Harmonisation of data flagging?

(submitted by M. Schultz and H. Koide)

"The purpose of data flagging is to obtain, at the end of the processing of the measurements, a time series of mole fractions that represents ambient conditions and to clearly identify artefacts as such. No entries should ever be removed from the original (raw) data set. Samples designated as not representing atmospheric composition should be identified [...]. The periods of automatic and/or manual calibration or maintenance as well as instrument problems should be clearly flagged. Instrumental problems are sometimes not obvious and identifying them in the time series may require significant experience." (from GAW report 209 – ozone measurement guidelines)

1. Motivation

Currently, there is no standardized, GAW-wide data flagging scheme, and the amount and quality of data quality information varies widely between data centers and even within data centers between variables. An initial discussion in the Reactive Gases SAG (RG-SAG) which resulted from the writing of new measurement guidelines for tropospheric ozone (GAW report 209) yielded the suggestion to investigate the suitability of existing data flagging schemes for wider adoption within the GAW program. The proposal that came out of the RG SAG was to adopt the alphabetical system that was first introduced for greenhouse gas data by the NOAA CMDL laboratory. However, it became quickly evident that this scheme may not cover all needs of all topic groups, and – more importantly – that some data centers may have to meet other requirements due to their obligations in other national or international programs. Hence, the objective of implementing a GAW-wide flagging scheme cannot mean that this must become mandatory for all data centers. Furthermore, the flagging scheme does not necessarily have to model the way how data are stored in the respective data centers, but it should primarily be seen as option for outputting data in a standardized, documented format to answer user requests; in particular in the framework of interoperable data systems.

The present document summarizes the proposed extensions of the NOAA flagging scheme for greenhouse gases and compares it to the numerical scheme that is used in EBAS (http: //ebas.nilu.no). A first attempt is made to establish a mapping of flag values from EBAS to the proposed GAW scheme. Finally, a short discussion attempts to summarize the advantages and potential shortcomings of the proposal.

2. The NOAA flagging scheme for greenhouse gases

2.1. The NOAA flagging scheme for greenhouse gases

The WDCGG in GAW Report No. 188 (WMO, 2009b) describes limited flags based on a NOAA standard procedure first presented in WMO (2003). This system uses three characters for the flag represented here by ABC. The characters can be either a period or an alphanumerical character, e.g. "..." or "X.." or ".Y.". The characters in "ABC" flag represent

the following information: "A" represents measurement information, e.g. special measurement conditions; "B" represents environmental conditions (e.g., background, pollution episode, biomass burning etc) and "C" is an operator defined variable for particular uses appropriate to that station.

The description on the latest flagging of NOAA ESRL global air sampling network is available from their FTP server (e.g.,

ftp://ftp.cmdl.noaa.gov/ccg/co2/flask/README_surface_flask_co2.html):

Column A QUALIFIER (GAW: REJECTION) flag. An alphanumeric other than a period (.) in the FIRST column indicates a sample with obvious problems during collection or analysis. This measurement should not be interpreted.

Column B SELECTION flag.

An alphanumeric other than a period (.) in the SECOND column indicates a sample that is likely valid but does not meet selection criteria determined by the goals of a particular investigation.

Column C INFORMATION flag. An alphanumeric other than a period (.) in the THIRD column provides additional information about the collection or analysis of the sample.

In CO_2 case, the flags listed in table 2.1 are applied, where samples are collected in pairs and the pair difference is used for the evaluation of the data with the threshold of 0.5 ppm..

Flag	Description	Operations
	(3 periods) good pair	retained
	(D <= 0.5 ppm)	
H	high member of bad pair;	retained
L	low member of bad pair	retained
I	sample has also been measured by another lab as part of an	retained
	intercomparison experiment	
.X.	flagged automatically as an outlier, greater than 3 sigma from a	selected
	fitted curve	
.Z.	flagged manually as an outlier (this is necessary to prevent	selected
	distortion of the curve used for automated data selection)	
+	high member of bad pair	rejected
	low member of bad pair	rejected
*	off scale or broken flask	rejected
N	rejected due to error in sampling or analysis	rejected
A	rejected due to error in analysis	rejected
Т	sample collected as part of a methods test; not used in data	rejected
	analysis	

