Uncertainty, Stability and Traceability in Global Monitoring of Atmospheric Composition and the Role of WMO/GAW Central Calibration Facilities – Reality and Plans

Herman G.J. Smit (1), Gao Chen, Julian Groebner, Bradley Hall, Stelios Kazadzis, Alberto Redondas, Martin Steinbacher, Joele Viallon, Roeland Van Malderen, Christoph Zellweger, Shinya Takatsuji, Robert Wegener, Alfred Wiedensohler, Chris Lehmann

(1) Research Centre Jülich, Institute of Energy and Climate Research: Troposphere (IEK-8), 52425-Juelich, Germany (Email: h.smit@fz-juelich.de)

Motivation:

Reporting of measurement uncertainties and meta data (traceability and stability) is of growing interest and crucial when merging observational data from different platforms to address long term changes or when comparing and validate numerical models

Theme 1: Atmospheric Chemistry and Physics

BIPM-WMO Workshop on Metrology for Climate Action

On-line meeting on 26-30 September 2022.

Outline

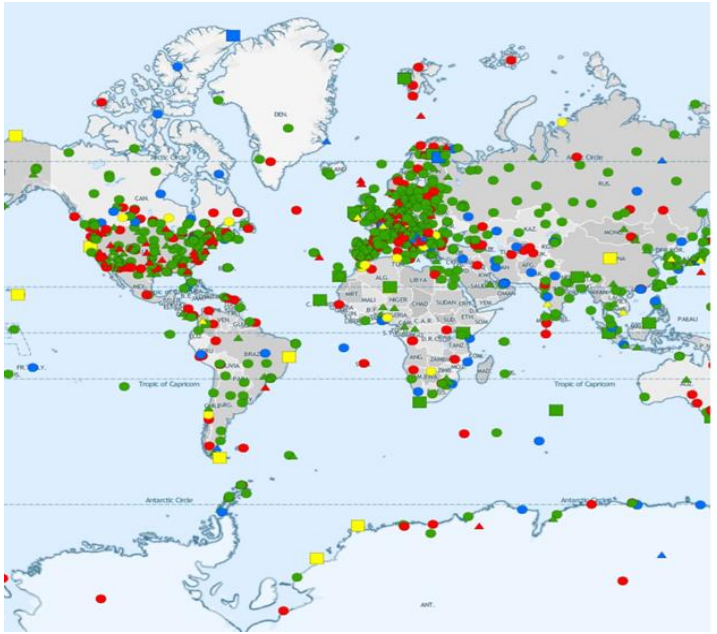
1. Introduction to WMO/GAW and its QA/QC Frame Work
2. GAW-Workflow within the new WMO-Organisation
3. Expert Team on Atmospheric Composition Measurement Quality
4. Traceability and Uncertainty within GAW
5. Overall Uncertainty and Data Quality Reporting within GAW
6. Outlook: Concept of Monitoring and Evaluation of GAW-QA/QC

GAW = Global Atmosphere Watch

GAW: Mission to Observe Atmospheric Composition

Better understanding of the increasing influence of human activities on Atmospheric Composition and subsequent environmental impacts through:

- ❑ Global network of stations doing long term quality controlled observations.
- ❑ Detect and document changes in atmospheric composition and its impact on air quality, weather and climate.
- ❑ Understand the underlaying processes and their causes.
- ❑ Service to public and policy makers



