Santos¹², C. Grüning¹², K. Faloon¹⁴, D. Beecher¹⁵, C. Monahan¹⁵, S. G. Jennings¹⁵, C. D. O'Dowd¹⁵, A. Marinoni¹⁶, H.-G. Horn¹⁷, P. H. McMurry¹⁸, Z. Deng²⁰, C. S. Zhao²⁰, M. Moerman²⁰, B. Henzing²¹, G. de I. 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 Laurent², Haeyoung Lee³, Sunin Kim⁴, Lukas Emmenegger¹, Martin Steinbacher¹, and Brigitte Buchmann²

ELEMENTA
Science of the Anthropocene

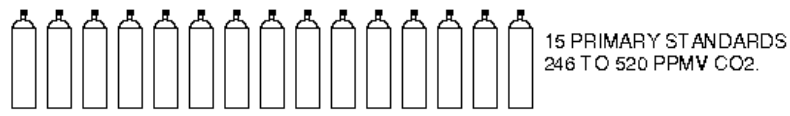
Tarasick, D. et al. 2019. Tropospheric Ozone Assessment Report: Tropospheric ozone from 1877 to 2016, observed levels, trends and uncertainties. Elem Sci Anth, 7: 39. DOI: https://doi.org/10.1525/elementa.376

REVIEW

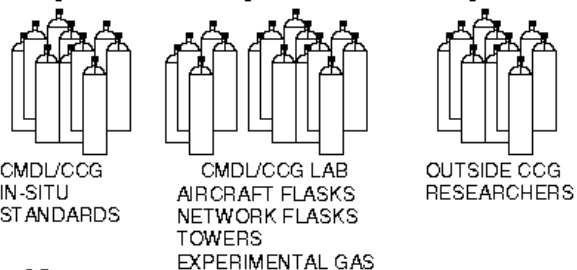
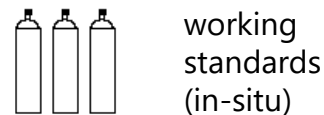
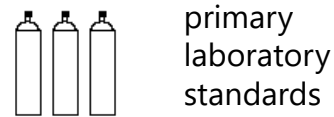
Tropospheric Ozone Assessment Report: Tropospheric ozone from 1877 to 2016, observed levels, trends and uncertainties

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, Prodomos 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

Key consideration – traceability and calibration



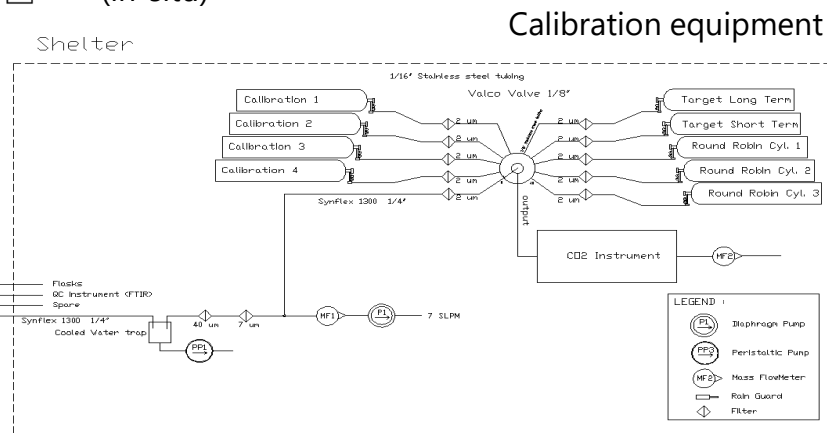
station operators



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]

