

# Manual for the

## Use of Real-Time Oceanographic Data Quality Control Flags

Version 1.0 January 2014



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## **Revision History**

Date	Revision Description	Notes
January 2014	Original Document Published	

## **Endorsement Disclaimer**

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## Acknowledgements

Thanks to all who assisted in the preparation of this document by providing content and reviewing drafts. Special thanks to the Data Management and Communications (DMAC) committee members. Appendix A contains the names and organizations affiliations of all those who contributed to this data QC flag manual.

## Acronyms and Abbreviations

AOOS	Alaska Ocean Observing System	
BOA	Board of Advisors	
CDIP	DIP Coastal Data Information Program	
CeNCOOS	Central and Northern California Ocean Observing System	
CO-OPS	Center for Operational Oceanographic Products and Services	
DCP	Data Collection Platform	
DMAC	Data Management and Communications	
GCOOS	Gulf of Mexico Coastal Ocean Observing System	
GLOS	Great Lakes Observing System	
GOOS	Global Ocean Observing System	
IOC	Intergovernmental Oceanographic Commission	
IOOS	Integrated Ocean Observing System	
MARACOOS	Mid-Atlantic Regional Association Coastal Ocean Observing System	
MBARI	Monterey Bay Aquarium Research Institute	
NANOOS		
NCDDC		
NDBC	· · · · · · · · · · · · · · · · · · ·	
NERACOOS	Northeastern Regional Association of Coastal Ocean Observing Systems	
NOAA		
NODC		
NOS		
PaclOOS	Pacific Islands Ocean Observing System	
QARTOD	Quality-Assurance/Quality Control of Real-Time Oceanographic Data	
QA	Quality Assurance	
QC	Quality Control	
RA	A Regional Association	
RCOOS	COOS Regional Coastal Ocean Observing System	
SCCOOS	S Southern California Coastal Ocean Observing System	
SECOORA	ORA Southeast Coastal Ocean Observing Regional Association	
SIO	Scripps Institution of Oceanography	
UNESCO	SCO United Nations Environmental, Scientific, and Cultural Organization	
USACE	U.S. Army Corps of Engineers	
WHOI	Woods Hole Oceanographic Institution	

## **Document Purpose**

The U.S. Integrated Ocean Observing System (IOOS) has issued Quality Assurance/Quality Control of Real-Time Oceanographic Data (QARTOD) manuals to be used for identifying the quality of oceanographic data in real time. This data QC flag manual provides information to operators of ocean observing systems about the purpose and protocols of marking or flagging data, so that subsequent use of the data can be properly controlled by both users and automated processes.

Please reference this document as:

U.S. Integrated Ocean Observing System, 2013. Manual for the Use of Real-Time Oceanographic Data Quality Control Flags. 19 pp.

## **Terms and Definitions**

Data Quality Flag	Metadata associated with a specific data point indicating the results of one or more QC tests.	
Operator	An entity or organization that has deployed and maintained oceanographic sensors and is currently providing data in real time.	
Real Time	Data are used or ingested without delay or further post-processing.	
Data User	A middle or endpoint entity desiring information, but not necessarily knowledgeable in methods used to obtain the information.	
Summary Flag	A single flag set to the lowest value of all QC flags within the data record.	
Data Record	An observation or collection of observations and supporting metadata treated as a stand-alone entity.	

## Background

#### **Need for Flags**

Real-time oceanographic data are employed for a wide variety of applications and users. Some applications/users may require that only data of the highest quality be used, and others may seek an indication that a data point is questionable. Some users may prefer the delivery of all data, to be quality controlled using their own criteria. Successful use of the data will depend upon the knowledge, skills, and diligence of the user. Erroneous use of bad data or questionable/good data identified as bad can have serious consequences. For example, specific data points collected during a sudden increase in wind speed resulting from a localized summer thunderstorm may be outside expected wind speeds. However, the automated deletion of such data results in a loss of vital information concerning the weather event.

Operators of observing systems may be best suited to determine the quality of their observations and to document their findings by generating metadata to accompany the observations. Information generated by software in real time about the data quality is referred to as data quality flags, which become an embedded part of the output data stream. As such, the first value added by generating data quality flags is that the quality of the data has been considered at all—sometimes data flow without any evaluation of their quality.

