INTEGRATED OCEAN OBSERVING SYSTEM

# Manual for

## Real-Time Quality Control of Dissolved Oxygen Observations

A Guide to Quality Control and Quality Assurance for Dissolved Oxygen Observations in Coastal Oceans

**Version 2.0**
**April 2015**

QARTOD
QUALITY ASSURANCE OF REAL-TIME OCEANOGRAPHIC DATA

## Document Validation

INTEGRATED OCEAN OBSERVING SYSTEM

### U.S. IOOS Program Office Validation

Zdenka S. Willis — 04/03/2015

Zdenka S. Willis, Director, U.S. IOOS Program Office — Date

### QARTOD Project Manager Validation

J. Swaykos — 04/03/2015

Joseph Swaykos, NOAA National Data Buoy Center — Date

### QARTOD Board of Advisors Validation

Julianna O. Thomas — 04/03/2015

Julianna O. Thomas, Southern California Coastal Ocean Observing System — Date

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## Revision History

| Date | Revision Description | Notes |
| --- | --- | --- |
| 12/2012 | Original Document Published | |
| 04/2015 | Updated Document Published | • Revised *Document Validation* page (page i).<br>• Added Request to Manual Users (page v).<br>• Updated *Acronyms and Abbreviations* (page viii).<br>• Added *Definitions of Selected Terms* to the front matter of document (page ix).<br>• Updated section 1.0 to reflect publication of other manuals and the DO manual update (pages 1-3).<br>• Updated list of sensors that measure DO (page 5).<br>• Added text to address data uncertainty (page 8).<br>• Updated graphic examples of mobile platforms (pages 10 and 11, figs. 3-1 and 3-2).<br>• Changed flags to meet standard adopted by U.S. IOOS in 2014 (page 9 and 10 and Tests 1 through 11).<br>• Added a Location Test to the list of required DO QC tests (pages 12, 14, and 21).<br>• Updated section 4.0 to reflect update of DO manual and publication of other manuals (pages 24 and 25).<br>• Edited for consistency across manuals and repaired broken links (various pages).<br>• Revised appendix A based on feedback from BOA, operators, and others (pages A-1 through A-6).<br>• Revised appendix B to reflect current U.S. IOOS leadership and additional contributors to the version 2.0 of this manual (pages B-1 through B-2). |
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## Endorsement Disclaimer

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## Request to Manual Users

**To help gauge the success of the QARTOD project, we need to be aware of groups working to utilize these QC tests. We request that manual users notify us of their efforts or intentions to implement QARTOD processes by sending a brief email to data.ioos@noaa.gov or posting a notice at http://www.linkedin.com/groups?gid=2521409.**

# Acknowledgements

**QARTOD VI** participants met at the National Data Buoy Center on 31 July-1 August 2012. We thank them for their valuable contributions to the creation of this manual.


**L-R:** Dick Crout (NOAA/NDBC), Emma Weston (NOAA/NDBC), David Wolgast (CalCOFI), Kay Howard-Strubel (UCONN), Scott Kendall (Grand Valley State University), Helen Worthington (CO-OPS/REMSA), Ray Toll (NOAA/NDBC/SAIC), Grace Cartwright (VIMS), Darvene Adams (EPA-Region 2), Dennis Demcheck (USGS/LA Water Science), Doug Wilson (NOAA/CBIBS), Melissa Ide (Baruch Institute/NERRS/CDMO), Josh Kohut (Rutgers), Mark Bushnell (CO-OPS/REMSA).

**Not pictured but attended or participated remotely:**

Carol Janzen (Sea-Bird); Mike Lizotte (YSI), and Ian Walsh (WET Labs®)

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Finally, we are grateful to our DO Manual update committee (appendix B) for reviewing the original manual and offering suggestions for improvement.

## Acronyms and Abbreviations

| | |
|---|---|
| ACT | Alliance for Coastal Technologies |
| AOOS | Alaska Ocean Observing System |
| AUV | Autonomous Underwater Vehicle |
| BOA | Board of Advisors |
| CalCOFI | California Cooperative Oceanic Fisheries Investigations |
| CBIBS | Chesapeake Bay Interpretive Buoy System |
| CDMO | Centralized Data Management Office |
| CeNCOOS | Central and Northern California Ocean Observing System |
| CO-OPS | Center for Operational Oceanographic Products and Services |
| CRC | Cyclic Redundancy Check |
| CTD | Conductivity, Temperature, and Depth |
| DCP | Data Collection Platform |
| DMAC | Data Management and Communications |
| DO | Dissolved Oxygen |
| GCOOS | Gulf of Mexico Coastal Ocean Observing System |
| GLOS | Great Lakes Observing System |
| GOOS | Global Ocean Observing System |
| IMOS | Integrated Marine Observing System |
| IOOS | Integrated Ocean Observing System |
| MARACOOS | Mid-Atlantic Regional Association Coastal Ocean Observing System |
| mg/L | Milligrams per Liter |
| NANOOS | Northwest Association of Networked Ocean Observing Systems |
| NCDDC | National Coastal Data Development Center |
| NDBC | National Data Buoy Center |
| NERACOOS | North Eastern Regional Association of Coastal Ocean Observing Systems |
| NERRS | National Estuarine Research Reserve System |
| NIST | National Institute of Standards and Technology |
| NOAA | National Oceanic and Atmospheric Administration |
| NODC | National Oceanographic Data Center |
| PacIOOS | Pacific Islands Ocean Observing System |
| QARTOD | Quality Control/Quality-Assurance of Real-Time Oceanographic Data |
| QA | Quality Assurance |