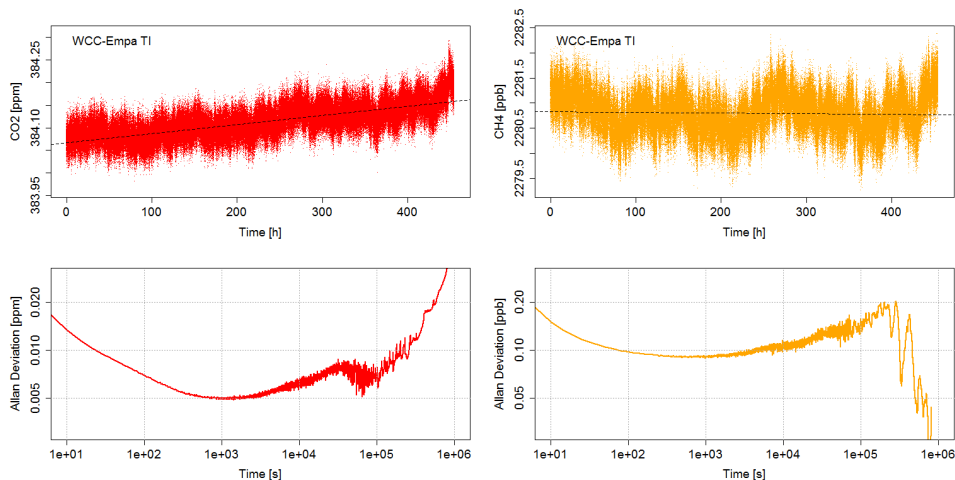
<https://www.esrl.noaa.gov/gmd/ccl/airstandard.html>