GAW-Global Network of Observation Stations
https://gawsis.meteoswiss.ch

>> Promote a "value chain" from observations to services

Classes of GAW-Global Measured Variables

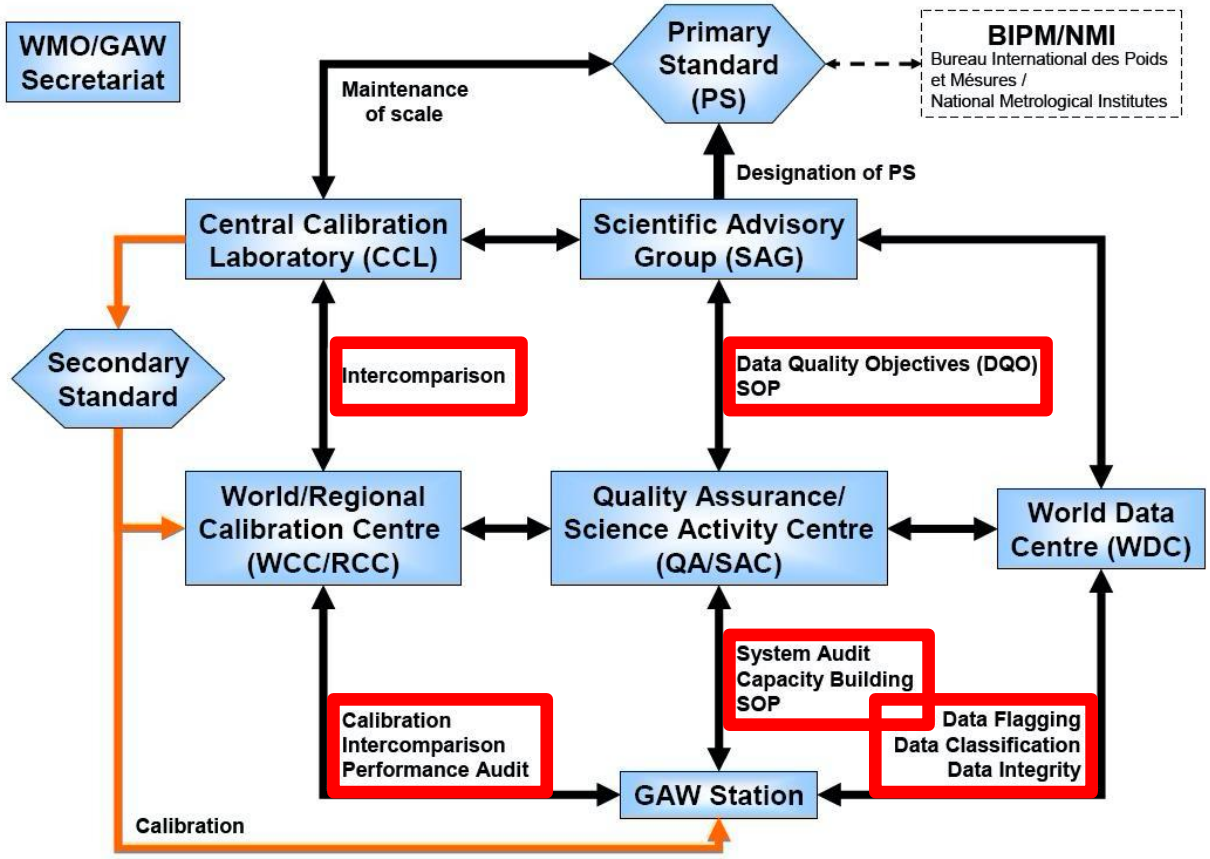
1. **Greenhouse Gases:** CO2, ^{13}CO2, CH4, N2O, SF6, (CFC's)
2. **Reactive Gases:** O3-Surface, CO, VOC, NOX, SO2, H2
3. **Ozone:** TCO (Dobson/Brewer), Sondes, Lidar, Umkehr, µWave
4. **Aerosols:** Physical Properties, Optical Depth, Chemical Properties
5. **Total Atmos. Depos.:** Wet & Dry Deposition
6. **Solar Radiation:** Ultra-Violet (UV) and Visible

GAW measurements are **long term and quality controlled** made within the GAW-QA/QC management framework that started in beginning of 1990's

Present QA/QC-Framework of WMO/GAW

GAW-Station = Class of Measured GAW Variables:

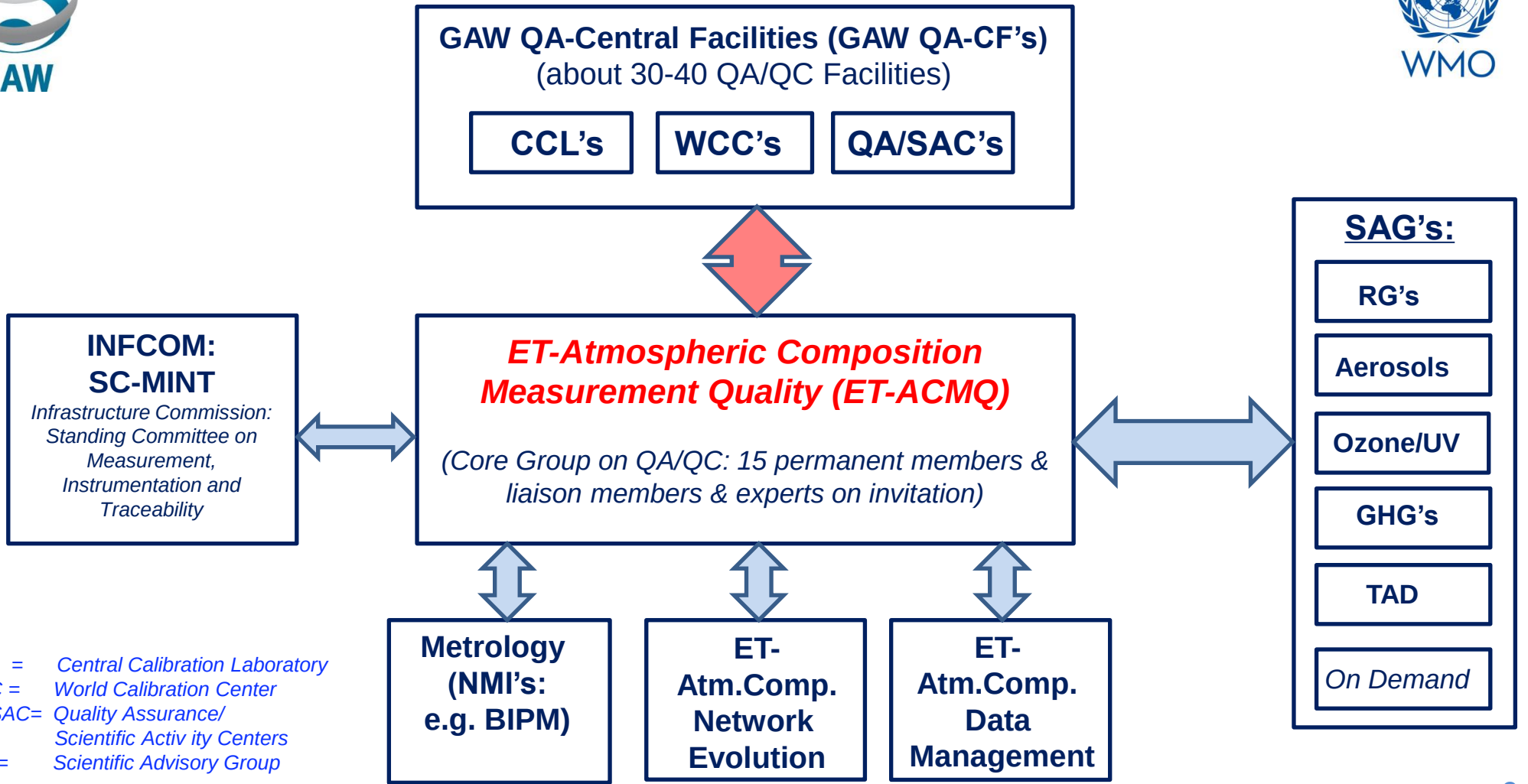
- GHG's
- RG's
- O3
- Aerosols
- TAD
- Radiation (UV-Vis.)



QA/QC schemes for the different classes of measured variables are coordinated independently from each other

New **ET-ACMQ** <u>also</u> for coordination among the different classes of measured variables

Interaction ET-ACMQ within GAW-Infrastructure



CCL. = Central Calibration Laboratory
WCC = World Calibration Center
QA/SAC= Quality Assurance/ Scientific Activ ity Centers
SAG= Scientific Advisory Group

GAW-QA/QC: Expert Team on Atmospheric Composition Measurement Quality (ET-ACMQ)

Mission

Bridging the QA/QC efforts in the different observation networks through:

- **Standardization and Harmonization** of **common** QA/QC components in the different observation networks:

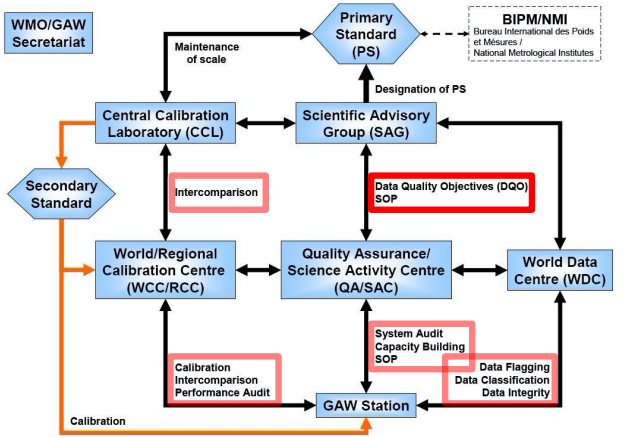
  >>>> What do we have? and What can we improve?

