Schweizerische Eidgenossenschaft
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Federal Office of Meteorology and Climatology MeteoSwiss

WMO

GAW

Empa
Materials Science and Technology

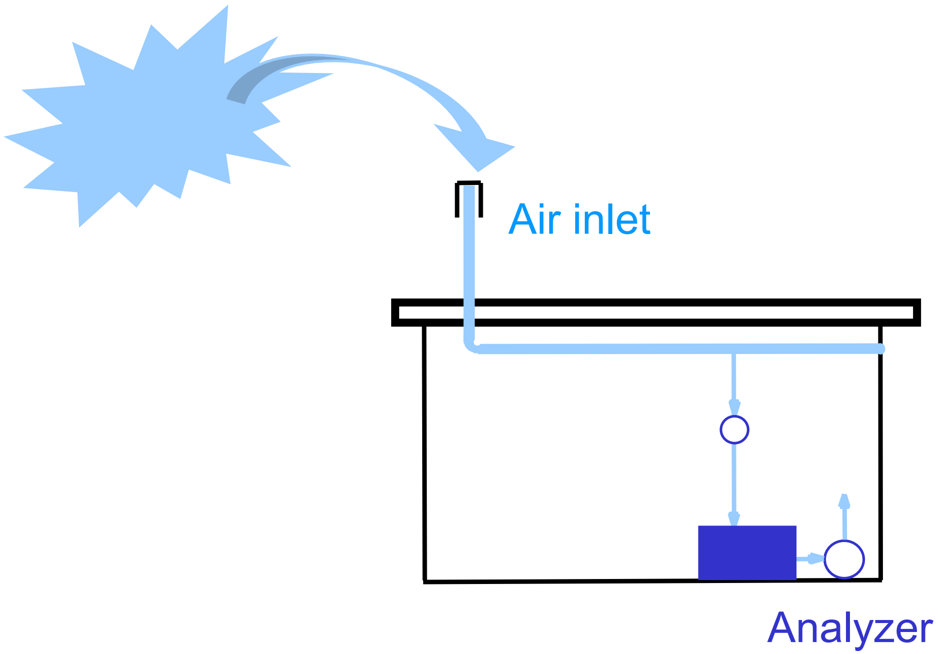
Data handling and evaluation, measurements uncertainty

Martin Steinbacher

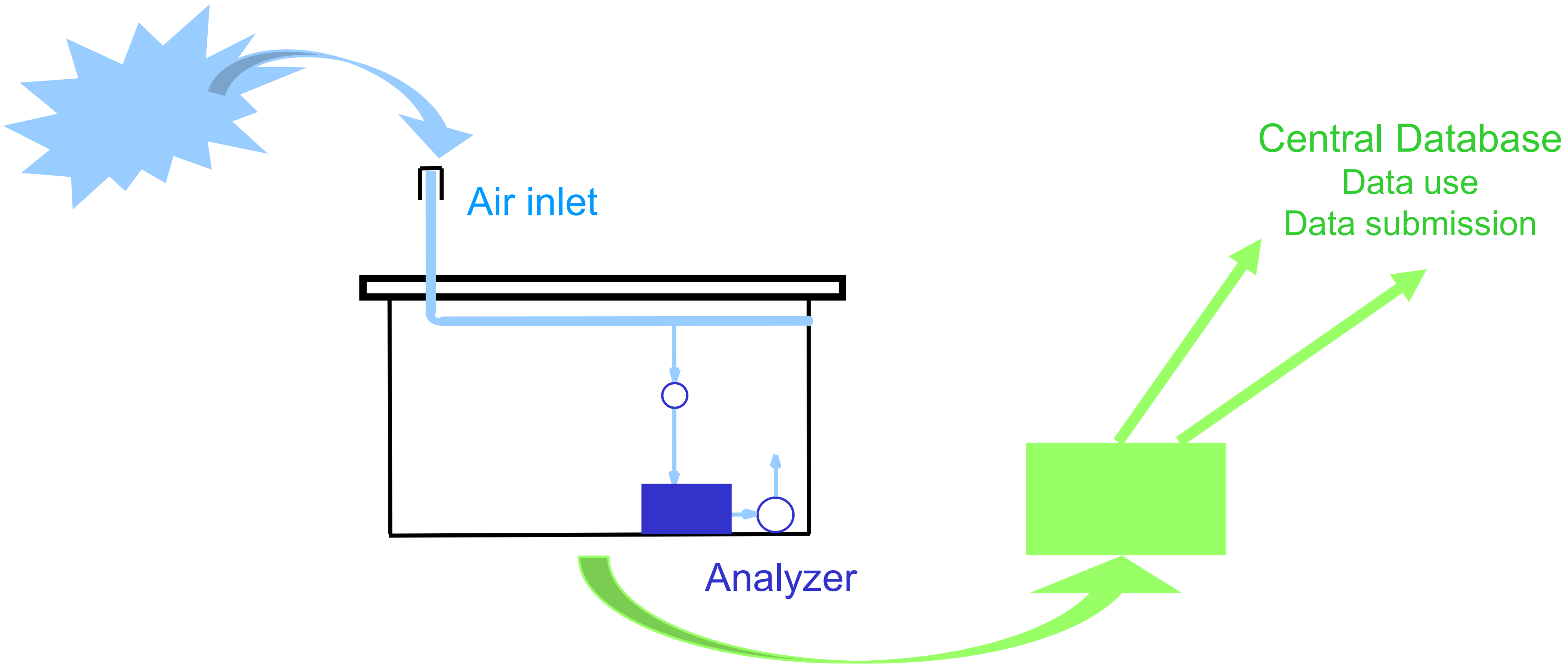
Empa, Laboratory for Air Pollution/Environmental Technology, Dübendorf, Switzerland

Training of KMD staff, Duebendorf, 28 June till 02 July 2018

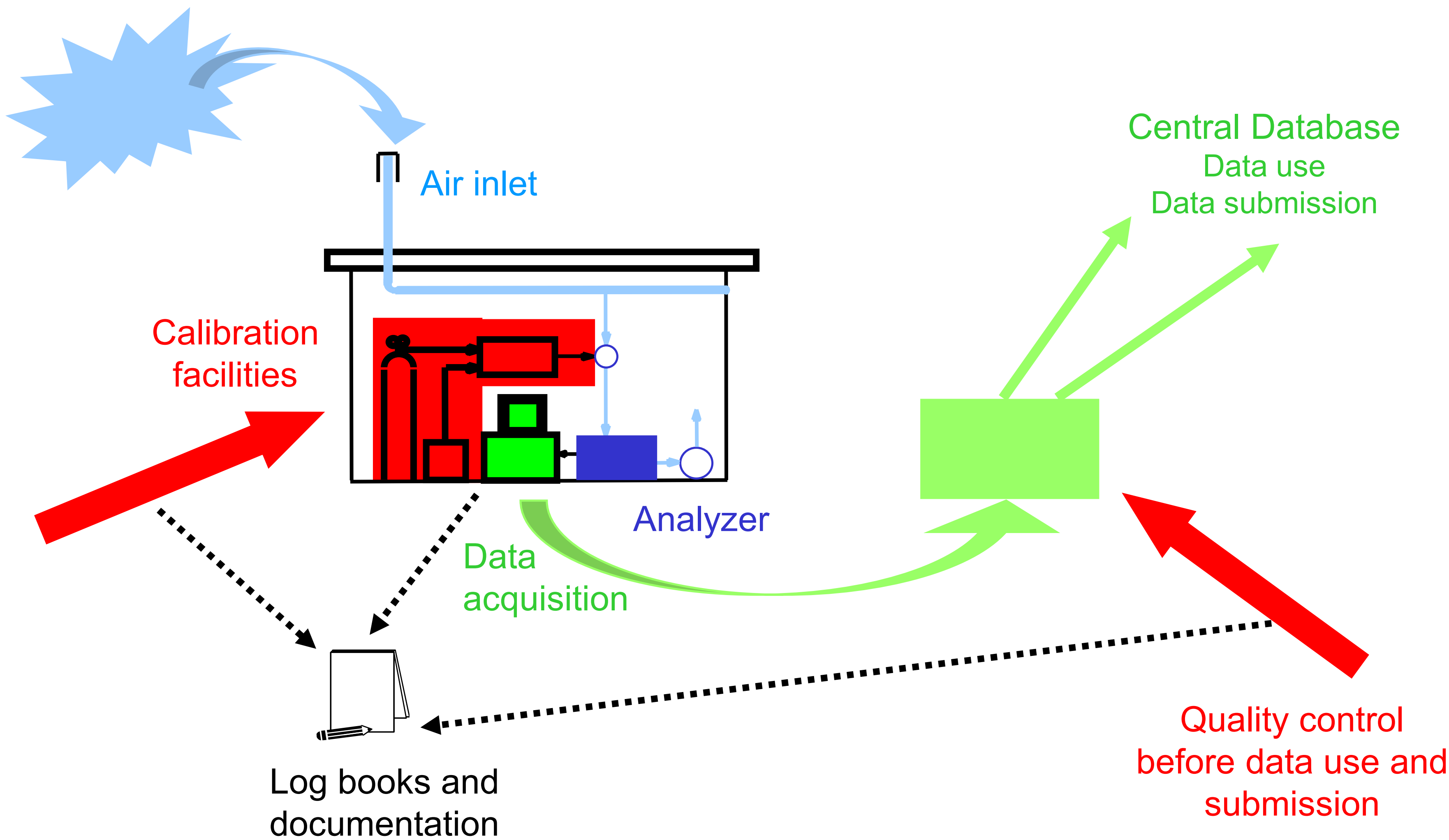
Requirements for air quality measurements