#### **Multiple Standards**

The Intergovernmental Oceanographic Commission/United Nations Environmental, Scientific, and Cultural Organization (IOC/UNESCO) issued a document (hereafter referred to as IOC 54:V3) (UNESCO 2013) with seven examples of flag schemes. Other flag scheme examples exist, including those from the EuroGOOS (European Global Ocean Observing Systems DATA-MEQ Working Group (Pouliquen et al. 2011) and the National Oceanic and Atmospheric Administration (NOAA) National Ocean Service (NOS) Center for Operational Oceanographic Products and Services (CO-OPS) (Evans et al. 2003). Some flag schemes may simply assign a good or bad rating, which is sufficient for operators/users who desire only good data. At the other extreme, flag schemes can generate a detailed indication of why a data point has been flagged, which is helpful to those responsible for troubleshooting and repairing a sensor.

#### Acceptance of Standards and Need for Flag Translators

U.S. IOOS/QARTOD must accommodate a wide variety of operator QC capabilities. Most operators do not collect sufficient data to justify accepting only the best data and discarding lower quality data—all data can have value to some users. Some operators have highly evolved QC processes in place, and they are not inclined to replace those processes. Other operators may set a few rudimentary min/max thresholds to eliminate outlier data, which, without a flagging scheme, could be interpreted as a data gap. Operators may also have limited resources to implement additional processes/flags.

Diversity in flag schemes is no different than that found worldwide in language, currency, engineering units, etc. One overarching standard may evolve over time, but meanwhile, a near-term solution is to create metadata translation tables to convert one standard to another. Both IOC 54:V3 and *Ocean Quality Flag Schemes and Mapping between Them* (Schlitzer 2013) provide good examples of such translations.

## **U.S. IOOS Data Flag Protocol**

#### Identification and Selection of an Existing Standard

IOC 54:V3 was issued in 2013, shortly after the first IOOS/QARTOD QC manual was published. A review of the various existing flag standards indicated that the standard suggested in early QARTOD manuals nearly matched the "Primary Level" scheme presented in IOC 54:V3. Rather than adhere to two nearly identical standards, IOOS/QARTOD decided to accept the IOC 54:V3 scheme and modify one existing QARTOD manual (Dissolved oxygen) to conform to IOC 54:V3.

#### **Definition of the Accepted Standard**

The IOC 54:V3 Primary Level flagging standard (UNESCO 2013) is shown in table 1.

Value	Primary-Level Flag Short Name	Definition
1	Good	Passed documented required QC tests
2	Not evaluated, not available or unknown	Used for data when no QC test performed or the information on quality is not available
3	Questionable/suspect	Failed non-critical documented metric or subjective test(s)
4	Bad	Failed critical documented QC test(s) or as assigned by the data provider
9	Missing data	Used as place holder when data are missing

Table 1. Primary Level Flagging Standard

U.S. IOOS/QARTOD discourages use of the *Flag 2 Not Evaluated* flag, as this violates the very first of the *Seven QARTOD Data Management Laws*, which is that "every real-time observation distributed to the ocean community must be accompanied by a quality descriptor" (NOAA 2009).

#### **Advanced Flagging Schemes**

In IOC 54:V3, a two-tiered flag scheme is proposed, but only the Level 1 tier is described. Likewise, U.S. IOOS/QARTOD adopts only the Level 1 flags but encourages the use of Level 2 flags for additional documentation that may be of use to operators and data users. Level 2 flags may be closely related to a specific sensor and consequently more challenging to translate to another standard. Several examples of such flags are taken from IOC 54:V3 and expanded in table 2.

 Table 2. Example of quality control tests and data processing history (IOC 54:V3)

Globally impossible value (exceeds low or high thresholds)	
Monthly climatology standard deviation test (exceeds warning or failure thresholds)	
Excessive spike check (exceeds warning or failure, low or high thresholds)	
Excessive offset/bias when compared to a reference data set (exceeds warning or failure, low or high thresholds)	
Unexpected X/Y ratio (e.g., chemical stoichiometry or property-property X to T, S, density, among others)	
Excessive spatial gradient or pattern check ("bullseyes")	
Below detection limit of method	

#### **Summary Flags**

Operators may generate summary flags for the convenience of data users. A summary flag is set to the highest level flag found in the detailed tests outlined in U.S. IOOS data quality manuals, such as the *QARTOD Manual for Real-Time Quality Control of In-Situ Surface Wave Data* (U.S. IOOS 2013). For example, if any tests generate a *Flag 4 Bad* flag, then the summary flag is set to *4 Bad*. This provides a simple check that users can invoke when they require only a basic level of QC. U.S. IOOS/QARTOD does not require use of the summary flag.