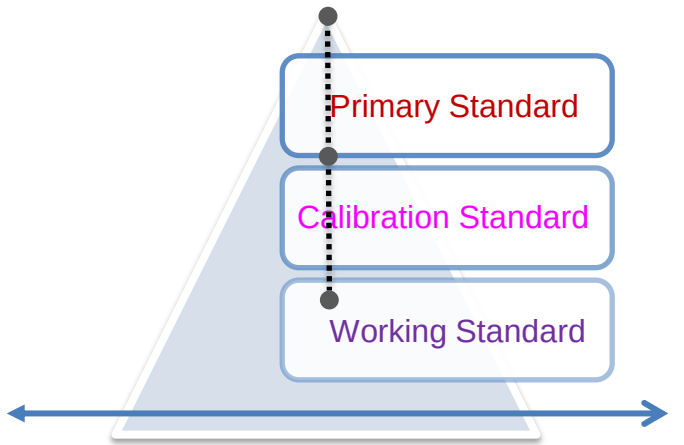
- **Monitoring and Evaluation of QA/QC** of the measurements done in the different observation networks: Develop and establish a common QA/QC Evaluation frame work (using e.g. templates for protocolls etc.)

  >>>> Quality assessed data in the different data centers

ET-ACMQ Direct Interaction with Metrology Community: Traceability and Uncertainty

- Traceability in GAW: What about measurement uncertainty?
- Which uncertainty shall be included?
- Measurement compatibility? How to compare measurements in time and space? Intercomparsion made “blinded”?
- How to maintain calibration chain short?
- How to maintain long-term stability?
- Are uncertainty on primary standards now comparable to DQO?
- How far GAW-CCL taking part in CIPM key comparison programme



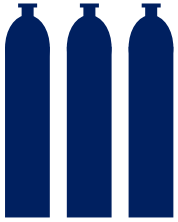


What about the measurement uncertainty?

➢ Among the different classes of measured variables there is a large inhomogeneity >>> **Need for harmonisation**

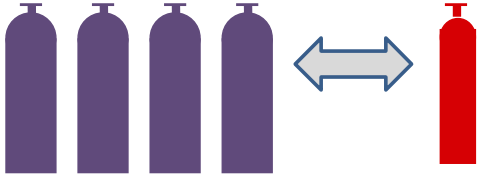
Traceability & Uncertainty: Example of GreenHouse Gases (GHG's)

Primary Standards



- Created or analyzed by absolute methods:
  - gravimetry
  - manometry (CO_2)
- Traceable to SI through mass, temperature, pressure

SECONDARY



Used to define instrument response on dedicated calibration systems

Dissemi-nated

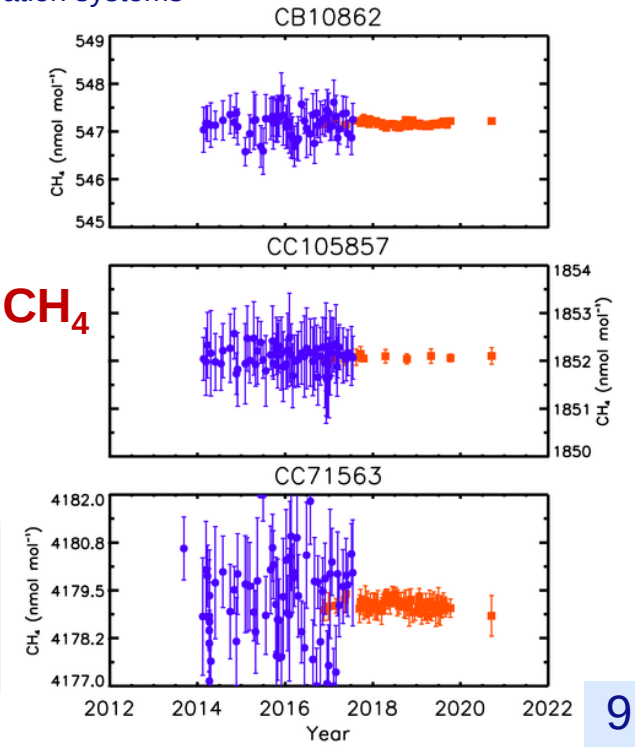
At present GHG's report **total uncertainty** and **scale transfer uncertainty**

