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Federal Office of Meteorology and Climatology MeteoSwiss





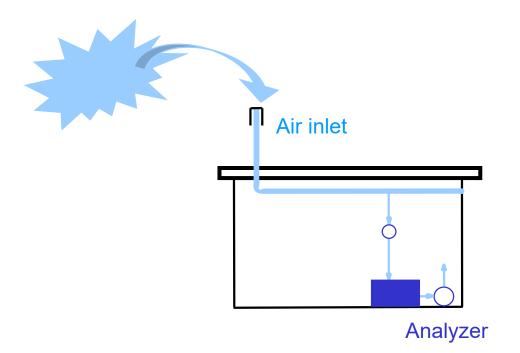
Data handling and evaluation, measurements uncertainty

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

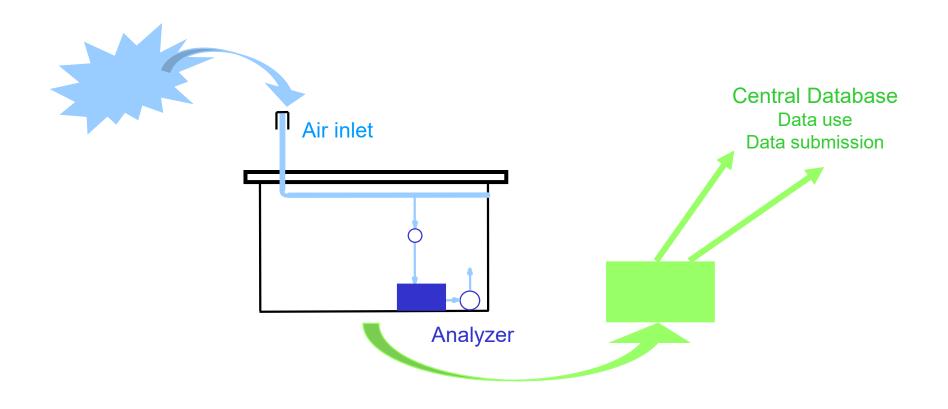
Requirements for air quality measurements



martin.steinbacher@empa.ch, Laboratory for Air Pollution/Environmental Technology



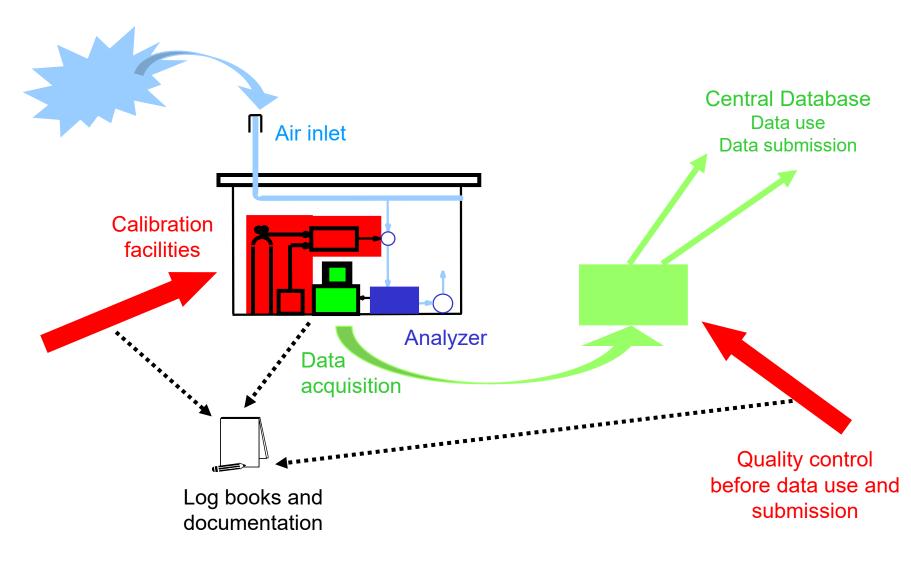
Requirements for air quality measurements