ICOS RI, 2020

Key consideration – frequency of calibration and QA/QC

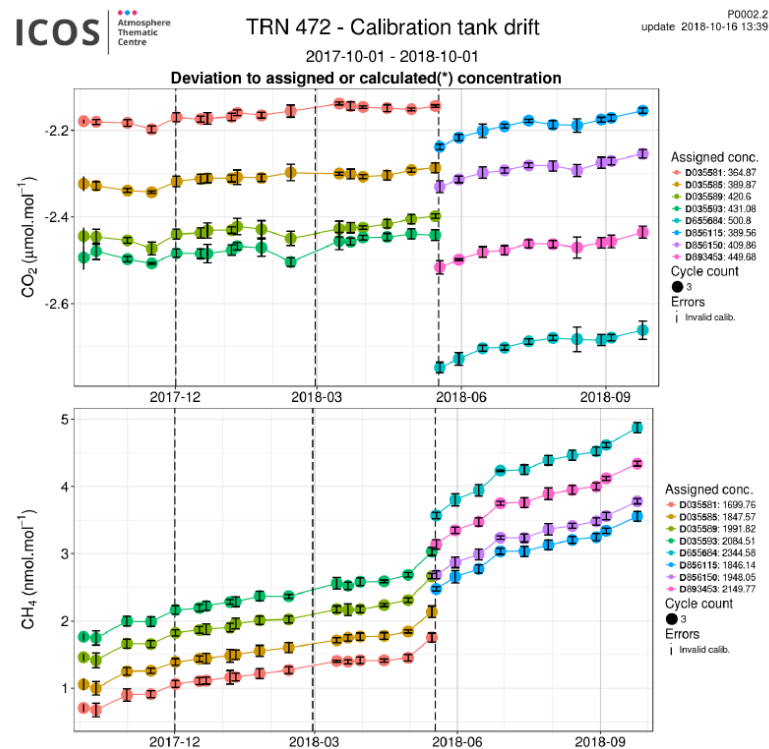
laboratory tests



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

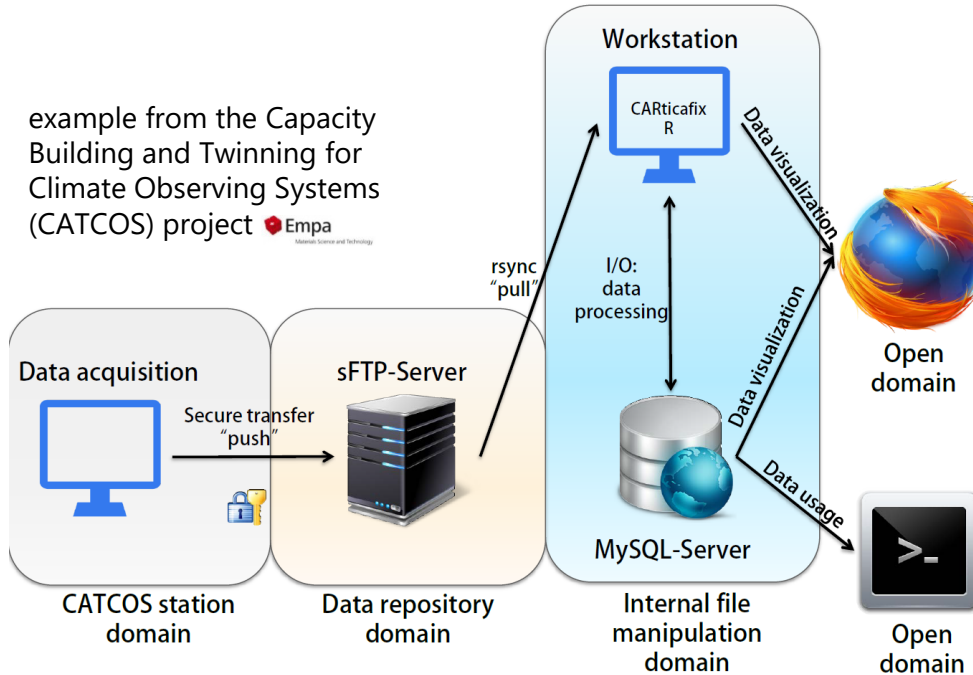


Yver-Kwok et al., 2020

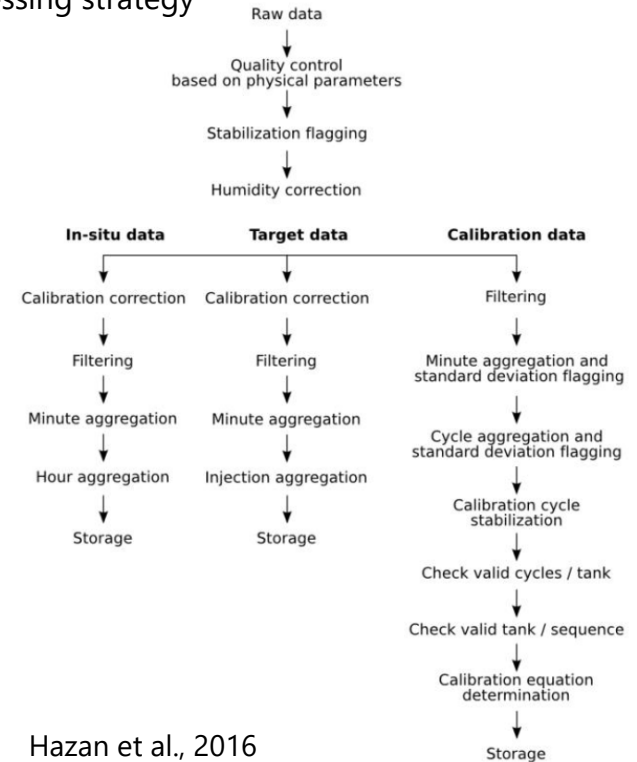
Key consideration – data Management

overall concept

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



data processing strategy



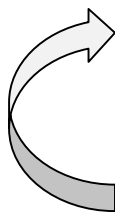
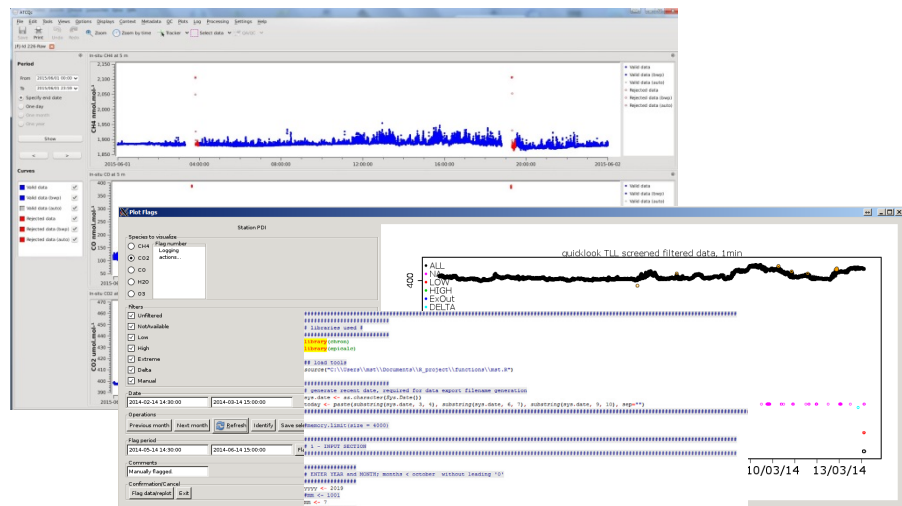
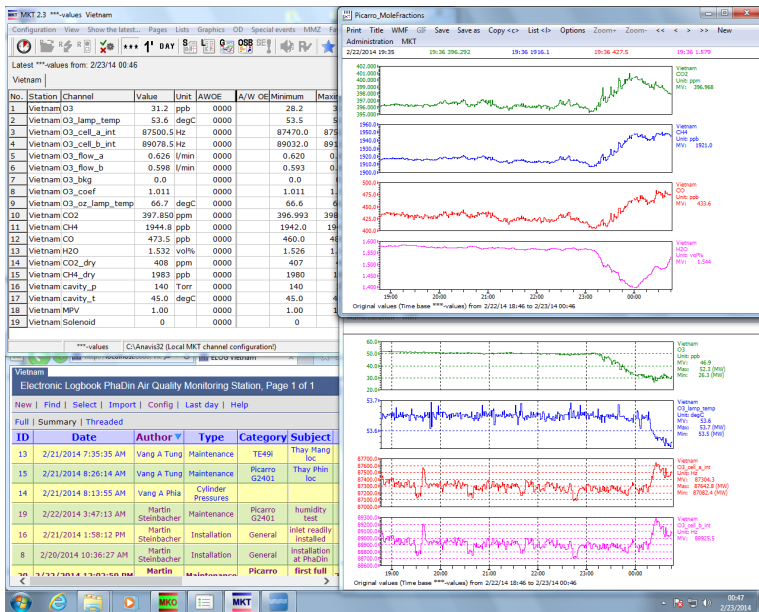
Hazan et al., 2016