Table 2.1. Flags for CO₂ surface flask sampling network of NOAA ESRL

The basic idea behind this scheme is that users can easily select valid data that are suitable for analysis in the context of the measurement programme (i.e. background concentrations) by looking for all data points that are marked "…". Any other flag value indicates that caution must be exerted when using the data or that the data are considered invalid. For example, in the context of evaluating atmospheric chemistry transport models, one is often interested also in measurements under polluted conditions. Therefore, data filtering for this application will typically accept "…" and ".X." as valid data.

2.2. Further deliberation on a flagging scheme at NOAA

Another direction recently developed by NOAA/ESRL (Ken Masarie, personal communication) is giving freedom to PIs with only limited standard flagging because of the difficulty to consolidate standard flagging which is suitable and agreeable to all PIs running different measurement programs using different protocols and detection methods.

NOAA originally developed the 3-character flagging strategy back in the early 1990s when focused primarily on making surface flask and surface in situ measurements at remote locations. As their measurement focus expanded to include continental sites and vertical profiles, the flagging strategy could not accommodate the varied and more complex measurements. Therefore, the idea of "internal" and "external" flags is developed.

The external flag is the 3-character QC flag with which most data users are familiar ("use", "don't use", "use-with-caution"). They have preserved the meaning of each column and have standardized the characters that will appear in the external flag (see table XXX below). Internal flag strategies and character assignments can be freely developed within each project to meet the needs. Pls can assign as many internal flags as they require to do their work. For example, a single surface PFP CO₂ measurement may have several internal flags each identifying some issue pertaining to the collection, measurement, or perhaps an anomalous influence on the air sample. Some internal flags characters have been standardized to have the same meaning across all projects. However, in general, NOAA/ESRL will NOT attempt to standardize the meaning of internal flag characters between projects as it imposes an unnecessary constraint. Therefore, it is possible that the same internal character flag may have a different meaning between projects. This is not ideal but is not considered as a serious problem.

For every measurement, they can derive a 3-character external flag from its assigned internal flags. Each lab/project is responsible for defining the logic or developing the algorithm required to translate their internal flags into the new standardized external flag.

The character set for external flags is

C = collection M = measurement B = both collection and measurement

U = unknown

S = selection

A few examples are shown in Table 2.2:

Flag	Information
	valid measurement that is representative of the sampling site
C	measurement rejected due to a problem during sample collection (typically affects all
	compounds measured)
М	measurement rejected due to a problem during air analysis
В	measurement rejected due to problems during collection and analysis
U	measurement rejected but we cannot determine with certainty whether the problem
	was with collection, analysis, or both.
C	a problem was noted during collection but we do not believe it warrants rejection. Use
	with caution.
M	a problem was noted during measurement but we do not believe it warrants rejection.
	Use with caution.
B	a problem was noted during both collection and measurement but we do not believe
	it warrants rejection. Use with caution.
.S.	valid measurement but for some reason is not representative of the sampling site. PIs
	(via README files) will be required to describe what "some reason" means.

This system is continuing to be refined and the 2nd column selection flag will expand to include a few other characters besides "S" in future. Therefore, users should expect NOAA data distributions always to include the external flags.

3. Extensions to the NOAA scheme

3.1. From tropospheric ozone measurement guidelines

GAW report 209 presents new guidelines for tropospheric ozone measurements and contains a section on data processing including data quality flagging. This is based on the NOAA 3-character approach and extends it by defining a list of suitable flag values for preliminary or invalid data.