| | |
|---|---|
| QC | Quality Control |
| RA | Regional Association |
| RCOOS | Regional Coastal Ocean Observing System |
| REMSA | Research, Environmental, and Management Support |
| SAIC | Science Applications International Corporation |
| SCCOOS | Southern California Coastal Ocean Observing System |
| SD | Standard Deviation |
| SECOORA | Southeast Coastal Ocean Observing Regional Association |
| UCONN | University of Connecticut |
| UNESCO | United Nations Educational, Scientific, and Cultural Organization |
| URL | Uniform Resource Locator |
| USGS | United States Geological Survey |
| VIMS | Virginia Institute of Marine Science |
| WHOI | Woods Hole Oceanographic Institution |
| WOCE | World Ocean Circulation Experiment |

## Definitions of Selected Terms

This manual contains several terms whose meanings are critical to those using the manual. These terms are included in the following table to ensure that the meanings are clearly defined.

| | |
|---|---|
| Codable Instructions | Specific guidance that can be used by a software programmer to design, construct, and implement a test. These instructions also include examples with sample thresholds. |
| Data Record | One or more messages that form a coherent, logical, and complete observation. |
| Message | A standalone data transmission. A data record can be composed of multiple messages. |
| Operator | Individuals or entities responsible for collecting and providing data. |
| Quality Assurance (QA) | Processes that are employed with hardware to support the generation of high quality data. (section 2.0 and appendix A) |
| Quality Control (QC) | Follow-on steps that support the delivery of high quality data and requires both automation and human intervention. (section 3.0) |
| Real Time | Data are delivered without delay for immediate use; time series extends only backwards in time, where the next data point is not available; and there may be delays ranging from a few seconds to a few hours or even days, depending upon the variable. (section 1.0) |
| Thresholds | Limits that are defined by the operator. |

## Preface

On 30 March 2009, President Barack Obama signed the Integrated Coastal and Ocean Observation System (ICOOS) Act of 2009 into law. The act authorizes the establishment of a National Integrated Ocean Observing System (IOOS) and codifies a governance structure within which that System will operate.

The ICOOS Act of 2009 provides the structure and foundation for the development of a U.S. IOOS built upon a national-regional partnership. U.S. IOOS broadly consists of contributions from both Federal and non-Federal assets and capabilities to advance the utility of marine observations by creating a system to rapidly and systematically acquire and disseminate ocean, coastal, and Great Lakes data and data products to meet critical societal needs.

High quality marine observations required sustained quality assurance (QA) and quality control (QC) practices to ensure credibility and value to operators and users. QA practices involve processes that are employed with hardware to support the generation of high quality data, such as a sufficiently accurate, precise, and reliable sensor with adequate resolution. Practices such as sensor calibration, calibration checks, and/or in-situ verification, including post deployment calibration; proper deployment considerations, such as measures for corrosion control and anti-fouling, solid data communications; adequate maintenance intervals; and creation of a robust quality control process are also part of QA. QC involves follow-on steps that support the delivery of high quality data and requires both automation and human intervention. QC practices include such things as format, checksum, timely arrival of data, threshold checks (minimum/maximum rate of change), neighbor checks, climatology checks, model comparisons, signal/noise ratios, verification of user satisfaction, and generation of data flags (Bushnell 2005).

Although QA and QC are inter-related, the guidance provided to U.S. IOOS-affiliated operators and users in this manual is specific to the QC of real-time data. It is further specific to data collected from instruments located in bays and/or coastal environments, not those deployed in the deep open ocean. It is also specific to sensors employing semi-permeable membranes or florescence-based detectors. The guidance identifies eleven QC tests—some are required, others are strongly recommended or suggested. Each test contains the codable instructions for implementation and assumes the involvement of highly knowledgeable scientists, engineers, programmers, and technicians. Suggestions for QA best practices are provided in appendix A as a courtesy to the manual user.