	Total uncertainty (2-sigma)	Scale transfer uncertainty (2-sigma)
CH_4	3.5 ppb	0.2 ppb
CO_2	0.2 ppm	0.02 ppm
N_2O	1 ppb	0.2 ppb
SF_6	0.08 ppt	0.02 ppt

Scale transfer uncertainty can improve with time as newer instruments and methods are implemented (e.g. CH_4 improved by factor of five with new instrument)

[Source: Brad Hall et al., NOAA/GML, 2020]

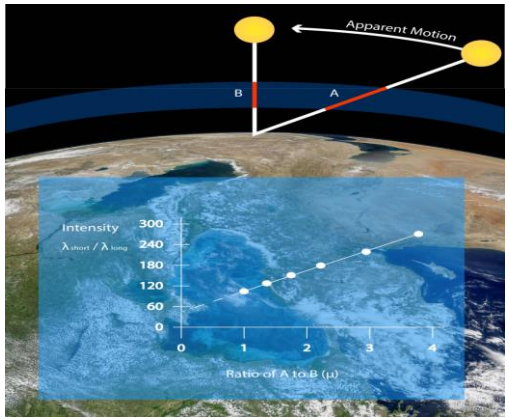
CH_4



- However, important is to have an uncertainty budget of ALL contributing parameters such as instrumental, sampling, calibration, etc….
- For better understanding of the key parameters contributing to the total uncertainty

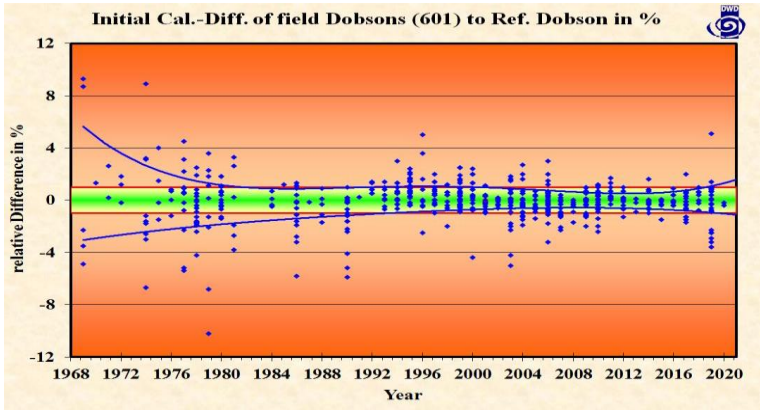
Traceability & Uncertainty: Example of Total Column Ozone (Dobson/Brewer)

Primary Standard:
Reference Instrument (Langley Calibration)



Secondary Standard:
Travel Reference

Intercomparison Campaigns:
Calibration with Travel Reference



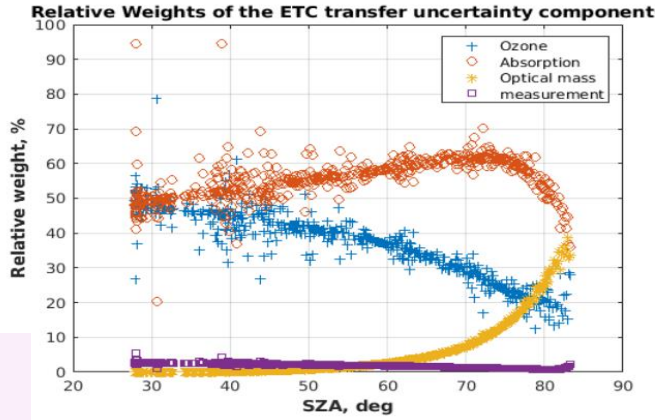
[Source: Ulf Köhler, DWD & McConville, NOAA/GML]

Uncertainty Budget Analysis for Brewer Instrument: Work in progress by Parra-Rojas and Redondas et al.)