Table 3.1. Suggested flags for tropospheric ozone data based on the scheme originally
suggested by WMO (2003). [from GAW report 209]

Flag	Measurement	Environment	Operations
Х	initial unprocessed and	no special conditions	no special
	unvalidated		conditions
U	processed unvalidated	no special conditions	no special
			conditions

C	calibration, zero or span	no special conditions	no special conditions
l	bad data, no special conditions	no special conditions	no special conditions
S	special study, not to be included in the ambient measurements data set,	no special conditions	no special conditions
	processed and validated	no special conditions	no special conditions
.Y.	processed and validated	background conditions	no special conditions
.N.	processed and validated	non-background conditions (not specified),	no special conditions
.В.	processed and validated	biomass burning influence,	no special conditions
.R.	processed and validated	urban plume,	no special conditions

Table 3.2: Specification of flags for invalid data

Flag	Measurement
I.P	Positive outlier value
I.N	Negative outlier value
I.R	Too rapid change in mixing
	ratio
I.C	Consistency problem
	between two analyzers
I.V	Extreme variability (lower or
	higher than normal)
I.Z	Drift in zero measurement
I.S	Drift in span value

3.2. From the European IGAS project

IGAS (http://igas-project.org) is a EU framework 8 project to enhance the usability of passenger aircraft data (IAGOS; http://www.iagos.org/IAGOS) in operational and research contexts. One of the IGAS work packages in IGAS is concerned with the documentation of data quality. After some internal discussion the team decided to further explore the NOAA-derived flagging scheme presented in section 3.1 with further modifications described below. In particular, the IGAS team saw no use in the second column () and kept it only for consistency with the original scheme and the proposed GAW scheme.

The system is presented in Table *** and additional flag values are defined below.

Table 3.3: Proposed flagging scheme for IAGOS ozone data [from IGAS project report, 2013]

Flag	Qualifier	Selection	Information
	(Measurements)	(Environment)	(Operations)
X.X	raw		unvalidated
P	valid		preliminary, passed automatic tests
D	valid		delayed mode
	valid		final validated data
N	valid		valid data, but noise exceeds
			threshold
L	valid		valid data with larger uncertainty
Z	valid		valid data with drift in zero
			measurement
I.X	invalid		reason unknown
I.R	invalid		out of range: exceeds instrument
			specification
I.S	invalid		stationarity
1.0	invalid		outlier (spike)
I.J	invalid		step
I.N	invalid		noisy
I.L	invalid		larger uncertainty
I.Z	invalid		drift in zero measurement
I.T	invalid		T aircraft used

Criteria for selection of . or I, e.g. :

- ... uncertainty < 2 σ %
- ..L uncertainty 2 -4 σ
- I.L uncertainty > 4 σ

Qualifier(Measurements)

X: raw

.: valid

I: invalid

C: calibration, zero or span

S: special study, not to be included in the ambient measurements data set

Information (Operations)

------General------D: delayed mode J: step L: larger uncertainty N: noisy O: outlier (spike) P: preliminary, passed automatic tests R: out of range S: stationarity V: final X: raw (unvalidated or reason unknown) Z: drift in zero measurement doc_6.2_data_flagging_schemes.docx

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------ specific for RH Measurement------T: T aircraft used

-----specific for NOy Measurements C: bad efficiency of converter Y: bad sensitivity

WARNING: A "P" in the 3rd column of the QC flag indicates the measurement result is preliminary and has not yet been carefully examined by the RI. The "P" flag is removed once the quality of the measurement has been determined.

3.3. The approach in Integrated Carbon Observation System (ICOS) Atmospheric Thematic Center (ATC)

The Integrated Carbon Observation System (ICOS) Atmospheric Thematic Center (ATC) takes charge of the central data center for atmospheric measurements in European ICOS framework (http://www.icos-infrastructure.eu/). The current flagging system adopted in ATC and their future plans are briefly described (Lynn Hazan, personal communication).

Following the principle that the primary objective of data quality flagging for most users is to find valid data and that the identification of valid data must be easy and unambiguous, ATC developed a simple flagging scheme: the data is either valid or invalid.