Key consideration – data Management

IT (hardware and software) resources are needed

on-site

central data processing unit



log book (meta data management) !

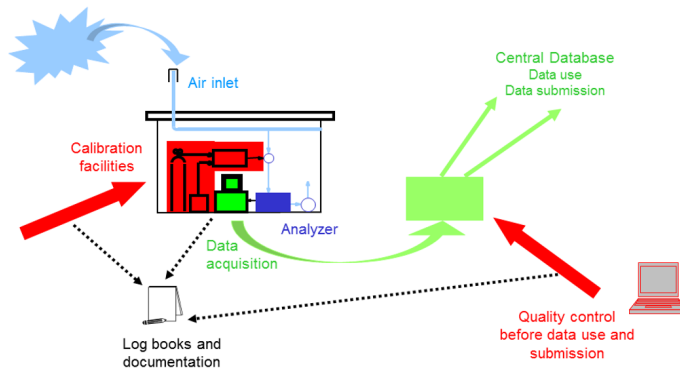
Conclusions – infrastructure requirements

Measurement site infrastructure

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

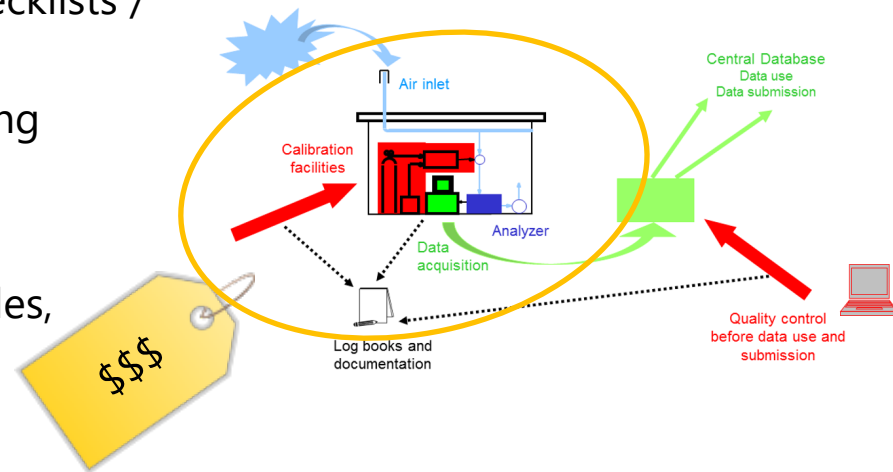
Instrument(s) and periphery

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



Conclusions – more general

- 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

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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Zellweger et al., Recent advances in measurement techniques for atmospheric carbon monoxide and nitrous oxide observations, *Atmospheric Measurement Techniques*, 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, *Atmospheric Measurement Techniques*, 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 !