Requirements for air quality measurements







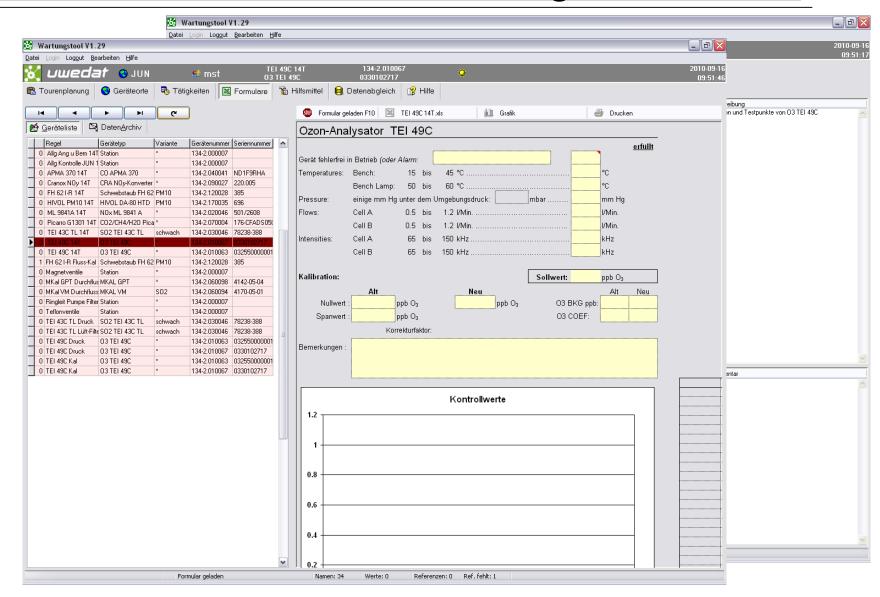
- maintenance
- documentation
- data format / data flagging
- uncertainty estimation
- use of other information



- 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





Documentation – Meta data management

El_Tololo Pha_Din LGR_N2O_CO_23r

	ectronic Logbook Los G				23r, Page 1 of	1						
Full Summary Threaded												
ID	Date	Author	T	pe Category	Subject	Event Date	Text					
20	3/26/2013 12:46:21 PM	mst134			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					
19	1/10/2013 8:22:52 AM	mst134	N20/0	CO-23d General	Passwords	1/9/2013 10:21:20 AM	New passwords set under the Lunix Environment lgr: su: /					
18	1/9/2013 10:41:08 PM	mst134	MultiP	ortUnit CalgasPressur	pressure in e reference gases	1/9/2013 10:39:58 AM	port; gas; regulator; upstreamP; downstreamP; overflow [m]/min]; comments port2; E-085; SS1412151; 142; 2;					
17	12/19/2012 11:51:41 AM	mst134	N2O/0		transmitted maintenance parameters according to instrument intensity.							
16	12/19/2012 11:48:23 AM	mst134	N20/0	Submit Preview Back Fields marked with * are required								
15	12/19/2012 11:38:00 AM	mst134	N20/0	Entry time: Author*: Type*:		3/26/2013 12:46:21 P mst134 MultiPortUnit	M					
14	12/7/2012 3:04:31 PM	mst134	N20/0	Category: Subject:		Tests - (Add Category					
13	12/7/2012 2:04:12 PM	mst134	MultiP	Event Date:	DM3000 membrane		Year: 2013 12 v: 46 v: 15 v O					
12	12/7/2012 2:02:16 PM	mst134	N20/0	port; gas; regulator; upstreamP; downstreamP; overflow [ml/min]; comments port2; E-085; S51412151; 135; 2.0; old: 95-120; new 95-120 port3; E-085; S5141278; 100; 2.0; old: 120-180; new 55-80								
11	12/4/2012 9:20:25 AM	mst134	N20/0	port5; E-084; SS1417 flows while measuring	489; 77;	2.0; old: no of the port with the port of	<pre>vverflow (downstreamP drops to 1.2bar, when reset to 2bar, overflow 150 : new: 40-70; target gas with the hardware switch inside the multiportunit</pre>					
10	10/5/2012 8:55:58 AM	mst134	N20/0	port2; E-085; SS1412 port3; E-088; SS1415 port4; E-087; SS1412 port5; E-084; SS1417	788; 100; 132; 82;	2.0; 90 2.0; 35 2.2; 55 2.0; old: no c	overflow : new: 30; target gas					
9	8/16/2012 12:49:23 PM	mst134	N2O/0									
8	8/8/2012 5:08:37 PM	mst134	N20/0									
Encoding: HTML ElCode Plain ESuppress Email notification Resubmit as new entry												
				Attachment 1:			Browse_ Upload					
				Submit Preview Ba	ck		ELOG V2 5 22465					