As ICOS is handling both Near Real Time (NRT) data which are available after an automatic processing but before going through expert judgment and PI qualified data, it is important to inform the users if the data can be safely used (manual quality control was applied) or it should be used for preliminary studies only (NRT data). The instruments deployed under ICOS are generating high frequency data (second data), and they store original data as well as aggregated data (minute and hour). All the data are flagged and are available and ATC want to trace if the flag has been applied directly by the PI or if the PI has applied the flag on an aggregate mean and the quality control flag is only "propagated" to the higher frequency data. All the above descriptions lead to the following flags (table 3.4):

Flag	Information
U	Data correct before manual quality control
Ν	Data incorrect before manual quality control
0	Data correct after manual quality control
K	Data incorrect after manual quality control
R	Data correct after manual quality control and backwards propagation
Н	Data incorrect after manual quality control and backwards propagation

 Table 3.4
 Flagging scheme in ICOS Atmospheric Thematic Center (ATC)

To trace what went wrong during the automatic processing, an additional internal flag can be provided on demand. This flag is displayed as a list of strings each reflecting a failing check on the data, for example the flag "Cavity temperature, Cavity pressure" will say that the temperature and pressure of the instrument were not meeting the requirements when the data was measured.

A classification flag is developed to indicate when it is possible the origin of air masses. Already implemented at two stations, using CO_2 data and meteorological information are: -Marine (Air mass coming from the sea) - Continental (Air mass coming from the continent). Other possible classifications could be: European, Baseline, Regional or local conditions.

ATC is planning to develop the following items for a near future:

* addition a second manual flag to allow the PIs to provide the reason why they have invalidated data or to allow them to provide useful information on data they have validated. The reasons will be taken from a list. This will allow having standardized flags.

* addition of a questionable boolean column for hourly data. Only invalidated hourly data could be questionable. When they will compute higher aggregates the percentage of not used questionable hourly data will be specify in an additional column to give the possibility for a user to request a data extraction including the questionable data for sensitivity test or whatever. On the other hand, it will be very easy to identify the questionable data in the hourly data files by looking at the new 'Questionable Data' flag (these files containing both valid and non-valid data)."

ATC's policy to allow PIs to use internal flags is somewhat similar with NOAA/ESRL's recent development (section 2.2).

4. Mapping of the numerical EBAS flagging scheme onto the proposed GAW scheme

In EBAS (http://ebas.nilu.no) a numerical flagging scheme is used which was defined primarily from requirements in the European Monitoring and Evaluation Programme (EMEP) and with input from the precipitation chemistry community. The EBAS flag values can be coded up to three times for each single data value, hence allowing for documentation of various processing levels (original PI, ???, data center). A full description of EBAS flags can be found at http:// ebas-submit.nilu.no/SubmitData/FullListofFlagsUsedforbrDataReporting/tabid/10569/Default.aspx. Here, we only reproduce those flags which have some relevance to the type of information that has been defined in the proposed GAW flagging scheme. The resulting mapping is 1:N, i.e. when an EBAS value is mapped, there is exactly one corresponding GAW flag, whereas there can be several EBAS values associated with the same GAW flagging value.

All flags are grouped in three categories: V (valid measurement), I (invalid measurement) or H (hidden and invalid measurements).

Table 4.1: Mapping between EBAS data quality flags and the proposed GAW and IGAS schemes

Flag	V/I/H	GAW	Description
Group 9: Missing flags			
999	Ι	I	Missing measurement, unspecified reason
990			Precipitation not measured due to snow-fall. Needed for
			historic data, should not be needed for new data
980	I	C	Missing due to calibration or zero/span check
900	Н		Hidden and invalidated by data originator
Group 8: Fla	gs for u	undefined	data elements
899	Ī		Measurement undefined, unspecified reason
890	1		Concentration in precipitation undefined, no precipitation
Group 7: Fla	gs use	d when th	ne value is unknown
799	1	I	Measurement missing (unspecified reason), data element
			contains estimated value
798	V	l	Measurement missing (unspecified reason), data element
			contains estimated value. Considered valid.
797	V		Data element taken from co-located instrument
784	1		Low precipitation, concentration estimated
783	1		Low precipitation, concentration unknown
782	V		Low precipitation, concentration estimated
781	V	I.N (?)	Value below detection limit, data element contains detection
-			limit
780	V	I.N (?)	Value below detection or quantification limit, data element
			contains estimated or measured value.
771	V	I.H (?)	Value above range, data element contains upper range limit
770	V	I.H (?)	Value above range, data element contains estimated value
750	1		H+ not measured in alkaline sample
741	V		Non refractory AMS concentrations. Don't include
			compounds that volatalises above 600 deg C
740	V		Probably biased gas/particle ratio
701	1	I.L (*)	Less accurate than usual, unspecified reason. (Used only
			with old data, for new data see groups 6 and 5)
Group 6: Me	chanica	al or instr	umental problem
699		I	Mechanical problem, unspecified reason
681		I	Low data capture
680	V		Undefined wind direction
679	V		Unspecified meteorological condition
678	V	I	Hurricane
677	1	I	Icing or hoar frost in the intake
676	V		station inside cloud (visibility < 1000 m)
675	V		no visibility data available
670	1		Incomplete data acquisition for multi-component data sets
669	I	I	Moist or wet filter, invalid
668	V		Moist or wet filter, valid
666		l	Filter damaged, invalid
665	V		Filter damaged, valid