U.S. IOOS/QARTOD does not dictate the methods operators use to implement data QC flags. Individual bits representing the five identified flag values (table 1) may be set, making data masking an easy task. More likely, operators will identify a character string that can detect more than the five values found in table 1. Operators are encouraged to provide code that can be used to read data and metadata, including these QC flags.

Evans et al. 2003 shows an example of a QC bit mask and a summary flag. The DQA (data quality assurance) bit mask consists of 32 zeros or ones, where one indicates a failure or warning. The definition of the bits varies with data type and may result in unused bits. The 32 bits are followed by a three-digit Data Quality Class Code. In the example below, the three (3) indicates there were no failures or warnings. For a more complete explanation, see <a href="http://www.tidesandcurrents.noaa.gov/publications/puff4.pdf">http://www.tidesandcurrents.noaa.gov/publications/puff4.pdf</a>. This example uses a salinity/temperature/pressure record with values of 3.55 PSU, 15.3 °C and pressure of 15.12 dBars and would read as:

#### 

Each bit is labeled as to its importance.

Info This is merely information; it does not reflect directly on the quality of	of the data.
---	--------------

- Warning This is a warning; the data quality may be affected.
- Failure The data has failed a real-time QA check; use at your own risk.
- Bit 0 Failure Salinity out of range
- Bit 1 Failure Salinity zero
- Bit 2 Failure Water temperature out of range
- Bit 3 Failure Time is > 6 minutes off
- Bit 4 Warning Salinity is flat
- Bit 5 Warning Water temperature is flat
- Bit 6 Failure No data
- Bit 7 Failure Barometric pressure is out of range

- Bit 8 Warning Barometric pressure is flat
- Bit 9 Failure Water temperature sensor disabled by CORMS<sup>1</sup>
- Bit 10 Failure Conductivity (salinity) sensor disabled by CORMS

An advanced character string flagging scheme can be found in a Scripps Institution of Oceanography (SIO) Coastal Data Information Program (CDIP) THREDDS (Thematic Real-Time Environmental Distributed Data Services) server that hosts the CDIP netCDF data sets (<u>http://thredds.cdip.ucsd.edu/thredds/catalog.html</u>). Table 3 shows the two-tier IOC flagging used by CDIP: waveFlagPrimary holds the IOC-recommended primary level values, and waveFlagSecondary holds additional information as assigned by CDIP QC routines, based on both the data type and sensor type (a Datawell directional Waverider).

Table 3. Example shows a two-tier flagging scheme (courtesy of the SIO CDIP team)

```
Web thredds.cdip.ucsd.edu/thredds/dodsC/cdip/archive/071p1/071p1_d17.nc.html
```

#### **waveFlagPrimary:** Array of 8 bit Bytes [waveTime = 0..22608] waveTime:

long\_name: primary wave QC flag FillValue: -127 valid\_min: 1 valid\_max: 9 flag\_values: 1, 2, 3, 4, 9 flag\_meanings: good not\_evaluated questionable bad missing reference: Ocean Data Standards, UNESCO 2013 - IOC Manuals and Guides, 54, Volume 3 Version 1 ancillary\_variables: waveFlagSecondary

#### waveFlagSecondary: Array of 8 bit Bytes [waveTime = 0..22608]

waveTime:|0:1:22608
long\_name: secondary wave QC flag
FillValue: -127
valid\_min: 0
valid\_max: 11
flag\_values: 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11
flag\_meanings: unspecified sensor\_issues Hs\_out\_of\_range Tp\_out\_of\_range Ta\_out\_of\_range
elevated\_check\_factors Hs\_spike Ta\_spike low\_freq\_energy\_spike excessive\_low\_freq\_energy
hf\_transmission\_errors\_fixed hf\_transmission\_errors\_present

The formatting and use of flags and other metadata, either through automated interoperability methods or human use, continue to evolve (see <a href="http://www.jcommops.org/dbcp/data/metadata.html">http://www.jcommops.org/dbcp/data/metadata.html</a>). Further information and training about metadata standards can be found at <a href="http://www.ncddc.noaa.gov/metadata-standards/metadata-training/course-one/">http://www.ncddc.noaa.gov/metadata-standards/metadata-training/course-one/</a>.