Documentation – Meta data management

	/agage/jung - GCWerks (Empa)		
File Help			
Save As Save C	hanges Delete File		
Directory File			
operations log			
tank press log 0901			
ports log 1001			_
hardware info 1101			
Tunfler			
check equilibration time for std.9: 70 seconds -> OK			
20.03.2012 (mst-rem) measurement shutdown after run 1523 due to envisaged po	wer outage in the evening		
21.03.2012 (mst-rem)			
restart of measurements with run 0826 to check if it ru measurement shutdown in order to save working standard			
-	yas as it is about to full empy		
<pre>11.04.2012 (mst-jun) restart of measurements, no peaksfor ECD channel, ECD t</pre>	emperature 47C (setpoint was set to 4C !)		
ECD temp setpoint set to 395C -> ECD temp comes up) is broken; dismantled and brought back to Empa -> no ambient air	r moscurements currently pessible	
new working std connected to port11		measurements currently possible	
afternoon old working std (E-064), port9 as std measure shutdown after run 2008	d vs. new working std E-073, port11		
20.04.2011 (mst-jun)			
new KNF pump installed, KNF N86KTE, SN 2.0614395, i.e.	membrane PTFE, valve and flippers Kalrez, euilibration time 50sec		
once more old std E-064 v(as std on port 9) vs new std equilibration time E-064: 60sec, E-073: 65sec	(E-0/5 (as tank on port 11).		
23.04.2012 (mst-rem)			
timefile, i.e. regular traget tank measurements enabled			
29.04.2012	il		
approx. 3h10 Local Winter Time till 15h20 LWT: power fa	Iture		
01.05.2012 (mkv-rem) Announced power failure. stopped run before power cut.	Power was cut at 18:15 LT and lasted at least 40 min (see medusa U	JPS).	
After that mkv finds jung to be running again, so mfi m instrument was off, may need to check back with mfi).	ust have restarted the instrument and the runs (unclear if the ent	.ire	
11.05.2012 (mst-jun)			
port of working std changed (before 11, now 9) as it wq	as connected to a temporary port (and tube) as long as		
the previous working std was still hooked up. donwstrea #			
check equilibrationtime for air measurements: 50sec ->	ок		
06.06.2012 (mkv-rem): announced power outage. Must have resulte drivers and restarts measurements (with an additional s	d in instrument shutdown. mfi must have restarted computer. mkv re td at beginning, will likely have to be flagged).	starts device	
18.06.2012 (mst-rem, UrsOtz-jun)			
flame of FID off, Urs reignites flame			
18.06.2012 till 19.06.2012 0750			
ecd3 and 4 don't change their setpoints, reason unknown functionality comes back again without intervention			
1201 (9 files)		Instrument Chromatograms Stripcha	art Results Edit
🔁 [Upda 🗖 /agage/ 🗖		💹 🕼 🖂 🄇	🔵 29 °C 🛛 Fri Jun 29, 13:19 🛛 🔒 Che 🔎
tual machine, press Ctrl+G.			

martin.steir

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.