Combined Standard Uncertainty: Gaussian propagation of errors

$$u_c^2(y) = \sum_{i=1}^{N} \left[\frac{\partial f}{\partial a_i}\right]^2 u^2(a_i) + 2 \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{\partial f}{\partial a_i} \frac{\partial f}{\partial a_j} u(a_i) u(a_j) R(a_i, a_j)$$

Uncertainty budget analysis taking all instrumental, atmospheric (incl solar), and sampling parameters into account

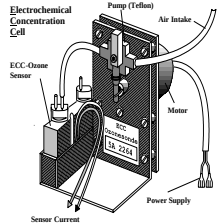


Goal

- **Measured data + Overall incl. key uncertainties + Meta data**
- **To be stored in the data archive**

Traceability & Uncertainty: Example of Ozone Sondes (O3S)

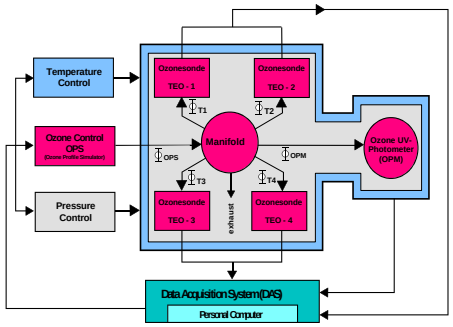
Balloon Ozonesonde



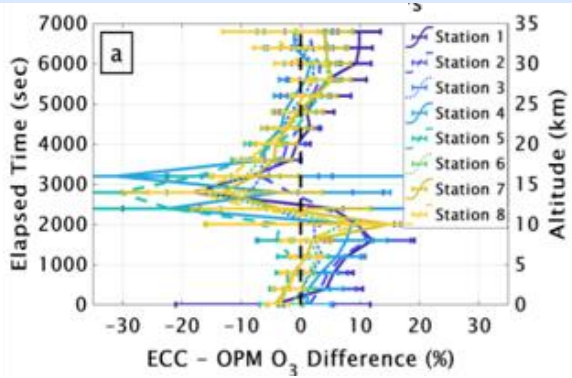
- Electrochemical Ozone sensor
- One way instrument
- No individual instrument calibration
- Only type calibration: JOSIE

Ozonesonde Types are calibrated against Ozone UV Photometer (OPM)
JOSIE: Juelich Ozone Sonde Intercomparison Experiment

WCCOS

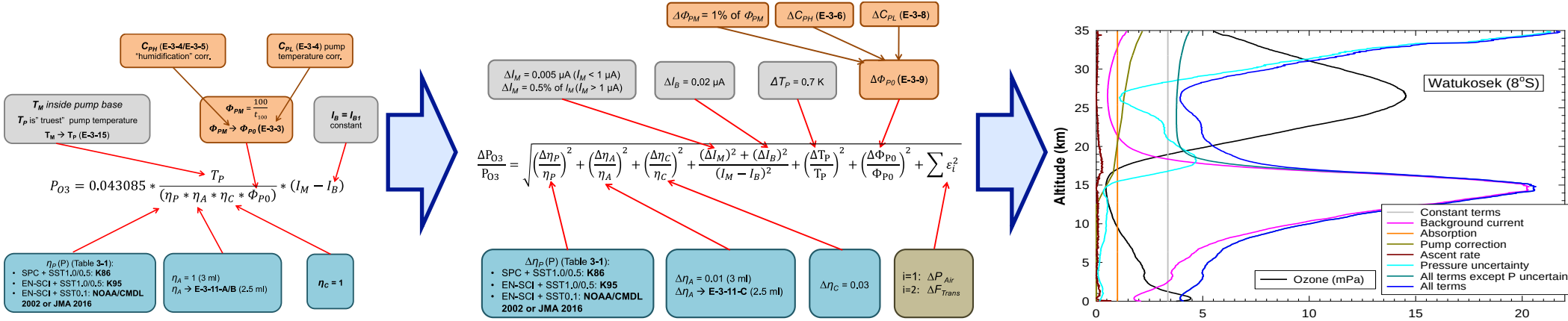


JOSIE



[Thompson et al., BAMS, 2019]

Uncertainty Budget Analysis for ECC-Ozonesonde: ASOPOS (2019-2021, WMO/GAW Report No. 268)



[Tarasick et al., ESS, 2021]

ASOPOS = Assessment of Standard Operating Procedures for OzoneSondes

Uncertainty Reporting (1) : Relevant VIM Keywords (JCGM 200:2012(E/F))

- Measurement uncertainty
- Random measurement error/measurement precision
- Systematic measurement error/measurement bias
- Detection limit
- Uncertainty budget
- Definitional uncertainty
- Standard measurement uncertainty
- Expanded measurement uncertainty
- Target measurement uncertainty (upper limit of uncertainty)

Storage of Data

Leading principle should be that ***each stored GAW-measurement*** should be traceable and consists of:

A. Measured value as obtained following the SOPs of the measuring GAW instrument.

B. Uncertainties in same physical quantity as measured value.

It consists of the uncertainty contributions of calibration, in-situ performance (incl. sampling) as described in the SOPs of the measuring GAW instrument.