## 1.0 Background and Introduction

The U.S. Integrated Ocean Observing System (IOOS) program has a vested interest in collecting high quality data for the 26 core variables (U.S. IOOS 2010) measured on a national scale (see sidebar). In response to this interest and as set forth in the ICOOS Act of 2009, U.S. IOOS continues to establish written, authoritative procedures for the quality control (QC) of real-time data through the Quality Assurance/Quality Control of Real-Time Oceanographic Data (QARTOD) program, addressing each variable as funding permits.

As of early 2015, six guidance manuals have been completed covering the QC of real-time data for each of the following core variables: dissolved oxygen (DO), currents, waves, temperature/salinity, water level, and wind. Additionally, U.S. IOOS produced the *Manual for the Use of Real-Time Oceanographic Data Quality Flags* (U.S. IOOS 2014), a guidance document to provide more information on the purpose of and protocols for flagging data in an automated system. A seventh manual covering ocean optics is in production.

This manual is the first in a series of updates to previously published manuals. The *Revision History* (see page iv) outlines the major changes to the original DO document. Other manuals will be updated as resources become available. Please reference this document as:

> U.S. Integrated Ocean Observing System, 2015. Manual for Real-Time Quality Control of Dissolved Oxygen Observations Version 2.0: A Guide to Quality Control and Quality Assurance for Dissolved Oxygen Observations in Coastal Oceans. 48pp.

**Background**

Ocean observers within the U.S. IOOS community represent a broad cross-section of organizations from the public, private, and academic sectors. One such organization was a grassroots group known as QARTOD (Quality Assurance of Real-Time Oceanographic Data). QARTOD participants included representatives from agencies and institutions with an interest in the quality assurance *and* quality control of oceanographic observations. With support from the National Oceanic and Atmospheric Administration (NOAA), QARTOD participants met to work toward the definition of minimum requirements in quality assurance/quality control (QA/QC) in four focus areas: waves, in-situ currents, CTD (conductivity, temperature and depth), and water quality (biogeochemical properties). QARTOD V yielded Seven Data Management Laws (NOAA 2009):

- Every real-time observation distributed to the ocean community must be accompanied by a quality descriptor.
- All observations are subject to some level of automated real-time quality test.

### 26 Core Variables

Acidity
Bathymetry
Bottom Character
Colored Dissolved Organic Matter
Contaminants
Dissolved Nutrients
Dissolved Oxygen
Fish Abundance
Fish Species
Heat Flux
Ice Distribution
Ocean Color
Optical Properties
Partial Pressure of $CO_2$
Pathogens
Phytoplankton Species
Salinity
Sea Level
Stream Flow
Surface Currents
Surface Waves
Temperature
Total Suspended Matter
Wind Speed and Direction
Zooplankton Abundance
Zooplankton Species

- Quality flags and quality test descriptions must be sufficiently described in the accompanying metadata.
- Data collectors independently verify or calibrate a sensor before deployment.
- Data collectors describe their method/calibration in the real-time metadata.
- Data collectors quantify the level of calibration accuracy and the associated expected error bounds.
- Manual checks on the automated procedures, the real-time data collected, and the status of the observing system must be provided by the observer on a time scale appropriate to ensure the integrity of the observing system.

The U.S. IOOS Program Office continued the effort by initiating the QARTOD Project to address the real-time QC issues of U.S. IOOS and the broader international ocean observing community, including the need for consistent practices for the QC of data. These practices, though different for each of the 26 core variables, help to ensure that consistent QC procedures are followed for data inputs to U.S. IOOS. Under this project, QARTOD VI convened to address the real-time QA/QC requirements for DO observations.

As part of the U.S. IOOS Data Management and Communications (DMAC) core services, the U.S. IOOS Program Office initiated a sustainable, community-based project to establish written authoritative procedures for the QC of real-time ocean sensor data collected for U.S. IOOS. This project is entitled QARTOD, and it formalizes cumulative efforts from previous meetings (also called QARTOD (www.ioos.noaa.gov/qartod/). All of the known QC programs in existence today provide parts to the solution, but none consolidates them in one document. The result of this effort is to develop consistent practices that can become formal U.S. IOOS guidance documents for data from the Regional Associations (RAs) and the ocean observing community at large.

The key objective of QARTOD is to sustain a process that will:

- Establish authoritative QC procedures for each of the 26 U.S. IOOS core variables (U.S. IOOS 2010) as necessary, including detailed information about the sensors and procedures used to measure the variables;
- Produce written manuals for these QC procedures;
- Define baseline QC procedures from the list of individual QC procedures and guidelines developed that can be used for certification of Regional Coastal Ocean Observing System (RCOOS) data providers;
- Facilitate QC integration with Global Ocean Observing System (GOOS) and other international ocean observation efforts;
- Engage the Federal agencies and RAs that are part of, or contribute to, U.S. IOOS that will use the established QC procedures; and,
- Work efficiently, without duplication of effort, to facilitate the implementation of common QC procedures amongst U.S. IOOS partners (U.S. IOOS 2012).