- 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

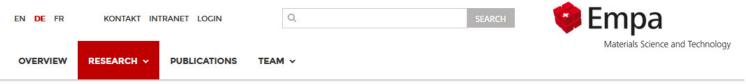
- ISO Guide for the Expression of Uncertainty in Measurements (GUM)
- Freely available on BIPM website http://www.bipm.org/en/publications/guides/gum.html





Terminology

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



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



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

Glossary

- Alphabetical list of terms
- SECTION 1 Quantities and Units
- SECTION 2 Measurement
- SECTION 3 Devices for Measurement

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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 | measurement quantity value | measurement | measurement accuracy | measurement bias | measurement error | measurement guideline (MG) | measuring instrument | measurement precision | measurement procedure | measurement repeatability | metrological comparability of measurement results | metrological traceability | metrological traceability chain | (mass) mixing ratio | (volume) mixing ratio | mole fraction | measurement model | precision | primary measurement standard | quality assurance | quality condition of measurement error | reference material | reference measurement standard | reference quantity value | reference scale | repeatability condition of measurement | resolution | secondary measurement standard | sensitivity of a measuring system | selectivity of a measuring system | selectivity of a measuring system | target cylinder (target gas) | tertiary standard | transfer measurement device | travelling measurement standard | true quantity value | Type A 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 \rightarrow measuring system, used with a specified \rightarrow measurement procedure, whereby it provides measured \rightarrow quantity values for one or more \rightarrow measurands such that the values of each measurand are independent of other measurands or other \rightarrow 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 ²⁸Si isotope and of the ³⁰Si isotope in silicon from a geological deposit without influence between the two, or from the ²⁹Si 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.

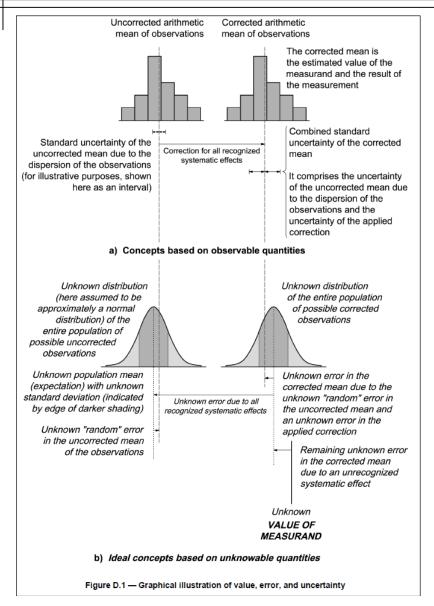
EXAMPLES (GAW)

- 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



 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.)

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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

					GAW Report No. 209
Component (y)	- Example of an uncertainty but Source	Distribution	Contribution to <i>u(x)</i>		
Imperfect calibration / linearity	Comparison between TS and OA	Rectangular	0.0017· <i>x</i> *		Guidelines for Continuous Measurements
Repeatability	Instrument stability	Rectangular	0.0016· <i>x</i>		Ozone in the Troposphere
Span drift	Instrument stability	Rectangular	0.0040· <i>x</i>	<u>@</u>	
Zero drift	Instrument stability	Rectangular	0.17	Wester Group, Wile WIMO-No. 1110	
Pressure P	Pressure measurement	Rectangular	0.0002·x		
Temperature T	Temp. measurement	Rectangular	0.0005· <i>x</i>		
H ₂ O interference	Interference in the UV		0.0060· <i>x</i>		
Other interferences	Interference in the UV		0.6		
Sampling loss (Inlet)	Inlet material, dirt	Rectangular	0.0014· <i>x</i>		

^{*} 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).