Requirements for air quality measurements



Requirements for air quality measurements



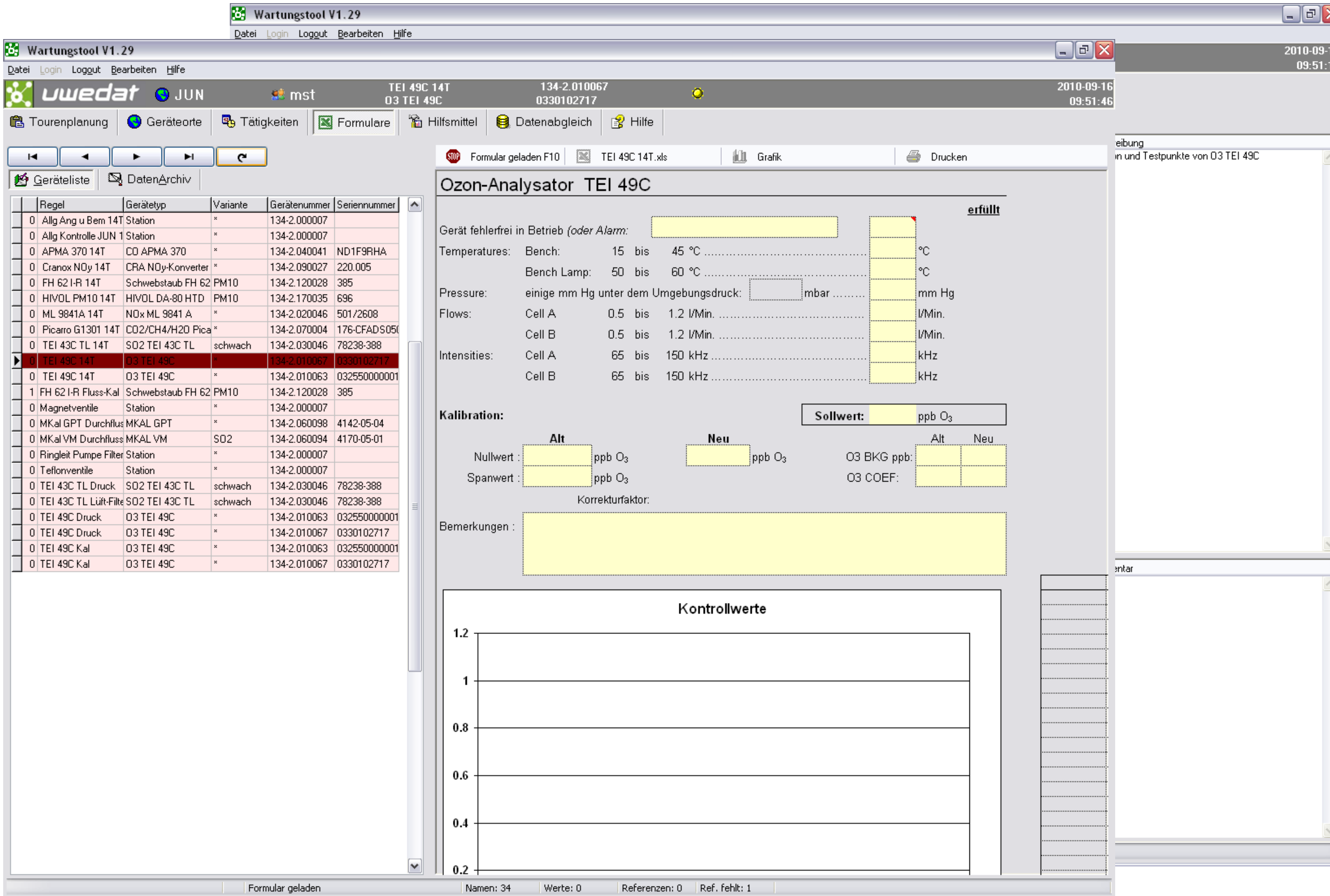
Contents

- maintenance
- documentation
- data format / data flagging
- uncertainty estimation
- use of other information

Instrument Maintenance

- Maintenance is an important factor to ensure continuous operation of an instrument. It improves both data availability and data quality.
- Download and backup raw data.
- Visualize (raw) data with graph plots.
- Basic instrument checks
  Check of general instrument operation
  Leak check, flow checks, pressure sensor checks, status of calibration gases …
- Further maintenance
  filter exchange, inlet line loss / tightness
- Develop a maintenance scheme (check list) for the individual analyzers.
- Consult instrument manual for specific maintenance recommendations.

Documentation – Meta data management



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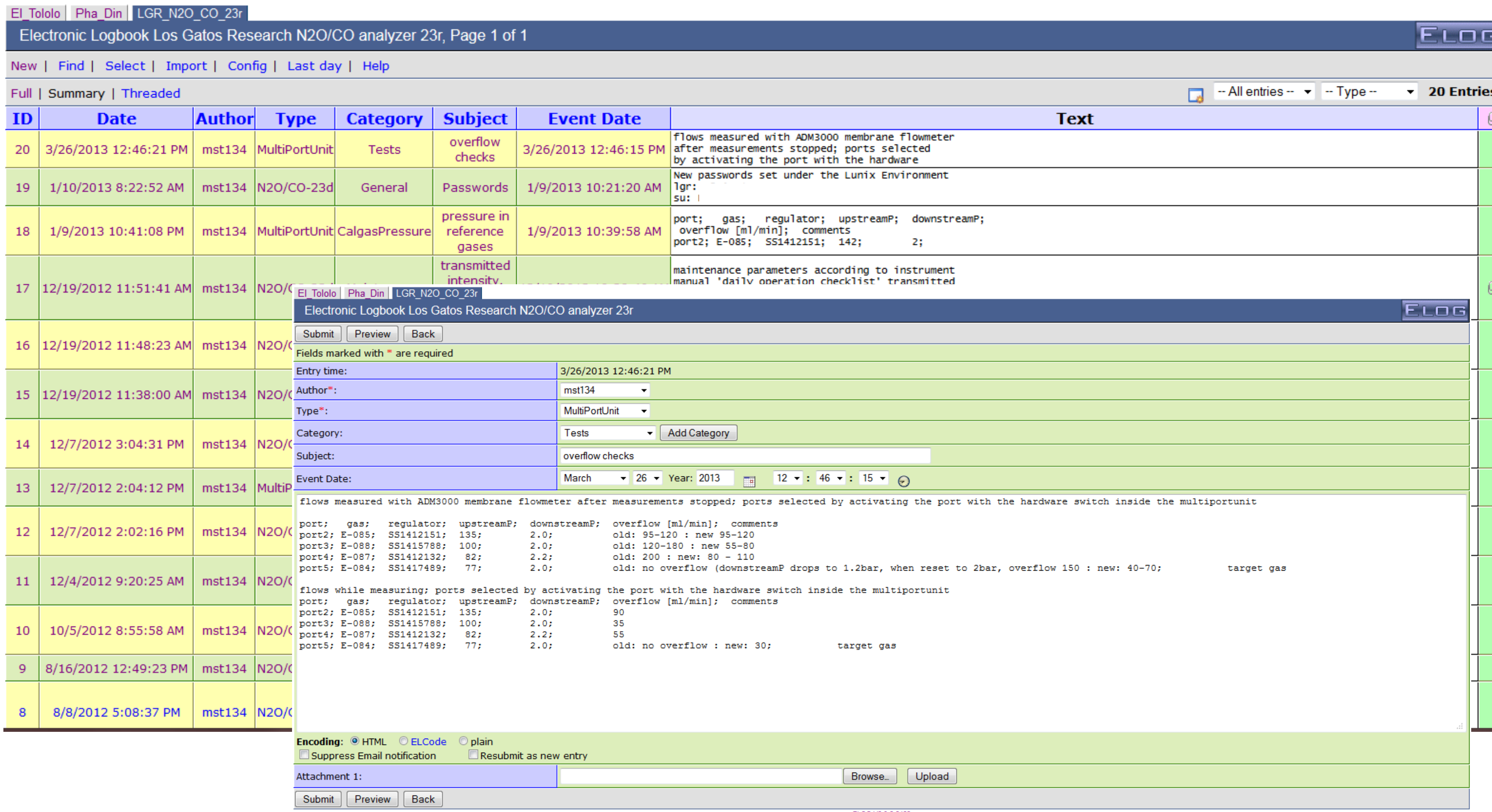