Each manual describes the individual QC tests to be applied to the data stream prior to data dissemination. For DO data, the manual describes eleven tests that are divided into three groups that are either required (group 1), strongly recommended (group 2), or suggested (group 3) for application prior to dissemination of data entered into the IOOS Data Assembly Centers. The time lag between the data collection and dissemination dictates the number and types of tests applied to the data stream (i.e., the real-time versus delayed-mode issue). The RA decides the applicability of the tests.

The description of each QC test will be sufficient for a skilled computer programmer to create software that implements the tests in different software environments. The description of individual tests includes:

- Assumptions of the algorithm or of the context in which it is applied: For example, with real-time data, an assumption for the $N^{th}$ data point might be that the $N+1^{st}$ data point is not available to the software implementation.

- Input thresholds: These thresholds are user-selected adjustable limits for the algorithm implementation. For example, for a gross value test, the minimum and maximum allowable values for the variable of interest are thresholds of the test. The chosen values for application of the test to coastal water temperature data would be different from those values chosen for land-based humidity data even though the logic of the test would be the same in each case. This value might also vary among sensor types where range differences might exist. It is important to note that specific threshold values vary by parameter, season, and geographic location.

- Individual flag syntax: The syntax chosen to represent the results of an individual QC test on a particular data value, or on an entire data set, is an important factor in data system interoperability. The code table of flag values should be described for each test. For binary tests in which the only allowable results are pass/fail, the syntax may simply be 0/1, but in tests in which the results can be characterized within a range, the specific meaning of each interval must be documented (U.S. IOOS 2012).

The completed manuals reside on the QARTOD website (www.ioos.noaa.gov/qartod/) so that they are easily accessible, citable, and dynamic, thus allowing for updates with the appropriate version control procedures in place. The website also includes items such as code libraries, procedures for testing data, and links to additional options for sharing information via social media.

## 2.0 Purpose/Constraints/Applications

This manual documents suggested standard test procedures for data QC from automated, in-situ DO concentration sensors that use either semi-permeable membrane or fluorescent-based technologies. DO observations covered by these procedures are collected as a measure of water quality along bays or coasts[1] in real-time or near-real-time settings.

Deep ocean DO observations used as water mass tracers are excluded because higher accuracies are required in more benign (i.e., less noisy) environments. In order to achieve these higher accuracies, more frequent calibrations and redundant measurements are needed but are rarely delivered in real time. Post-deployment calibration and trend removal associated with sensor drift and other delayed-mode QC practices are not part of the scope of this manual because generally they cannot be applied in near real time. Post processing provides a much higher level of QC and is a necessary and important step that U.S. IOOS will need to address in a process similar to this one. Appendix A addresses QA best practices, along with numerous post-processing and post-deployment calibration issues.

These procedures are written as a high-level narrative from which a computer programmer can develop code to evaluate data quality within a software program. This DO manual is a deliverable to the U.S. IOOS RAs and may be useful to the ocean observing community at large. It represents part of a series of QC manuals for U.S. IOOS core variables that have become formal U.S. IOOS guidance documents.

The goal is to provide guidance to the RAs and the ocean observing community to improve QC through agreed/documented/implemented standard processes. This manual presents a battery of eleven tests that are required, strongly recommended, or suggested. Although certain tests are recommended, thresholds can vary among and within the RAs. For example, the upper limit for DO observations for a buoy moored in deep coastal waters may not be suitable for use in a shallow, wind-mixed bay.

These practices for sensor QC of DO data were developed by operators with experience using a variety of sensors and sensor types. Table 2-1 provides several examples of the devices and the associated sensing technology employed. The operators must make the final determination of the applicability of these tests to their specific sensor(s), and they are encouraged to submit additional sensors to be included in the table.

[1]The coast means coasts of the U.S. Exclusive Economic Zone (EEZ) and territorial sea (http://oceanservice.noaa.gov/facts/eez.html) Great Lakes, and semi-enclosed bodies of water and tidal wetlands connected to the coastal ocean (U.S. IOOS 2006).

**Table 2-1.** Sensors commonly used to measure DO

| Sensor Technology | Sensor Name/Manufacturer |
|---|---|
| Optical | Aanderaa Oxygen Optode<br>ALEC Rinko Fast Dissolved Oxygen<br>Eureka Manta 2<br>Hach HydroLab LDO<br>Onset HOBO U26-001<br>Sea-Bird SBE 63<br>YSI Reliable Oxygen Sensor (ROX)<br>YSI EXO |
| Electrochemical | Sea-Bird SBE 43 |
| Electrochemical/Galvanic | Eureka Manta 2<br>Greenspan DO 300/350 series<br>RBR Global Oxygard<br>YSI Clark Membrane |
| | |

The process of ensuring data quality is not a straightforward one for DO sensors. QC procedures may be specific to a sensor technology or even to a particular manufacturer's model, so the establishment of methodology that is applicable to every DO sensor is challenging. The following paragraphs provide insight into the nature of these challenges.