 $u(O_3) = \sqrt{(0.81)^2 + (0.0089 \times O_3)^2}$ nmol mol⁻¹

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(14)

Example: Uncertainty of surface O3 measurements

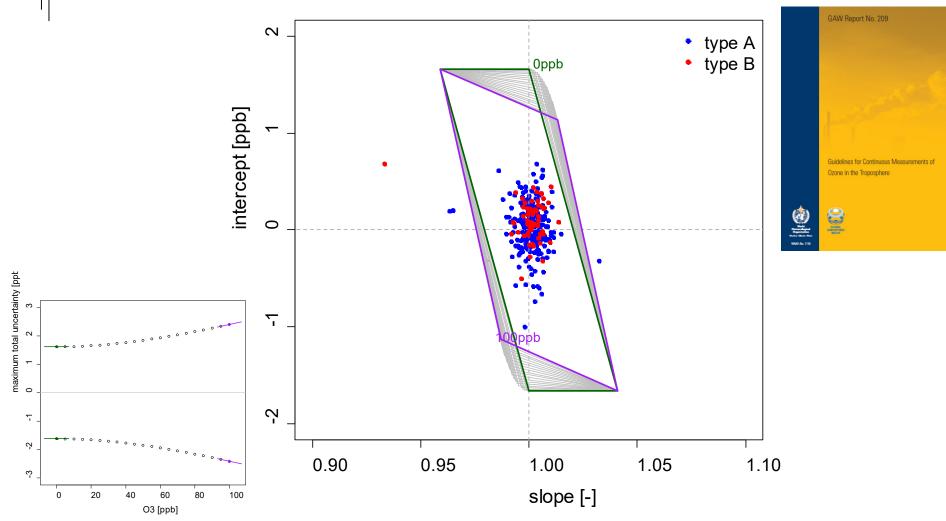
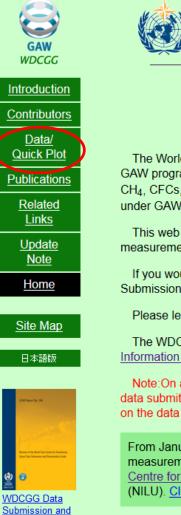


Figure 7 - Intercept vs. slope plot for 296 calibrations of various ozone analysers with transfer standards within the Swiss National Air Pollution Monitoring Network between November 2005 and November 2011 for two different types of UV absorption ozone instruments. The grey lines correspond to the uncertainties 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 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.



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



Welcome to the WDCGG Web Site

WMO Global Atmosphere Watch

World Data Centre for Greenhouse Gases

The World Data Centre for Greenhouse Gases (WDCGG) is one of the WDCs under the GAW programme. It serves to gather, archive and provide data on greenhouse gases (CO_2 , CH_4 , CFCs, N_2O , etc.) and related gases (e.g., CO) in the atmosphere and ocean, as observed under GAW and other programmes.

This web site provides information on greenhouse gases, including WDCGG publications and measurement data contributed by organizations and individual researchers around the world.

If you would like to submit data for the first time, please refer to the WDCGG Data Submission and Dissemination Guide.

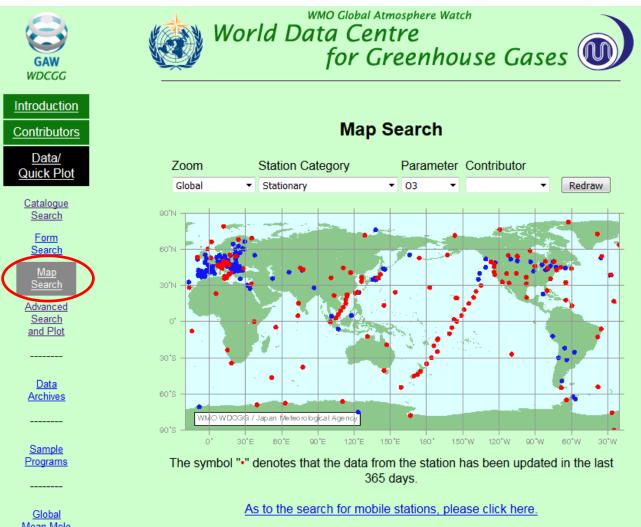
Please let us know if you would like to obtain older versions of archived data.