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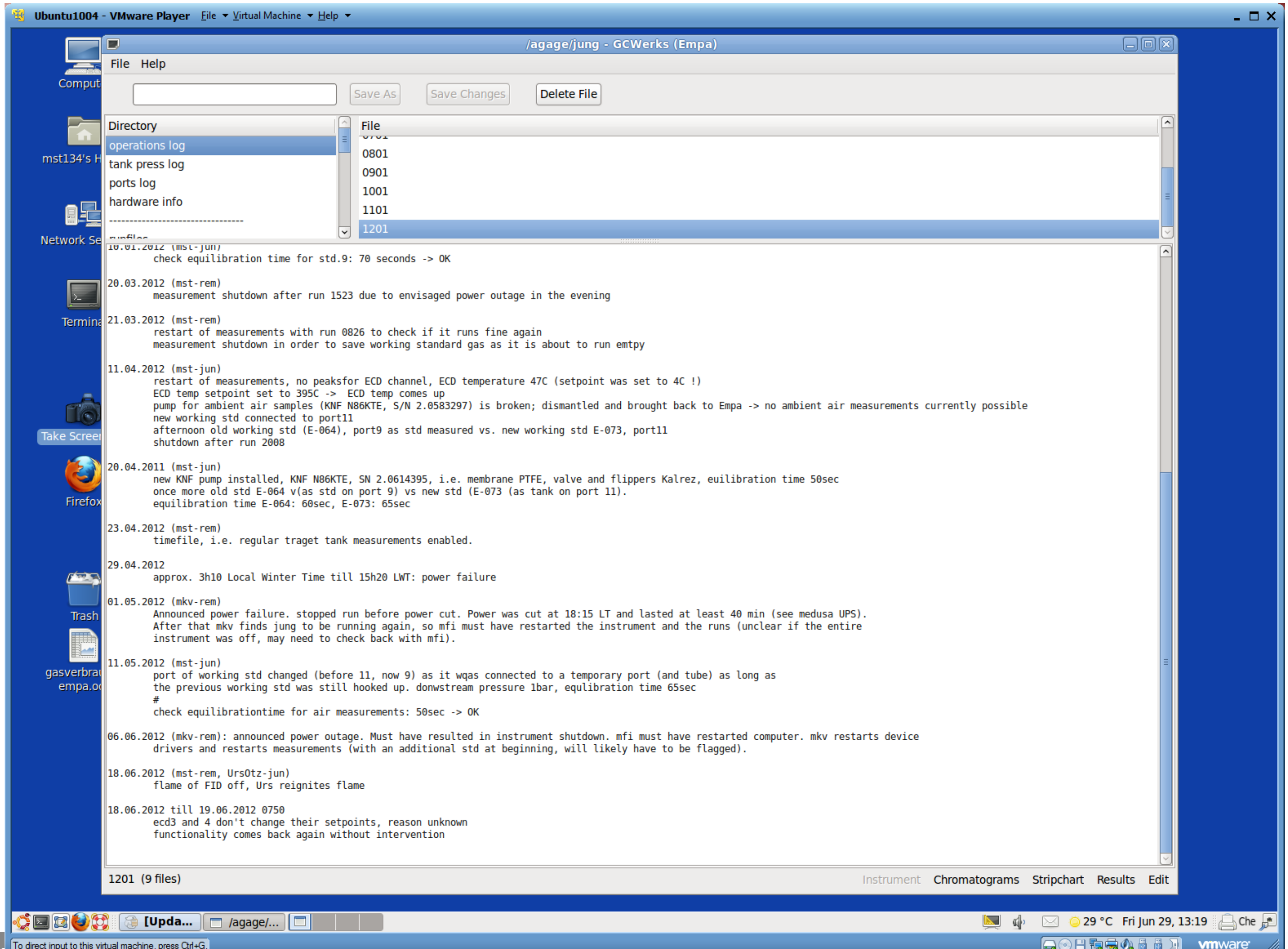

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Data flagging

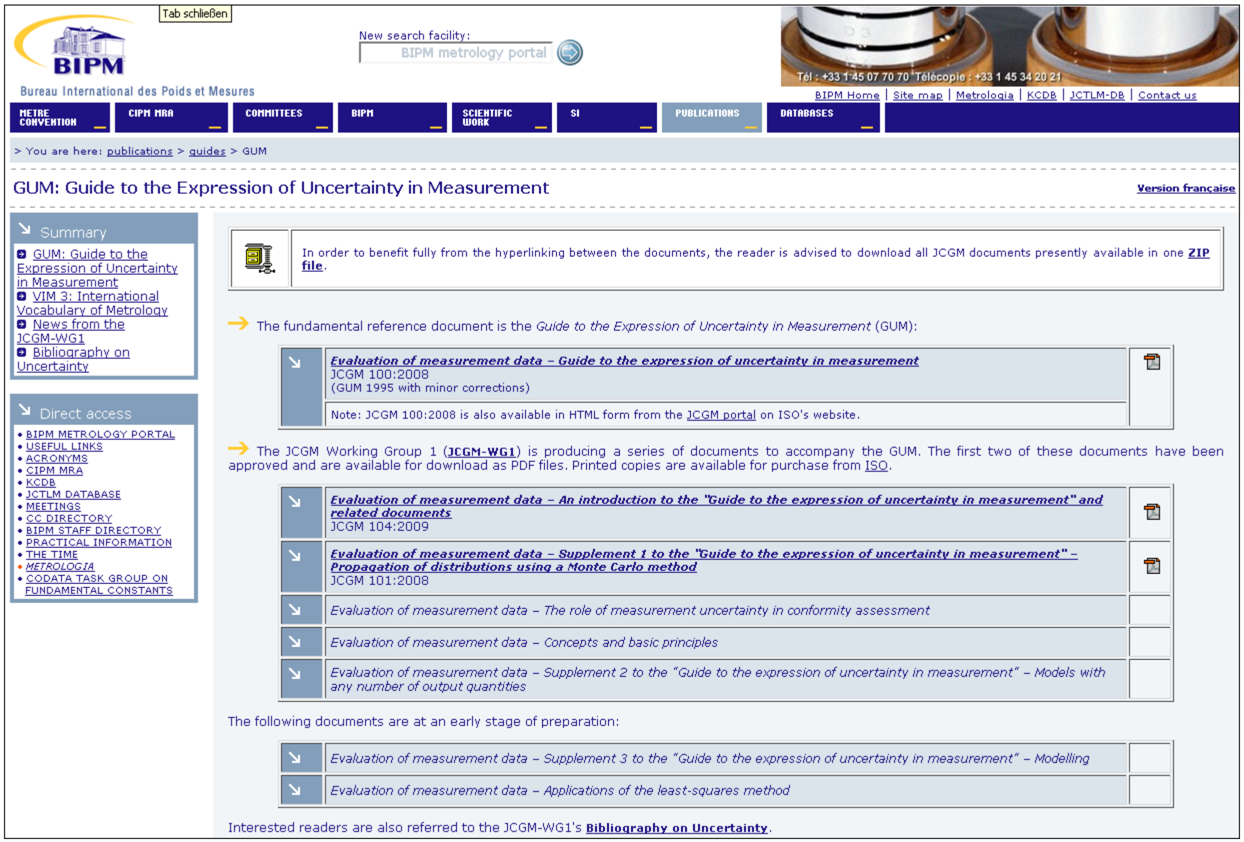
- Data need to be flagged for further data analysis.
- Ancillary instrument information (e.g. flows, temperatures, state of calibration valves) should be recorded by the data acquisition system for efficient data analysis.
- "Valid ambient data" should be used for scientific studies and data submission.
- All other data should NOT be deleted, but remain the data base with appropriate flags.

Uncertainty

- All data that is submitted / published / used should be associated with an uncertainty.
- However, data are often submitted or published without any uncertainty information.

Uncertainty

- ISO Guide for the Expression of Uncertainty in Measurements (GUM)
- Freely available on BIPM website http://www.bipm.org/en/publications/guides/gum.html



Terminology

http://gaw.empa.ch/glossary/glossary.html

EN DE FR KONTAKT INTRANET LOGIN SEARCH

Empa
Materials Science and Technology

OVERVIEW RESEARCH PUBLICATIONS TEAM

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

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WMO/GAW Glossary of QA/QC-Related Terminology

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

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

Table of Contents

Terminology

http://gaw.empa.ch/glossary/glossary.html

Glossary

Alphabetical list of terms

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

Terminology - Example

http://gaw.empa.ch/glossary/glossary.html

[4.13] selectivity of a measuring system #top#

selectivity

property of a →measuring system, used with a specified →measurement procedure, whereby it provides measured →quantity values for one or more →measurands such that the values of each measurand are independent of other measurands or other →quantities in the phenomenon, body, or substance being investigated [1]

EXAMPLES

1. Capability of a measuring system including a mass spectrometer to measure the ion current ratio generated by two specified compounds without disturbance by other specified sources of electric current.
2. Capability of a measuring system to measure the power of a signal component at a given frequency without being disturbed by signal components or other signals at other frequencies.
3. Capability of a measuring system for ionizing radiation to respond to a given radiation to be measured in the presence of concomitant radiation.
4. Capability of a mass spectrometer to measure the amount-of-substance abundance of the ^{28}Si isotope and of the ^{30}Si isotope in silicon from a geological deposit without influence between the two, or from the ^{29}Si isotope.

NOTES

1. In physics, there is only one measurand; the other quantities are of the same kind as the measurand, and they are input quantities to the measuring system.
2. In chemistry, the measured quantities often involve different components in the system undergoing measurement and these quantities are not necessarily of the same kind.
3. In chemistry, selectivity of a measuring system is usually obtained for quantities with selected components in concentrations within stated intervals.
4. Selectivity as used in physics (see Note 1) is a concept close to specificity as it is sometimes used in chemistry.

EXAMPLES (GAW)

1. A measuring system is highly selective for a specific trace gas (e.g. CO) mole fraction if its quantity value (e.g. 2 nmol/mol) is independent on quantity changes of the sample matrix (e.g. humidity changes).
2. Capability of gas chromatographic system to fully separate the peak of substance A from substance B in a chromatogram.