## 2.1 Temperature/Salinity

The DO sensor detects a measure of dissolved oxygen concentration, but the sensor response and DO concentration calculations also depend upon the quality of the temperature and salinity data. Corrections to the sensor output are required to account for the effects of temperature and salinity. These corrections occur internally in many instruments, and in these cases, failure of the instrument to collect accurate temperature and/or salinity data necessitates that the DO data be highlighted with a suspect or fail flag and reviewed during the QC process. Not all sensors make the temperature data available, and not all sensors measure conductivity. Some DO sensors require the user to input a fixed salinity that represents the likely value.

When expressing DO as a percentage of saturation, the user must consider the effects of temperature, salinity, and barometric pressure (e.g., Benson and Krause 1984; Garcia and Gordon 1992). The U.S. Geological Survey (USGS) maintains a useful Web page at http://water.usgs.gov/software/DOTABLES/ where these variables can be used for single point calculations or the generation of user-specified tables. Scripts (Fortran and MATLAB) for calculating DO saturation are available as part of the GSW Toolbox (www.teos-10.org/).

## 2.2 The Effect of Dynamic Environments on Sensor Data

DO measurements can be challenging for two reasons: DO is a non-conservative[2] variable, and dynamic coastal regions create rapid horizontal and vertical water mass changes. Tidal and meteorological events can create substantial steps in the DO time series. Other variations are induced by such things as seasonal stratification, upwelling, organic loading, increased biological activity (blooms), air-sea exchange, river inputs, and expected diurnal variations in DO due to day-night cycles in photosynthesis and respiration.

Panels 1-4 in fig. 2-1 show strong diurnal fluctuations, as well as strong variations caused by the storm. The example time series of temperature, salinity, DO as a percentage of saturation, and DO concentration in milligrams per liter was obtained during a demonstration deployment in Biscayne Bay, Fla. The demonstration period included the passage of Hurricane Fran on 28 August 2006. The decrease in temperature and introduction of abundant fresh water are clear and correlate well with the change in the DO signal shortly after the storm passed. Important to note, however, are the large diurnal swings in the data even in the absence of the storm passage. Although mixing associated with storms disrupts the diurnal signal, DO values as a percentage of saturation can swing from over 200% (and higher in coastal and estuarine waters) to near zero in less than 24 hours. The storm amplifies the range, reducing DO from over 200% to zero during the storm onset.

As with many other real-time QC challenges, the question is how to deal with extremes associated with a phenomenon (e.g., storm, spill, etc.) in a data time series, yet identify questionable data values that may have similar characteristics. One option is to allow a tighter QC requirement for the data, highlighting the event with a suspect flag and requiring a human review. This way, the event is both: a) acknowledged as substantial if real, and b) identified as potentially questionable in the absence of causal forces.

[2]Temperature and salinity are conservative properties because there are no sources or sinks of heat and salt in the interior of the ocean. Other properties, such as oxygen are non-conservative. For example, oxygen content may change slowly due to oxidation of organic material and respiration by animals. see http://oceanworld.tamu.edu/resources/ocng_textbook/chapter13/chapter13_03.htm.