The WDCGG starts operation as <u>DCPC (Data Collection or Production Centre) of WMO</u> Information System.

Note:On any publication using data from the individual station, the author must contact the data submitters concerning co-authorship or acknowledgements, and make proper descriptions on the data sources in their references.

From January 1st 2016, the responsibility related to archiving of reactive gases measurement data(except for CO) is transferred to <u>the newly established GAW World Data</u> <u>Centre for Reactive Gases (WDCRG)</u> hosted by the Norwegian Institute for Air Research (NILU). <u>Click here for the WMO official letter on this transfer</u>.

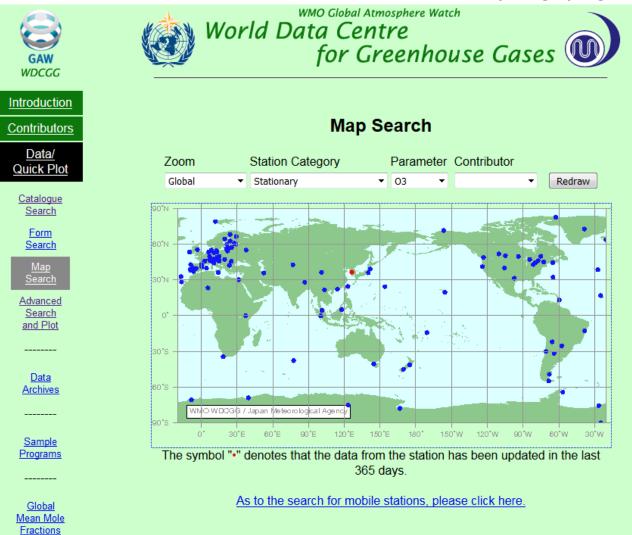
https://ds.data.jma.go.jp/gmd/wdcgg/





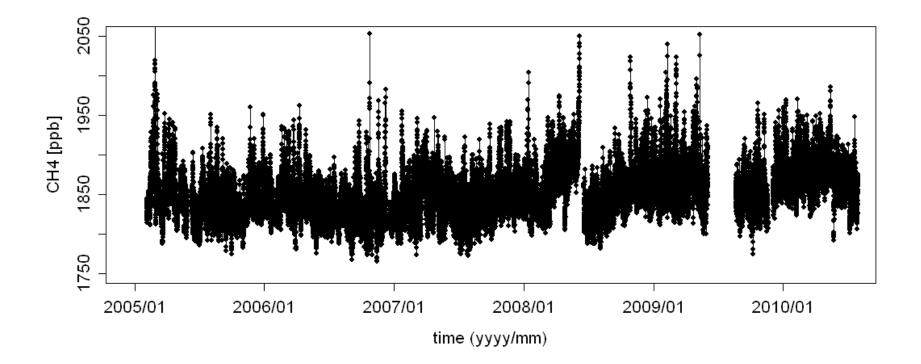


https://ds.data.jma.go.jp/gmd/wdcgg/





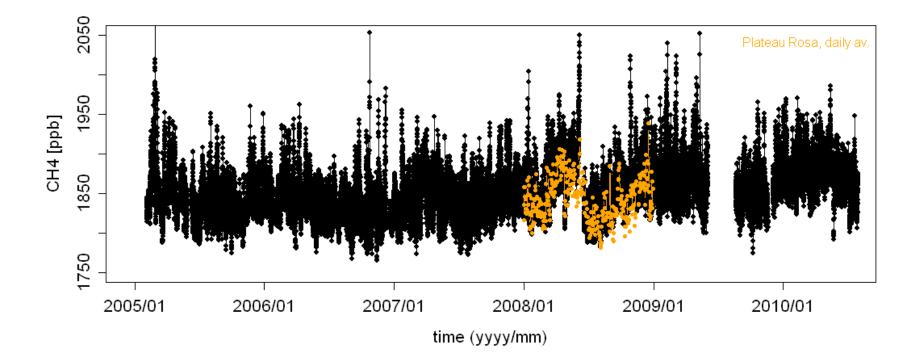
• it works well for longer lived species