Uncertainty

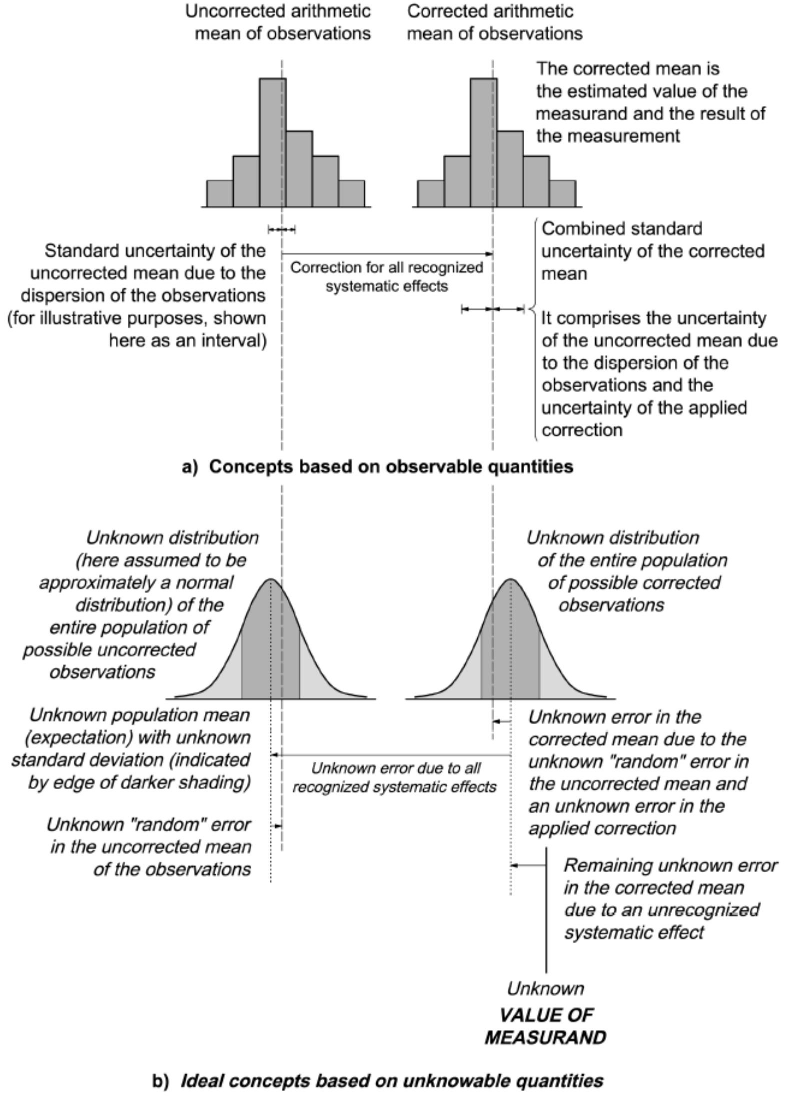


Figure D.1 — Graphical illustration of value, error, and uncertainty

- See ISO Guide for the Expression of Uncertainty in Measurements (GUM)

Example: Uncertainty of CO measurements

- Different factors contribute to the overall uncertainty of the measurements:

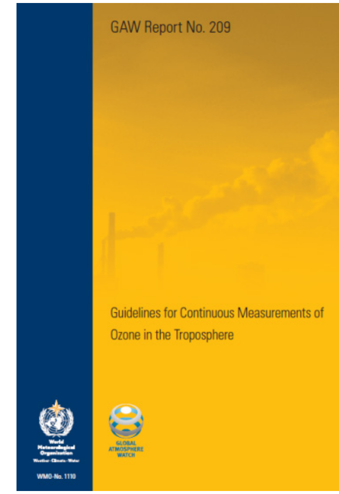
- Primary lab standard

- Secondary lab standard
- Zero air

- Repeatability
- Drift (zero)
- Drift (span)
- Linearity / deviation from the calibration function
- Pressure dependency
- Temperature dependency
- Interferences

- Sampling (artifacts, inlet loss etc.)

Example: Uncertainty of surface O3 measurements



9.4.3 Combined standard uncertainty of the ozone analyser

The uncertainty budget of the ozone analyser can also be estimated by combination of the contributions of the individual uncertainty components. An example of an assessment for an ozone analyser operated in the Swiss National Monitoring network is given below. The individual contributions to the combined standard uncertainty were estimated by either experimental data, manufacturer specifications or, in cases where no data was available, by expert judgment. Table 1 summarises the uncertainty budget for the measurement of ozone mole fractions [...]. The uncertainty components have been combined according to the methodology proposed by the Joint Committee for Guides in Metrology (2008).

Example: Uncertainty of surface O3 measurements

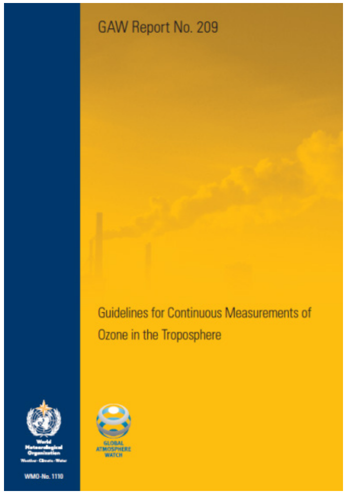


Table 1 - Example of an uncertainty budget of an ozone analyser

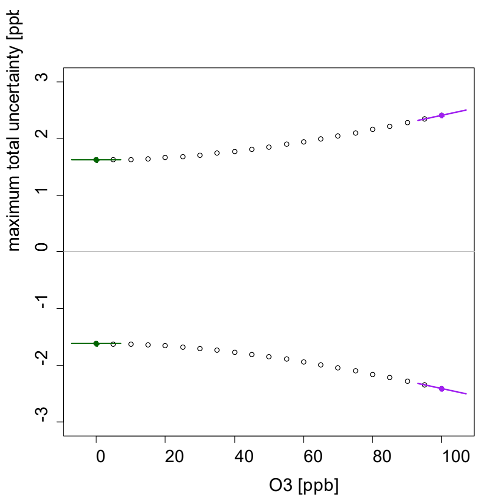
Component (*y*)	Source	Distribution	Contribution to *u(x)*
Imperfect calibration / linearity	Comparison between TS and OA	Rectangular	$0.0017 \cdot x^*$
Repeatability	Instrument stability	Rectangular	$0.0016 \cdot x$
Span drift	Instrument stability	Rectangular	$0.0040 \cdot x$
Zero drift	Instrument stability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

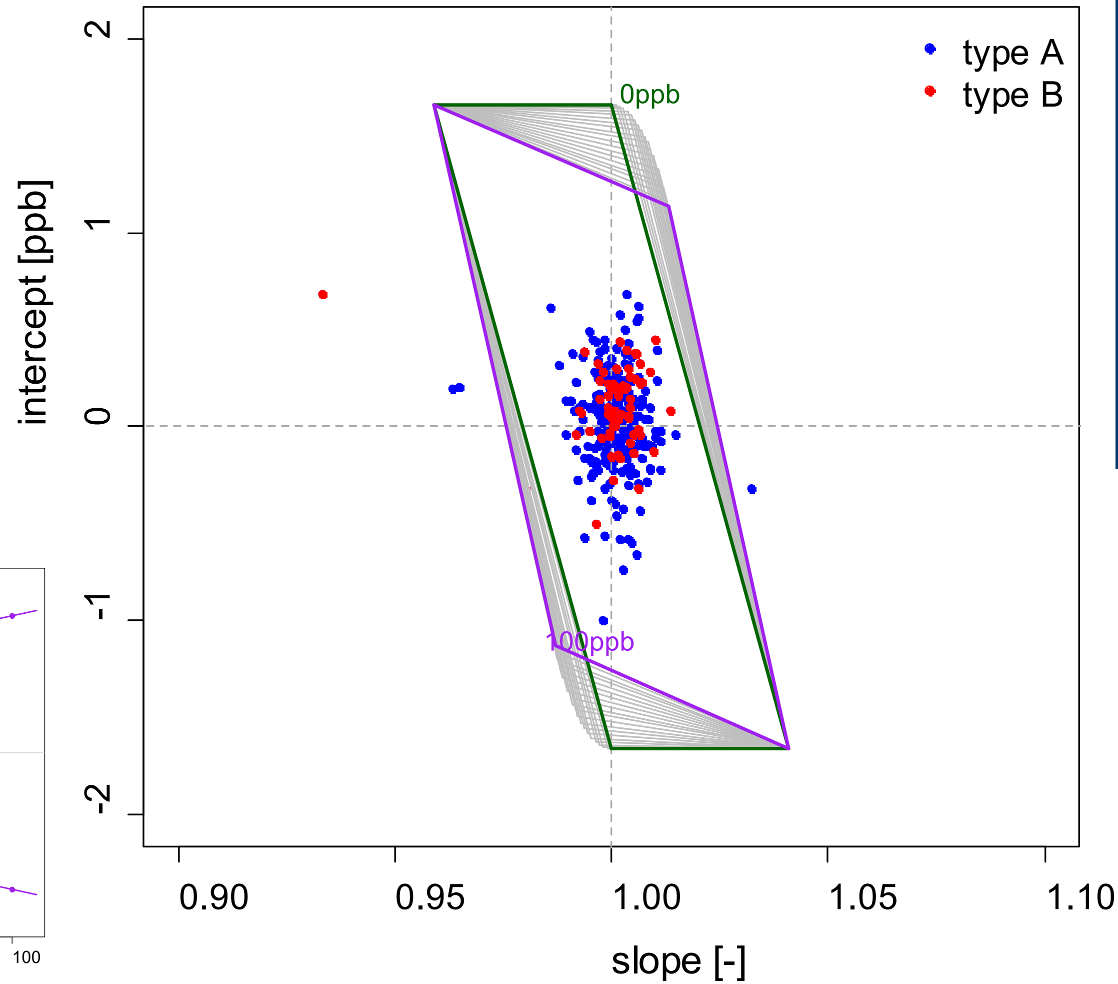
* *where x refers to ozone mole fraction*

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

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

Example: Uncertainty of surface O3 measurements





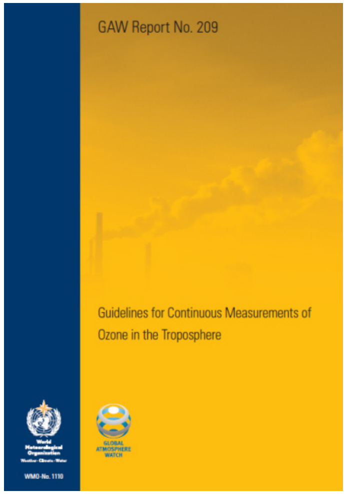


Figure 7 - Intercept vs. slope plot for 296 calibrations of various ozone analysers with transfer standards within the Swiss National Air Pollution Monitoring Network between November 2005 and November 2011 for two different types of UV absorption ozone instruments. The grey lines correspond to the uncertainties from Equation (14), expanded by a coverage factor k=2 for ozone mole fractions from 0-100 ppb. The uncertainties for 0 ppb and 100 ppb are highlighted in green and purple, respectively

From the GUM (3.4.8)

- Although this Guide provides a framework for assessing uncertainty,
  - it cannot substitute for critical thinking, intellectual honesty and professional skill.
  - the evaluation of uncertainty is neither a routine task nor a purely mathematical one
  - it depends on detailed knowledge of the nature of the measurand and of the measurement.
  - the quality and utility of the uncertainty quoted for the result of a measurement therefore ultimately depend on the understanding, critical analysis, and integrity of those who contribute to the assignment of its value.