#### **Application of Flags**

QC flags provide important information to those who may use the data to make important decisions in real time. The data and the metadata (including QC flag settings) provided in real time should be archived exactly as they were delivered to users. Therefore, data records containing QC flags set in real time should retain those flags permanently. Operators should have a high degree of confidence in the assigned QC flags. Post-processed records may yield a different finding, but these records should not overwrite the real-time records.

<sup>&</sup>lt;sup>1</sup> The Continuous Operational Real-Time Monitoring System serves as the primary automated QC system for NOAA/NOS/CO-OPS oceanographic and meteorological data.

However, there are limited instances where it is acceptable to change a real-time flag. In some cases, QC tests operate on a data point that may be one or more cycles old. For example, a spike check uses data points at  $N_{-2}$  and  $N_0$  to examine data point  $N_{-1}$ . In this case, the flag for the QC test on the data point  $N_0$  should be set to "2 Not evaluated, not available, or unknown." After receipt of the subsequent data point,  $N_0$  becomes  $N_{-1}$ , the spike test can be applied, and the flag can be changed as necessary. Operators and users must understand that some tests operate over several data points, and the determination of summary flags must also take this into consideration. The situation highlights the importance of users (both machine-to-machine and end users) evaluating the QC flags for several time-steps backward.

#### Summary

There are a wide variety of applications for and users of real-time oceanographic data. The quality of those data is dependent upon many factors, including the ability to apply QC flags to real-time data streams. This QC flag manual has been compiled considering multiple QC flagging schemes that have been documented by various sources. The flagging standard suggested in early QARTOD manuals nearly matched the "Primary Level" scheme presented in IOC 54:V3. Therefore, U.S. IOOS/QARTOD has accepted the IOC 54:V3 scheme as its data QC flag protocol.

Although content for this manual draws from many sources, it is primarily intended to support the existing QARTOD QC manuals—not to address flagging schemes globally. Guidance provided in this manual, like that in other U.S. IOOS manuals, also considers that operators have different skill levels and resources with which to apply QC flags. Some operators already employ advanced flagging schemes, while others use basic thresholds to flag outlier data.

U.S. IOOS/QARTOD maintains a code repository (<u>http://code.google.com/p/qartod/</u>) where operators may find or post examples of code in use and encourages operators to share examples of code that has been implemented.

Each QC manual is envisioned as a dynamic document and will be posted on the QARTOD website at <u>www.ioos.noaa.gov/qartod/</u>. This process allows for QC manual updates as technology development occurs for both upgrades of existing sensors and new sensors.

#### References

- Evans, M., French, G., and Bethem, T., 2003. Information Systems Branch PORTS Uniform Flat File Format (PUFFF) NOAA/NOS/CO-OPS, Silver Spring, Maryland. 32 pp. <u>http://tidesandcurrents.noaa.gov/publications/pufff4.pdf</u>
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- Schlitzer, R., 2013. Ocean Quality Flag Schemes and Mapping between Them, Version 1.4. Alfred Wegener Institute for Polar and Marine Research, Bremerhaven, Germany. 18 pp. <u>http://odv.awi.de/fileadmin/user\_upload/odv/misc/ODV4\_QualityFlagSets.pdf</u>
- U.S. Integrated Ocean Observing System, 2013. Manual for Real-Time Quality Control of In-Situ Surface
  Wave Data: A Guide to Quality Control and Quality Assurance of In-Situ Surface Wave Observations.
  61 pp.

http://www.ioos.noaa.gov/qartod/waves/

### **Useful Links**

U.S. IOOS Website http://www.ioos.noaa.gov/qartod/

Ocean Data Standards Pilot Project http://www.oceandatastandards.org/

Hydrographic Data Formats http://cchdo.ucsd.edu/manuals/pdf/90\_1/chap4.pdf

NetCDF Climate and Forecast Metadata Convention http://cf-pcmdi.llnl.gov/documents

Data Buoy Cooperation Panel Meta-T Pilot Project http://www.jcommops.org/dbcp/data/metadata.html)

NCDDC Metadata Training Course http://www.ncddc.noaa.gov/metadata-standards/metadata-training/course-one/

Marine Data Quality Flags http://library.oceanteacher.org/OTMediawiki/index.php/Marine Data Quality Flags

Argo Flag Scheme http://www.usgodae.org/argo/argo-dm-user-manual.pdf

Global Temperature-Salinity Profile Program QC Flag Scheme <u>http://www.nodc.noaa.gov/GTSPP/document/qcmans/qcflags.htm</u>

## Appendix A. QARTOD Data QC Flag Manual Team

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