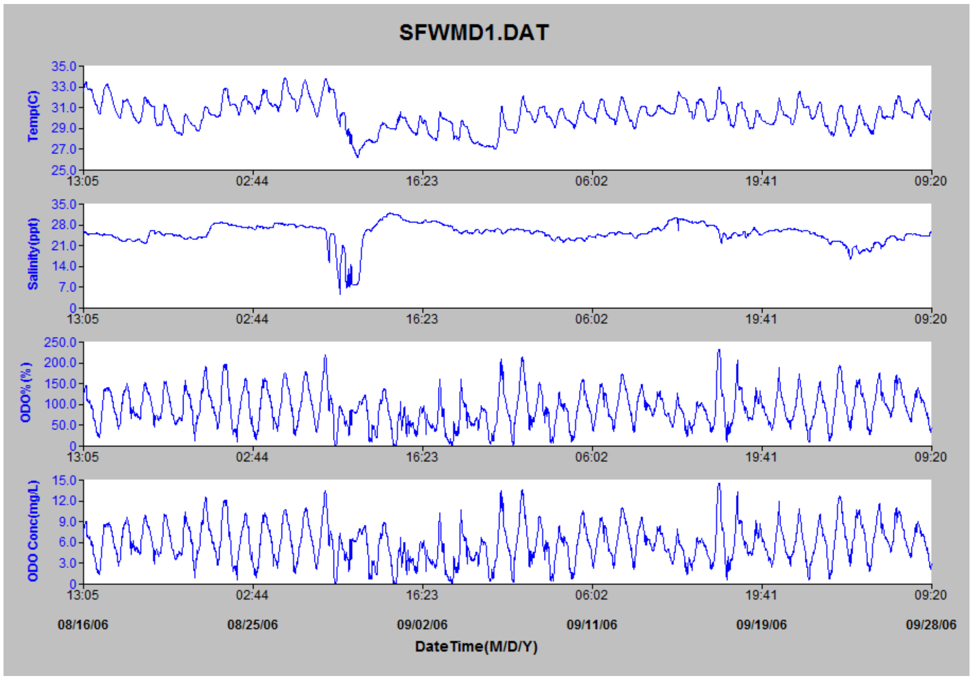


**Figure 2-1.** Panels 1-4 show temperature, salinity, DO percent, and DO concentration, respectively. The series tracks the passage of a hurricane and the effect it has on the time series before, during, and after the storm front passes (courtesy of Mike Lizotte, YSI).

## 2.3 Traceability to Accepted Standards

DO sensor accuracy and resolution are generally provided by the manufacturers of the DO sensors. Traditionally, DO sensor calibrations required Winkler/Carpenter titrations for traceable standardization (Carpenter 1965). While these titrations are not technically a NIST (National Institute of Standards and Technology) standard, equipment used to conduct the titration (weights and volumes) must be NIST traceable. Many other international standards exist and are equally valid. Sensor drift and shift require nearly continuous sensor/titration comparisons to ensure target reproducibility to the highest possible quality. Improvements to both the Clark-style membrane design DO sensors and especially the emergence of fluorescence-based sensors have dramatically improved calibration stability and in some cases, long-term durability. This stability, coupled with high quality manufacturer calibrations, can allow for longer deployments and less frequent sensor validations in some instances. Nevertheless, these sensors are still affected by bio-fouling and degradation of sensor parts (the optical foil and membranes used to protect them, for example). Therefore, QA activities affiliated with measuring oxygen in any aquatic environment still need to be established and recorded.

Some manufacturers use traceable mixed gases to calibrate DO sensors, claiming accuracies ≤1% (personal communication, Mark Bushnell [CO-OPS] and Mike Lizotte [YSI]). Users can readily conduct water-saturation verification tests (Lewis 2011) to confirm performance, and little more is required, especially in the coastal regimes considered herein.

## 2.4 Hardware Limitations

As an example of the impact of good QA, fig. 2-2 shows the step in DO as a percentage of saturation that was observed when swapping a sensor. The plot shows data recorded before and after replacement at the

First Landing Chesapeake Bay Interpretive Buoy System (CBIBS) buoy. The old sensor had become fouled and less responsive, showing just 50% saturation for this surface DO measurement. The replacement sensor immediately showed a much higher saturation percentage. Such steps in a time series during a sensor swap or cleaning provide valuable information for future service intervals and are highly dependent on both the site and season.

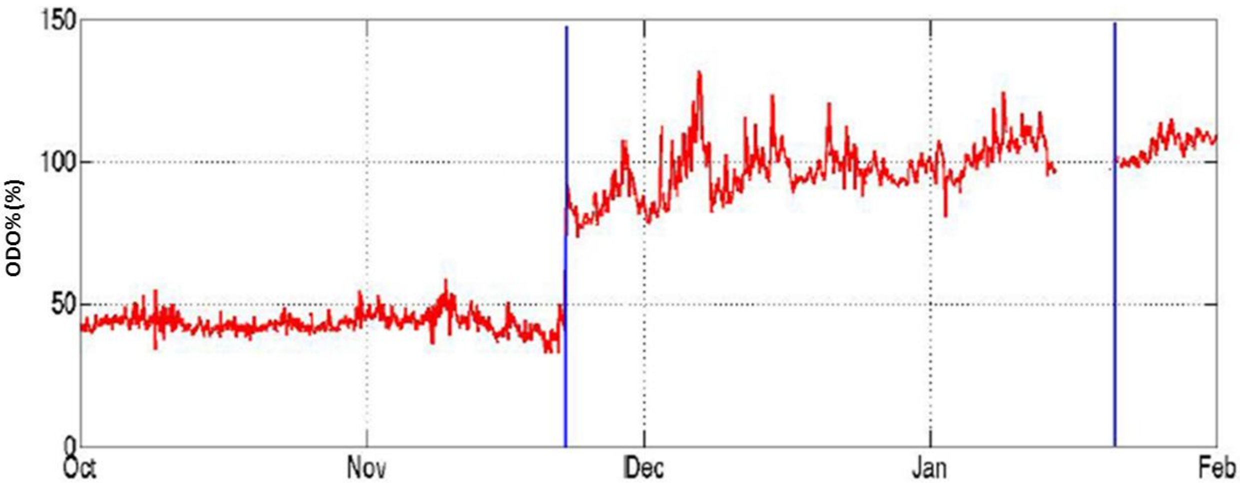


**Figure 2-2.** Note the abrupt shift in late November 2011 when the badly fouled sensor was replaced. The blue lines indicate the time of sensor replacement. Sensor replacement immediately shows higher saturation percentage. Note also apparent lack of a shift in January 2012 (courtesy of Doug Wilson, NOAA/CBIBS).