C. Flag Code Scheme:

(i) giving state of processing/validation (NRT, LO, L1, L2..) ;

(ii) reliability and representativeness.

D. Meta Data

Uncertainty Reporting (2) : Summary WDCGG (GAW-Data Center of GHG's)

Instrument	Dataset	Uncertainty Variable
Picarro/CRDS	CH4	'Value_unc, QC-flag, Scale
GC-MS	COS	value_std (standard deviation), value_unc (total measurement uncertainty), value_unc_short, value_unc_long, QC-flag
QA-OCOS	N2O	
Gamma Ray Spectrometer	7Be	
GC-ECD	CFC12	
DELTA-V (MS)	O2/N2	
Picarro/CRDS	CO2	
Licor (NDIR)	CO2	
HORIBA VIA-510	CO2	

Uncertainty Reporting (3) : Summary WOUDC (GAW-Data Center of Ozone and UV)

Instrument	Dataset	Uncertainty Variable
Brewer and Brewer MKII	Total Ozone	StdDevO3 of the Mean
Filter	Total Ozone	StdDevO3 of the Mean
DIAL/Lidar	Lidar (ozone profile)	Standard Error
Dobson	Umkehr N14	None
ECC Ozonesonde	Ozonesonde (ozone profile)	In progress
Kipp Zonen	Broadband (radiation)	None
Biospherical	Multiband (radiation)	None
Brewer MKIV	Spectral (radiation)	Err_O3 (?)

Uncertainty Reporting (4) : Summary of Data Quality Reporting in GAW

- Uncertainty reporting method highly consistent for each data center, while significant difference exists between the data centers
- Not all measurements report uncertainty, and some uncertainty variables have fill values only
- Some uncertainty definition is not readily available and consistency with metrological terms should be improved
- Standard deviation is commonly reported, which includes both measurement uncertainty and ambient variability
- Lack of reporting of Meta Data for data re-processing
- Missing of QC-flagging

Uncertainty and Data Quality Reporting in Future Practice

- Encourage reporting uncertainties and data quality information
- Increase uniformity among the data centers
- uncertainty quantities according to user needs and feasibility and link these quantities to VIM vocabularies
- Usable by those who are not familiar with the measurements
- Quantifiable by instrument scientists
- Promote use of VIM vocabulary
- Develop metadata standards common to all measurements as well as specific measurements
- Provide definitions readily usable by researchers and tag to VIM vocabularies
- Provide examples for different types of measurements to ensure usability