664	1	I.S	Instrument flow(s) too far off target value, considered invalid
663	1	l	Too high sampling flow, data considered invalid
662	V		Too high sampling flow, data considered valid
660	V		Unspecified sampling anomaly, considered valid
659	Ι	I	Unspecified sampling anomaly
658	1	l	Too small air volume
657	V	l	Precipitation collector overflow. Heavy rain shower (squall)
656	V	l	Wet-only collector failure, operated as bulk collector
655	V	I.C	Two samples mixed due to late servicing of sampler.
654	V		Sampling period longer than normal, observed values reported
653	V		Sampling period shorter than normal, observed values reported
652	V	l	Construction/acitivity nearby
651	V	l	Agricultural activity nearby
650	V	l	Precipitation collector failure
649	V	l	Temporary power fail has affected sampler operation
648	V	l	Snow sampler
644	V	I.L (*)	Low instrument precision and/or calibration issues
641	1	l	Aerosol filters installed incorrectly
640	V		Instrument internal relative humidity above 40%
635	I	l	Internal temperatures too far off target value, considered invalid
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530		I.N (*)	Invalid due to too low or too high recovery
521	V		Bactericide was added to sample for storage under warm
			climate. Considered valid
Group 4: Extreme or inconsistent values			
499	V	C (?)	Inconsistent with another unspecified measurement
498	V		Gold trap inconsistency in mercury monitor
478	1	I	Invalid due to inconsistency discovered through ion balance
			calculations
477	I	l	Invalid due to inconsistency between measured and estimated conductivity
476	V		Inconsistency discovered through ion balance calculations.
_			but considered valid
475	V		Inconsistency between measured and estimated
			conductivity, but considered valid
470	V		Particulate mass concentration higher than parallel mass
			concentration measurement with higher cut off; i.e
			PM1_mass > PM25_mass and PM25_mass > PM10_mass
460	1	I	Contamination suspected
459	1	I.P	Extreme value, unspecified error
458	V	I.P	Extremely high value, outside four times standard deviation
			in a lognormal distribution
457	V	I.N	Extremely low value, outside four times standard deviation in
			a lognormal distribution
456	1	I	Invalidated by data originator
451	1	I	Invalid due to large sea salt contribution
450	V	.N.	Considerable sea salt contribution, but considered valid
440	V		Reconstructed or recalculated data
420	V	U	Preliminary data
410	V	.N.	Sahara dust event
Group 3: Fla	gs for a	aggregate	ed datasets
395	Ĭ		Data completeness less than 90%
394	V		Data completeness less than 90%
393	1		Data completeness less than 75%
392	V		Data completeness less than 75%
391	1		Data completeness less than 50%
390	V		Data completeness less than 50%
382	V		More than 75% of the measurements are below detection
			limit
380	V		More than 50% of the measurements are below detection
			limit
370	V		For monthly averages with samples partly in two months, the
			number of days in each month is used for weighing the
			sample
Group 2: Exc	ception	flags as	signed by the database co-ordinator
299	V	C (?)	Inconsistent with another unspecified measurement
298	V		Gold trap inconsistency in mercury monitor
278	1	I	Invalid due to inconsistency discovered through ion balance
			calculations