Such steps in a time series during a sensor swap or cleaning provide valuable information for future service intervals and are highly dependent on both the site and season. Correcting a data shift like this is extremely difficult if not impossible, so servicing schedules and the technology used should be carefully considered. While the data in fig. 2-2 show what happens when fouling is not countered, it should be noted that improvements in anti-fouling measures and sensor technology are constant. For example, the second Alliance for Coastal Technologies (ACT) DO evaluation is underway as this updated manual is being written (http://www.act-us.info/Download/Evaluations/DOII/FINAL_DO_Sensor_Verification_Protocols_12_09_14.pdf). Results are expected in late 2015, and findings of significance will be incorporated in a later revision of this manual. All monitoring programs should investigate which technology best suits their application, the field service budget and data quality goals.

Also important, but beyond the scope of this document at present, is the determination and reporting of data uncertainty. Knowledge of the accuracy of each observation is required to ensure that data are used appropriately and aids in the computation of error bars for subsequent products derived by users. All sensors and measurements contain errors that are determined by hardware quality, methods of operation, and data processing techniques. Operators should routinely provide a quantitative measure of data uncertainty in the associated metadata. Such calculations can be challenging, so operators should also document the methods used to compute the uncertainty. The limits and thresholds implemented by operators for the data QC tests described here are a key component in establishing the observational error bars. Operators are strongly encouraged to consider the impact of the QC tests on data uncertainty, as these two efforts greatly enhance the utility of their data.

# 3.0 Quality Control

In order to conduct real-time QC on DO observations, the first pre-requisite is to understand the science and context within which the measurements are being conducted. DO measurements are dependent upon many things such as season, location, time of day, and the physical, chemical, and biological conditions where the measurements are being taken. The real-time QC of these observations can be extremely challenging. Human involvement is therefore important to ensure that solid scientific principles are applied to the process. Without credible science-based thought, good data might be discarded and bad data distributed.

Advances in oxygen sensor technology have eliminated many of the problems encountered in older devices. Some new sensors are immune to anoxic conditions and the resultant hydrogen sulfide, and some do not develop oxygen depletion at the detector interface.

Again, this manual focuses specifically on real-time data in coastal environments, so the operator is likely to encounter aspects of data QC where the flags and tests described in the following sections do not apply because the data are not considered to be real time. For example, for real-time QC, drift cannot be detected or corrected. Drift correction for DO sensors during post-processing is difficult even with a post calibration in hand because drift in DO sensors is not always linear. Drift is often caused by bio-fouling, usually results in a lower reading, and is accompanied by an attenuated response. Another example might be the ability of some data providers to backfill data gaps. In both of these examples, the observations are not considered to be real time for purposes of QC checks.

## 3.1 QC Flags

Data are evaluated using QC tests, and the results of those tests are indicated using flags in the data files. Table 3-1 provides a simple set of flags and associated descriptions. Operators may incorporate additional flags for inclusion in metadata records. For example, a DO observation may fail the gross range test and be flagged as having failed the test. Additional flags may be incorporated to provide more detailed information to assist with troubleshooting. If the data failed the gross range check by exceeding the upper limit, "failed high" may indicate that the values were higher than the expected range, but such detailed flags primarily support maintenance efforts and are presently beyond U.S. IOOS requirements for QC of real-time data. Flags set in real time should retain their original settings. Further post-processing of the data may yield different conclusions from those suggested in the initial real-time flags. However, by retaining the real time flag settings, the historical documentation is preserved.

**Table 3-1** Flags for real-time data (UNESCO 2013)

| Flag | Description |
|---|---|
| Pass=1 | Data have passed critical real-time quality control tests and are deemed adequate for use as preliminary data. |
| Not Evaluated=2 | Data have not been QC-tested, or the information on quality is not available. |
| Suspect or Of High Interest=3 | Data are considered to be either suspect or of high interest to data providers and users. They are flagged suspect to draw further attention to them by operators. |
| Fail=4 | Data are considered to have failed one or more critical real-time QC checks. If they are disseminated at all, it should be readily apparent that they are not of acceptable quality. |
| Missing Data=9 | Data are missing; used as a placeholder. |

## 3.2 Sensor Deployment Considerations

DO sensors can be deployed in several ways. Stationary sensor deployments are on fixed platforms or moorings where there is minimal movement either horizontally or vertically. Mobile platforms are available in a variety of configurations and require different real-time DO QC considerations. Mobile platforms are, in order of increasing complexity: fixed vertical profilers, mobile surface vessels, and vessels freely operating in three dimensions (e.g., gliders, floats, powered autonomous underwater vehicles or AUVs). Figures 3-1 and 3-2 provide examples of mobile platforms.