Comparison with other sites

https://ds.data.jma.go.jp/gmd/wdcgg/

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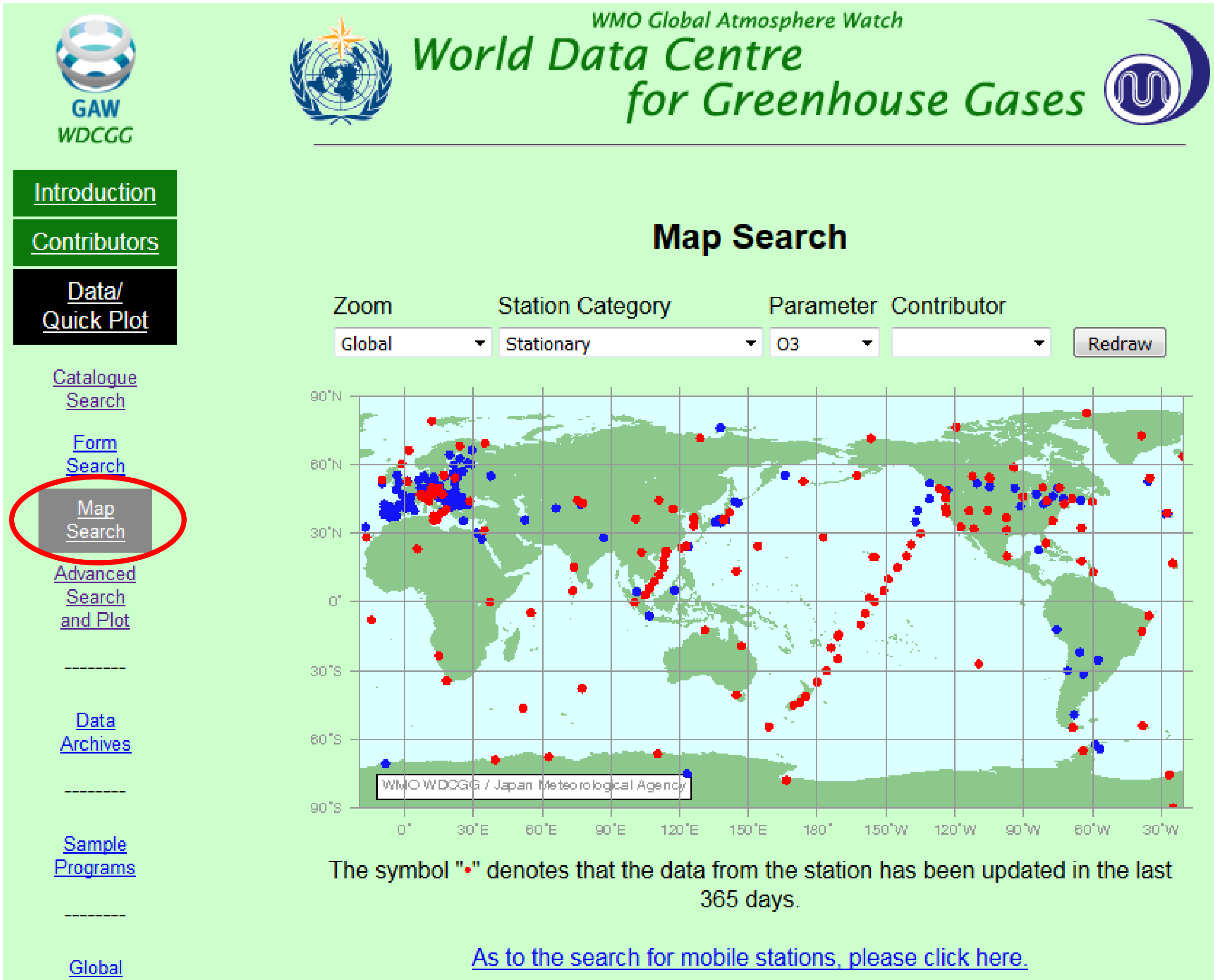

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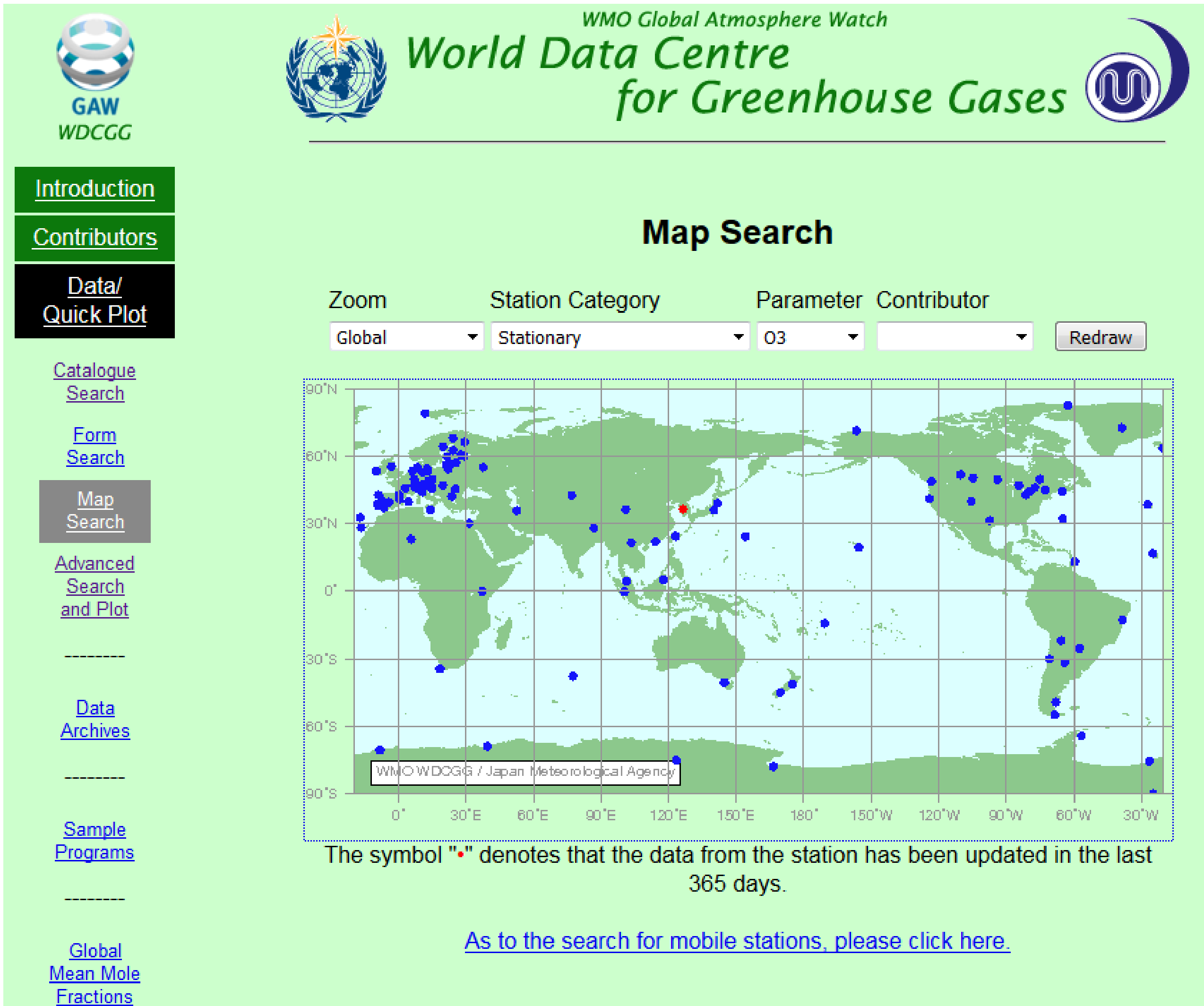
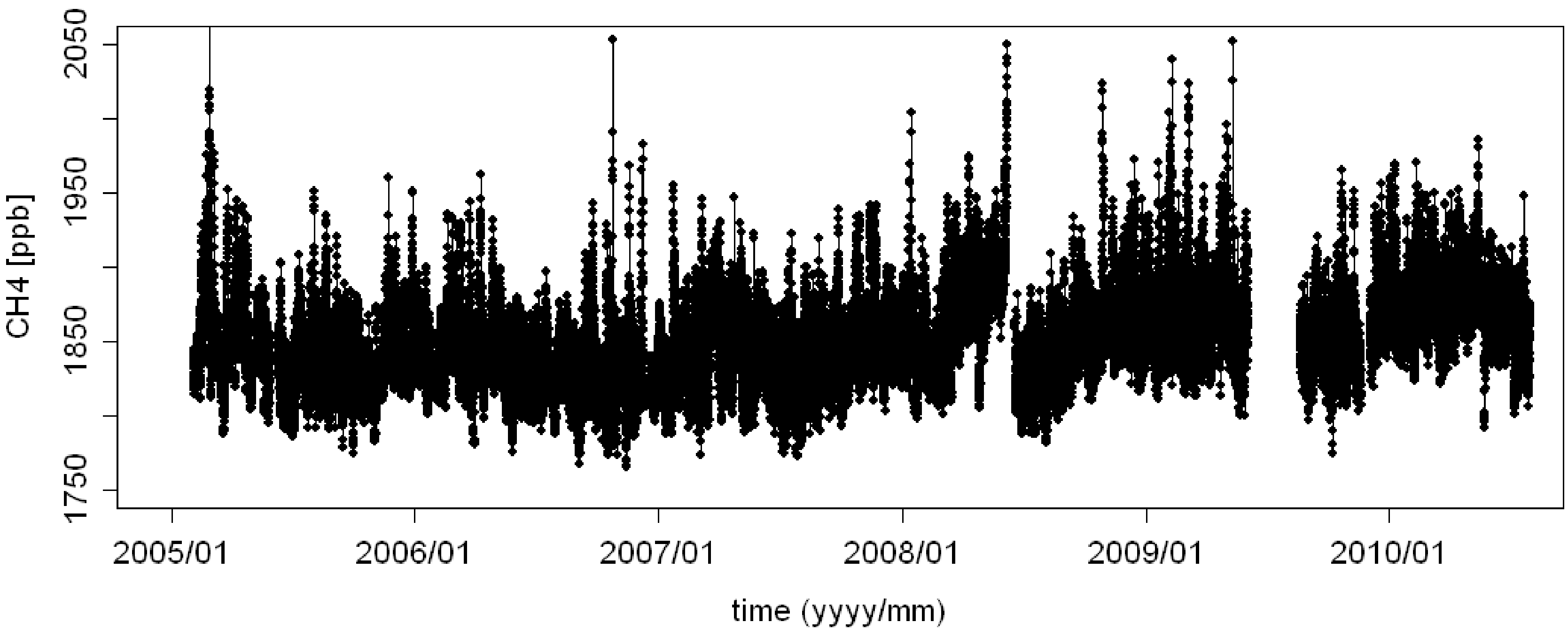