277	I	l	Invalid due to inconsistency between measured and estimated conductivity
276	V		Inconsistency discovered through ion balance calculations,
075			but considered valid
275	V		Inconsistency between measured and estimated conductivity, but considered valid
260	Ι	I	Contamination suspected
259	1	l	Unspecified error expected
258	V		Extremely high value, outside four times standard deviation in a log-normal distribution
257	V		Extremely low value, outside four times standard deviation in a log-normal distribution
251	1	I	Invalid due to large sea salt contribution
250	V		Considerable sea salt contribution, but considered valid
249	V		Apparent typing error corrected. Valid measurement
220	V		Preliminary data
211	V		Irregular data checked and accepted by database co- ordinator. Valid measurement
210	V		Episode data checked and accepted by database co-
			ordinator. Valid measurement
Group 1: Exception flags for accepted, irregular data			
191	V		Data not truncation corrected - Valid measurement
190	V		Not corrected for cross-sensitivity to particle scattering
189	V		Possible local contamination indicated by wind from
			contaminated sector (auto)
188	V		Possible local contamination indicated by low wind speed (auto)
187	V		Possible local contamination indicated by occurrence of new
			particles (auto)
186	V		Possible local contamination indicated by single scattering
			albedo (auto)
185	V		Possible local contamination indicated by wind direction or velocity
147	V		Below theoretical detection limit or formal Q/A limit, but a
			value has been measured and reported and is considered
			valid
120	V		Sample reanalyzed with similar results. Valid measurement
111	V		Irregular data checked and accepted by data originator. Valid measurement
110	V		Episode data checked and accepted by data originator.
			Valid measurement
103	V		CV of replicate ALPHA samplers > 15 %;. Valid
			measurement
102	V		CV of replicate diffusion tubes > 30 %. Valid measurement
101	V		Denuder capture efficiency < 75%. Valid measurement
100	V		Checked by data originator. Valid measurement
Group 0: Valid data			
000	V		Valid measurement

EBASflagsarefromhttp://ebas-submit.nilu.no/SubmitData/FullListofFlagsUsedforbrDataReporting/tabid/10569/Default.aspx(last updated in April 2012 by Anne Hjellbrekke). All flags are grouped in three categories: V(valid measurement), I (invalid measurement) or H (hidden and invalid measurements).

(*) from proposed IGAS flag list

During the RG SAG discussions in November 2013, K. Torseth (NILU) indicated that the level of detail contained in the EBAS flagging scheme is often not practical and most flag values are rarely, if ever, used.

5. Discussion

In the previous discussions and based on past experiences, a couple of design principles for data quality flagging schemes have emerged:

- 1. The scheme should be simple to implement and easy to understand. This increases acceptance and avoids errors in the implementation and use
- 2. The primary objective of data quality flagging for most users is to find valid data. Therefore, the identification of valid data must be easy and unambiguous
- 3. Given the increasing importance of NRT delivery of unvalidated data, a distinction between unvalidated (automatically processed) and validated data must be possible
- 4. Investigators should be able to provide some basic explanation of what went wrong with a measurement, but too much detail will lead to ambiguities and inconsistent use of flag values
- 5. Flag codings should be standardized so that automated data retrieval algorithms (interoperable systems) can interpret them (controlled vocabulary)

The three-letter approach originally defined by NOAA and extended for use in GAW as described in this document appears to fulfill most of these principles and has the advantage of being compatible with a standard that is widely used in the greenhouse gas community. One potential shortcoming is the lack of flag values for data operations performed by the data centers (e.g. correct rounding errors, compute mean values, etc.). It should be discussed how this information can be provided.

Agreement on at least a subset of flag values and on a scheme by which the validity or suitability of a given data point can easily be evaluated is essential for a universal data quality flagging system that can be used throughout GAW and beyond. A process for adding new flag codes should be defined and a custodian needs to be appointed who manages the controlled vocabulary on these flag values.

Such a flagging system would contribute to the "branding" of GAW as a network and allow the inclusion of data quality information in automated data retrievals or via filter settings at the world data centers.

While the proposed scheme may not be appropriate for all GAW thematic fields, we suggest that it can be adopted at least by reactive gases, greenhouse gases and ozone, unless another more suitable alternative comes up.