25 😢 Empa

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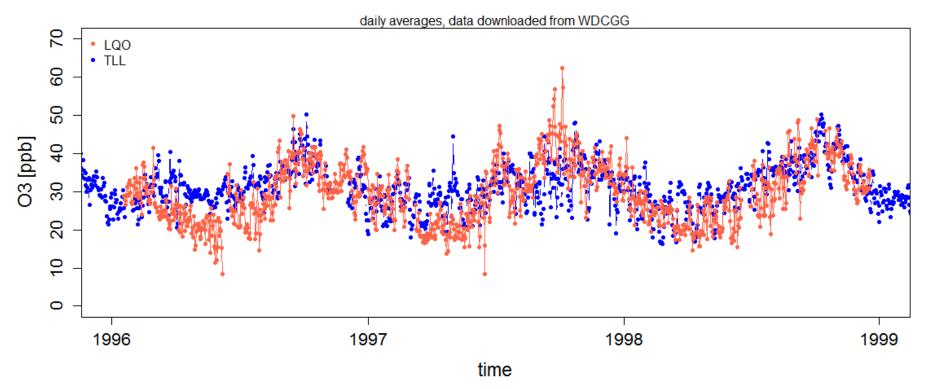
• it works well for longer lived species



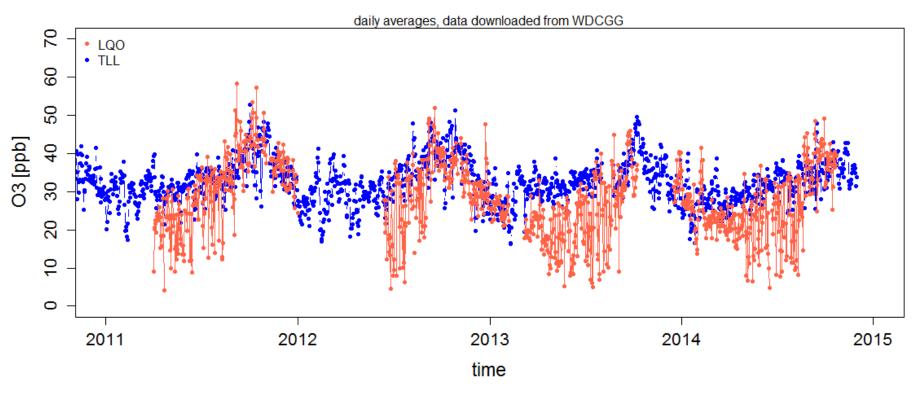


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• Large variability due to (local) formation and depletion of ozone makes a comparison more complex



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

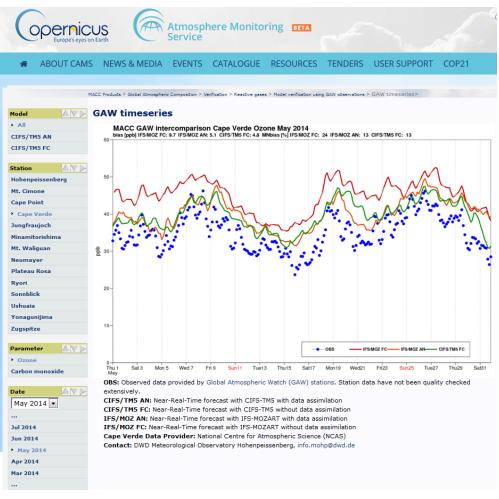


- Is it real or an instrumental artefact? Local knowledge is key to judge.
- Consult logbook entries, compare with other local data (air quality, meteorology)