Comparison with other sites

- it works well for longer lived species



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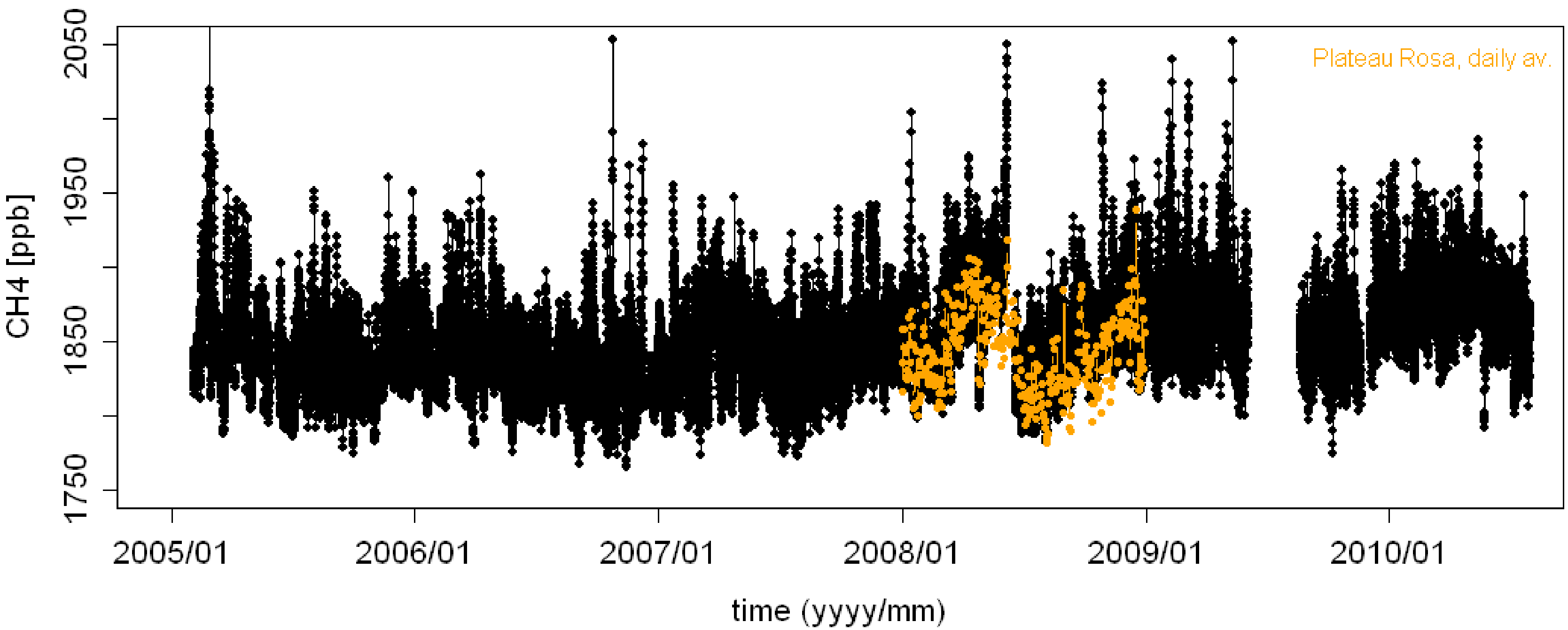
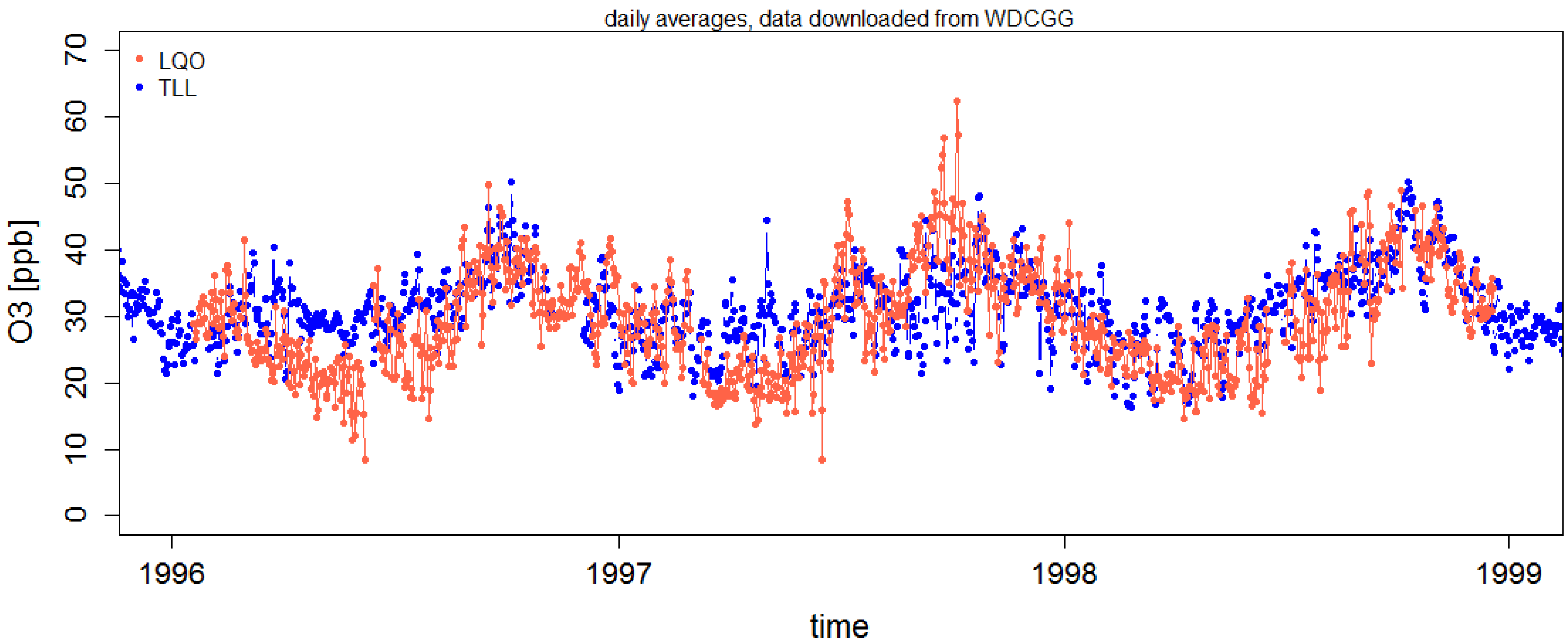


Comparison with other sites

- Large variability due to (local) formation and depletion of ozone makes a comparison more complex