GAW-QA/QC Evaluation Concept: Objectives

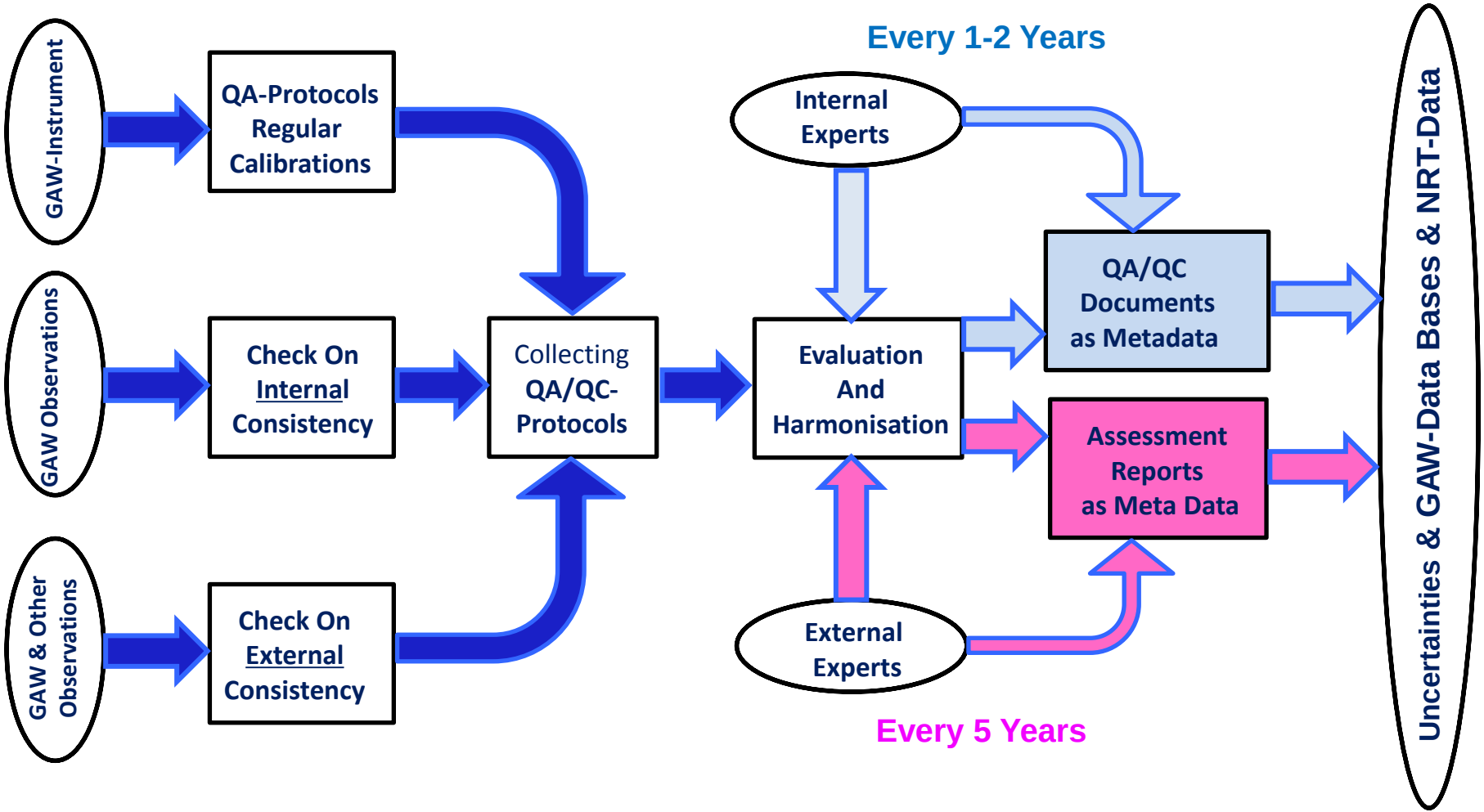
To establish procedures for regular documentation and evaluation of the quality of the GAW measurements and their harmonisation through developing and testing/evaluation of:

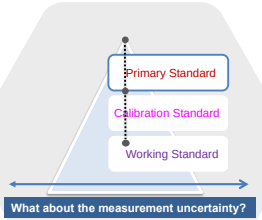
- **A harmonized QA/QC- concept based on the largest possible uniformity to achieve among the different observing systems**
- **QA/QC procedures and their traceabilitiy** (link to Metrology)
- **Tools to evaluate on internal and external consistency of the measurements.**

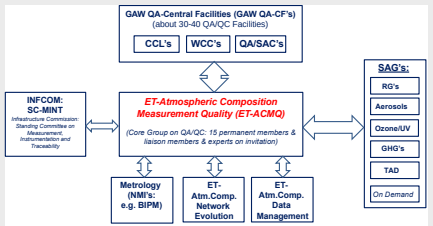
Essentially thereby is to ***obtain a full documentation*** of the standard operating procedures (SOPs) and quality control procedures for each instrument, making the measured data transparently ***traceable to established standards***.

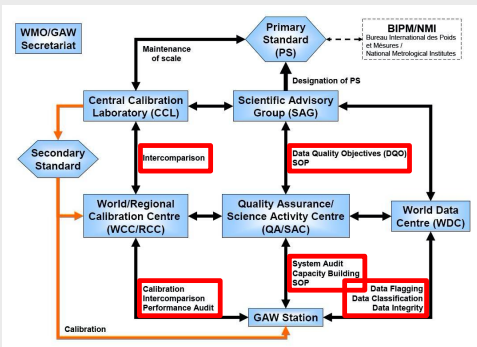
The overall goal thereby should be that these procedures will be ***established as an essential component of the QA/QC plan of the WMO/GAW and that they are monitored and regularly evaluated.***

Monitoring and Evaluation of GAW-QA/QC: Concept of Framework









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