Using model output information

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





or

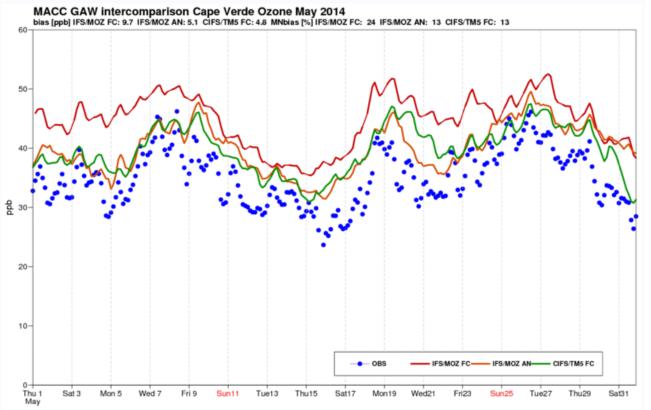


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Using model output information

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

GAW timeseries



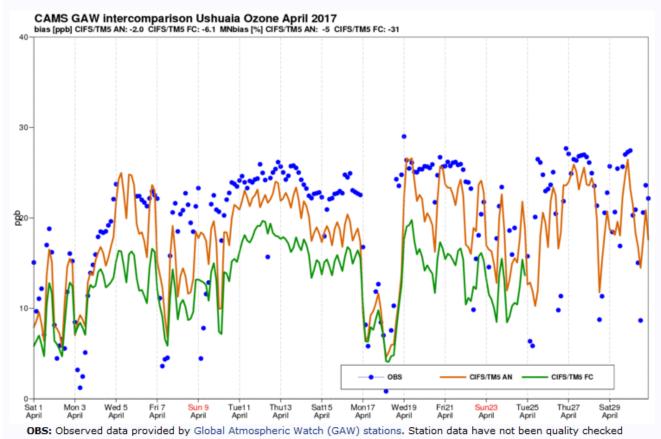
OBS: Observed data provided by Global Atmospheric Watch (GAW) stations. Station data have not been quality checked extensively.

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

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



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 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

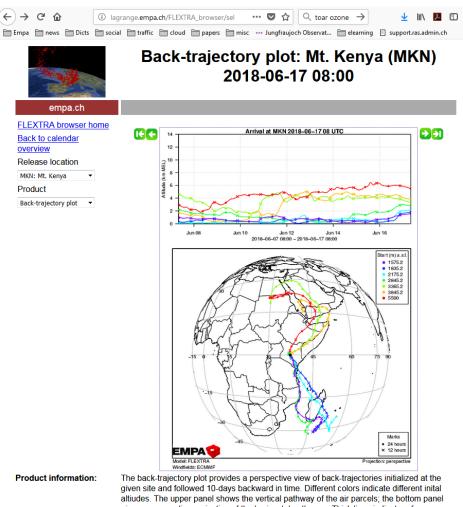
http://lagrange.empa.ch/FLEXTRA_browser/

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

98 Aug 2009

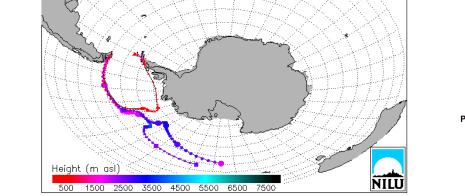
18:00

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



given site and followed 10-days backward in time. Different colors indicate different inital altiudes. The upper panel shows the vertical pathway of the air parcels; the bottom panel gives a perspective projection of the horizontal pathways. Thick lines indicate reference trajectories, thin lines (if available) give uncertainty trajectories started in a circle 0.25° around the site. Traveling times along the trajectory are marked by filled circles (24 h) and crosses (12 h). The calculations are based on the <u>FLEXTRA</u> model and driven by ECMWF windfields with a global resolution of 1° x 1° and 0.2° x 0.2° for the Alpine area (since 2006).





Ushuaia ▲ 500 m

●1000 m ■1500 m



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Federal Office of Meteorology and Climatology MeteoSwiss







Questions ?