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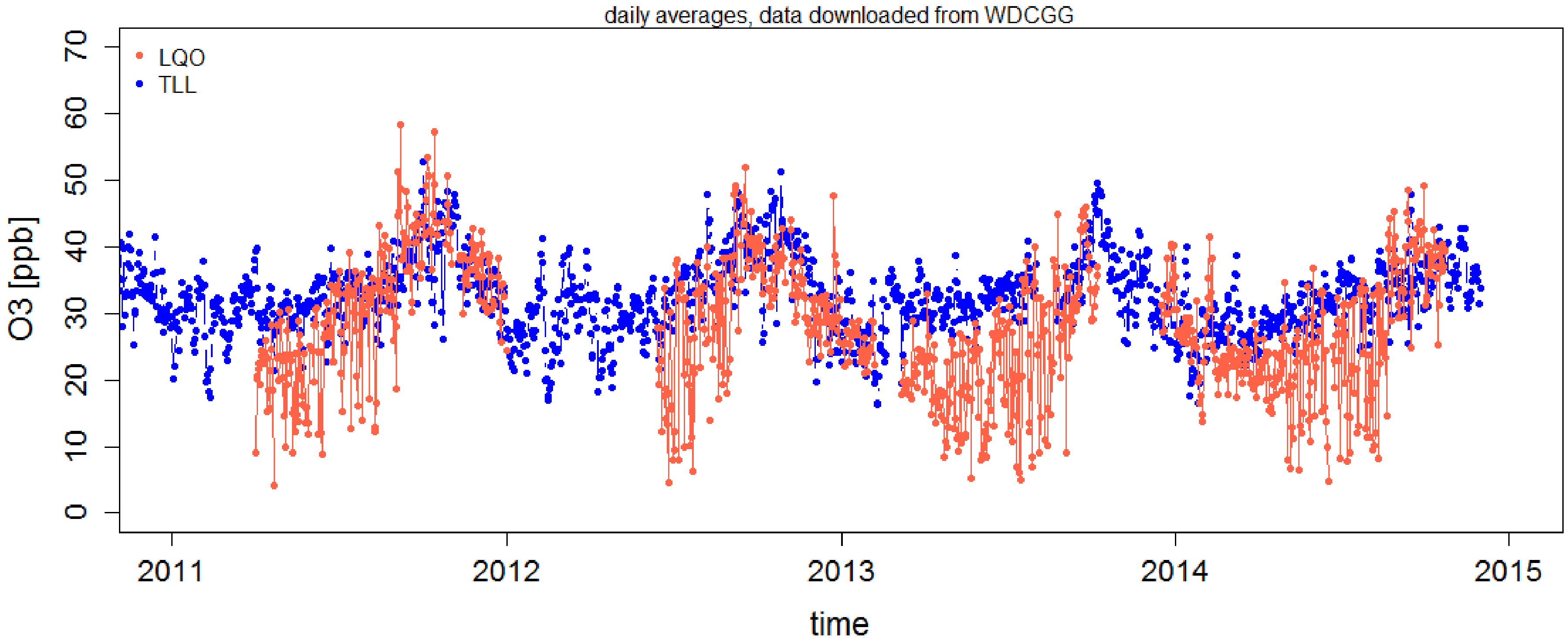
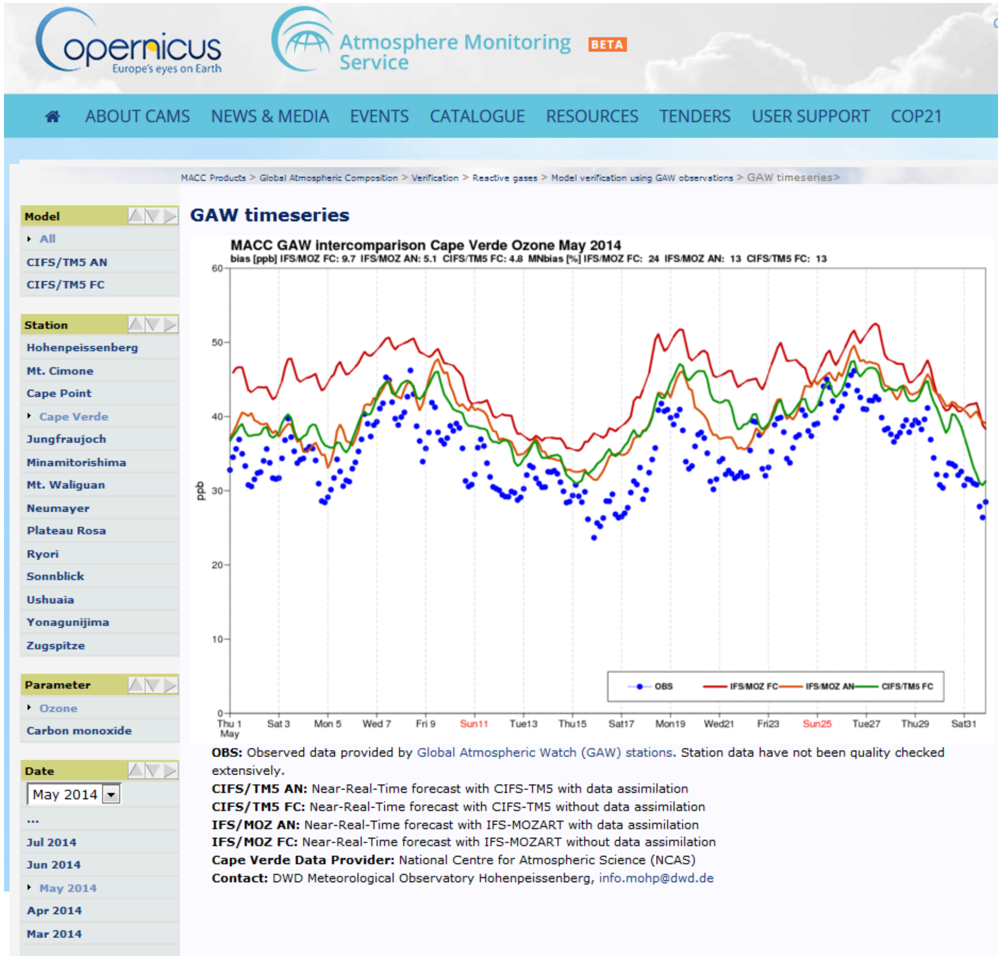


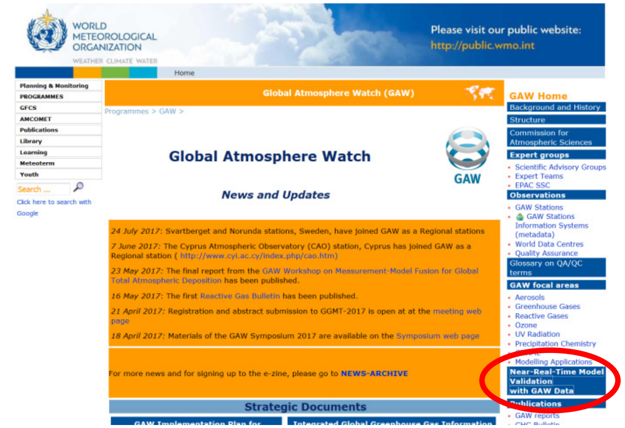
- Is it real or an instrumental artefact? Local knowledge is key to judge.
- Consult logbook entries, compare with other local data (air quality, meteorology)

Using model output information

http://gmes-atmosphere.eu/d/services/gac/verif/grg/gaw/gaw_station_ts/



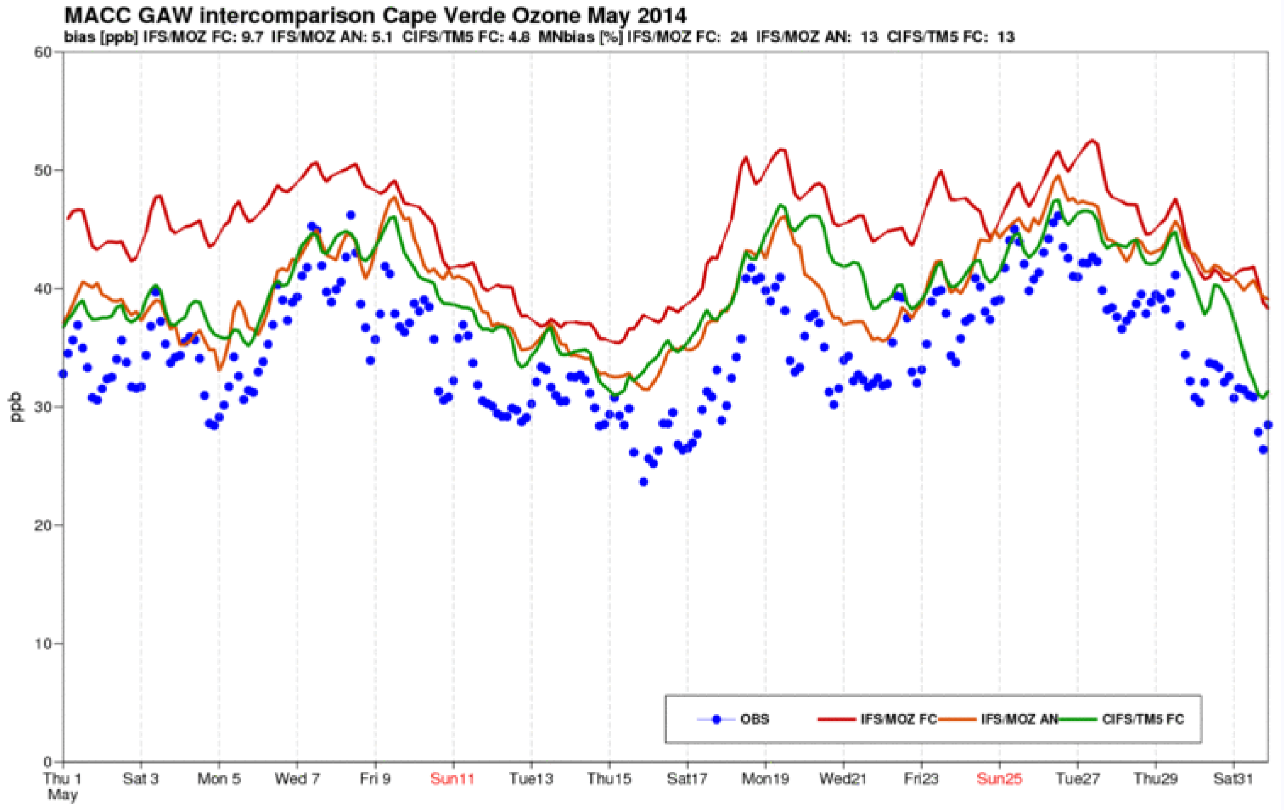
or



Using model output information

http://gmes-atmosphere.eu/d/services/gac/verif/grg/gaw/gaw_station_ts/

GAW timeseries



OBS: Observed data provided by Global Atmospheric Watch (GAW) stations. Station data have not been quality checked extensively.
CIFS/TM5 AN: Near-Real-Time forecast with CIFS-TM5 with data assimilation
CIFS/TM5 FC: Near-Real-Time forecast with CIFS-TM5 without data assimilation
IFS/MOZ AN: Near-Real-Time forecast with IFS-MOZART with data assimilation
IFS/MOZ FC: Near-Real-Time forecast with IFS-MOZART without data assimilation
Cape Verde Data Provider: National Centre for Atmospheric Science (NCAS)
Contact: DWD Meteorological Observatory Hohenpeissenberg, info.mohp@dwd.de

Using model output information

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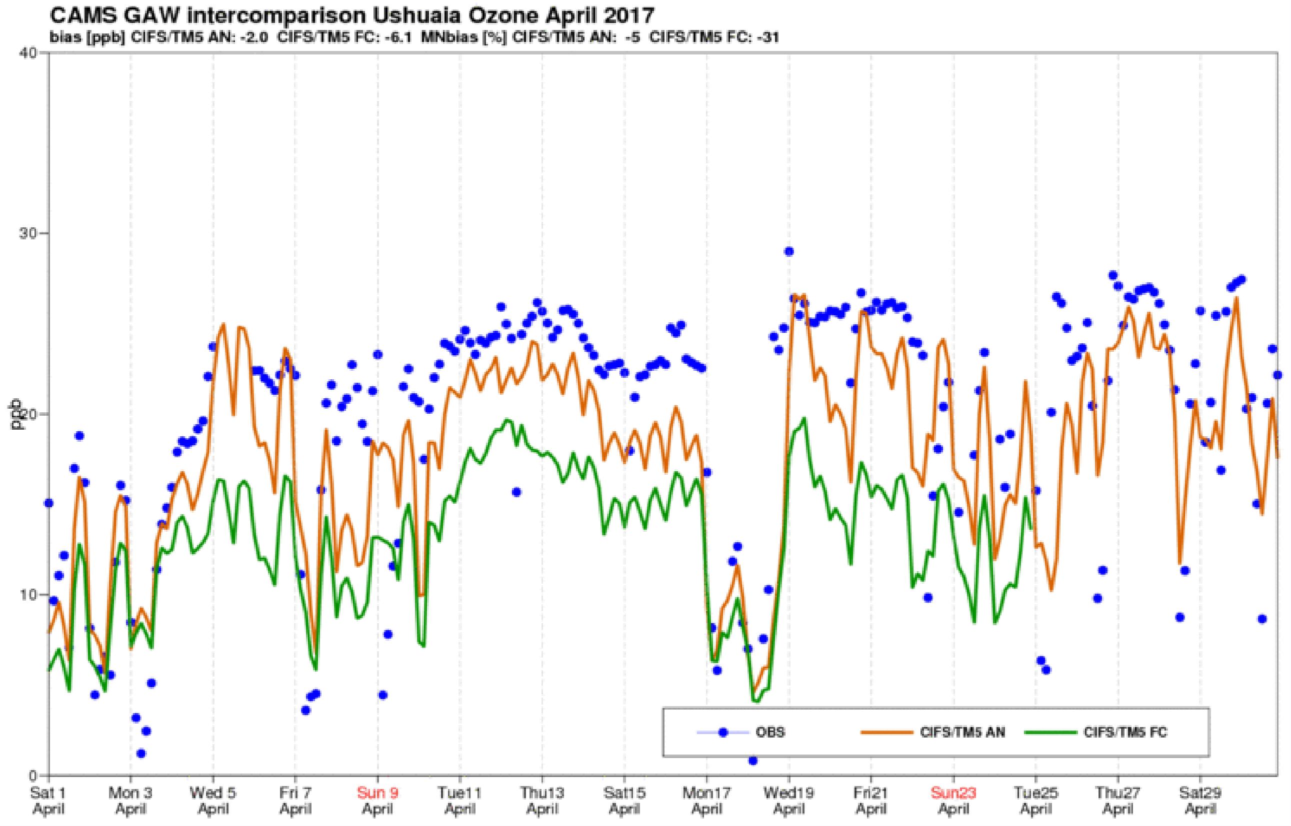

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IFS/MOZ FC: Near-Real-Time forecast with IFS-MOZART without data assimilation

Ushuaia Data Provider: National Meteorological Service

Contact: DWD Meteorological Observatory Hohenpeissenberg, info.mohp@dwd.de

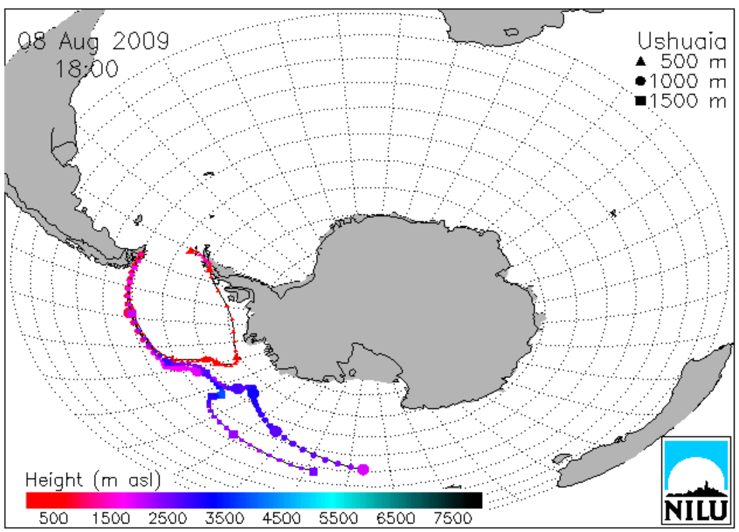
Using trajectory information

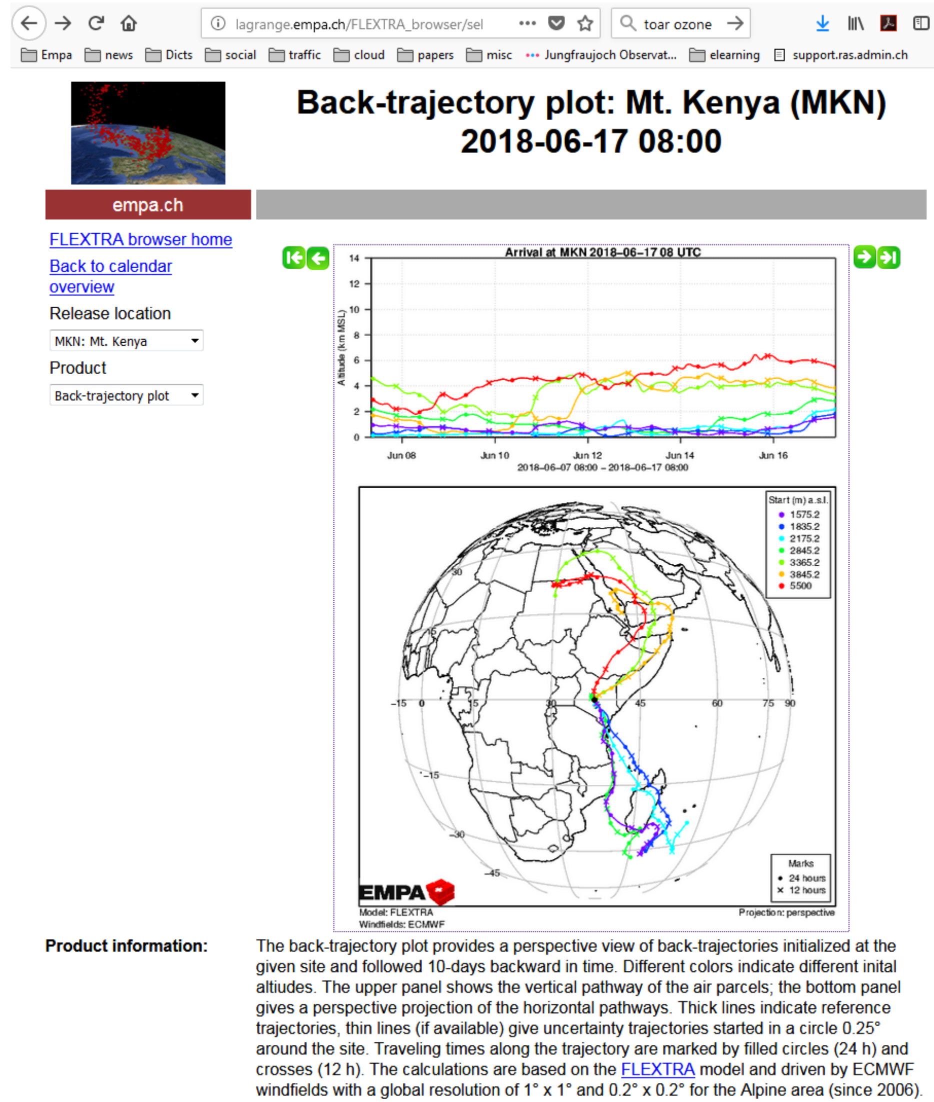
Available through the internet from various sources

http://lagrange.empa.ch/FLEXTRA_browser/

http://www.emep.int/trajectories.html

http://www.arl.noaa.gov/ready/hysplit4.html





Questions ?