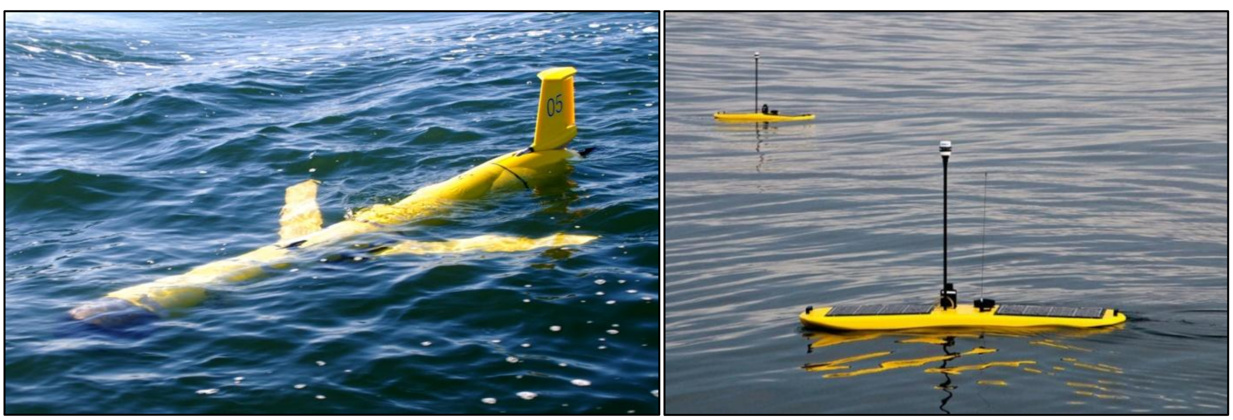


**Figure 3-1.** WebbGlider Profiler 3-D (L) (photo courtesy of Dr. Grace Saba) and Liquid Robotics Wave Glider Mobile Surface (R) (photo courtesy of Liquid Robotics).

**Figure 3-2.** WET Labs AMP C100 In-Situ Profiler (photo courtesy of WET Labs).

### 3.2.1 Fixed, In-Situ Vertical Profilers

Fixed vertical DO profiles can be obtained from a variety of systems, including rigid-mounted profiling systems, buoy/mooring climbers, surface or bottom tethered systems, or even routine repeated manual station occupations. In such cases, the tests described for a fixed sensor (see sections 3.3 and 3.4) either remain unchanged or are conducted along the vertical 'z' axis as well as along a time series of observations.

### 3.2.2 Mobile Surface Vessels

Examples of mobile surface vessels include manned vessels of opportunity and autonomously operated vehicles such as the Liquid Robotics Wave Glider fitted with DO sensors. Samples are obtained at a fixed depth along track. They may be sampled at fixed temporal or spatial intervals. Again, the tests described for a fixed sensor may remain unchanged, or they are conducted along the vessel track 's' or projections onto 'x' (longitude) and 'y' (latitude) coordinates as well as along a time series of observations.

### 3.2.3 3-D Profiler Vessels

Gliders, floats, and powered AUVs can provide DO observations in a wide variety of space/time configurations. They can be as simple as along track 's' observations, periodic vertical ascent profiles recorded following at-depth drifts (Argo profilers), or real-time processed down/up profiles (gliders). When applying increasingly complex real-time QC tests to increasingly complex deployments, challenges may arise. However, most of the eleven tests described in sections 3.3 and 3.4 can be applied with little modification.

## 3.3 Test Hierarchy

This section outlines the eleven real-time QC tests that are required and recommended for selected DO sensors. Tests are listed in order of increasing complexity, and generally, decreasing utility and are divided into three bins. The tests in group 1 are required for all DO data measurements collected for U.S. IOOS. Operators must consider each test in group 2 and group 3 to determine if it can be applied in their particular instance—

not all tests can be implemented in all situations. For example, under anoxic conditions, which are defined as a complete absence of DO, some of the eleven tests do not apply. Table 3-2 shows the test hierarchy.

**Table 3-2.** QC Tests in order of implementation

| | | |
|---|---|---|
| **Group 1** *Required* | Test 1<br>Test 2<br>Test 3<br>Test 4<br>Test 5 | Gap Test<br>Syntax Test<br>Location Test<br>Gross Range Test<br>Climatological Test |
| **Group 2** *Strongly Recommended* | Test 6<br>Test 7<br>Test 8 | Spike Test<br>Rate of Change Test<br>Flat Line Test |
| **Group 3** *Suggested* | Test 9<br>Test 10<br>Test 11 | Multi-Variate Test<br>Attenuated Signal Test<br>Neighbor Test |

Some effort will be needed to select the best thresholds, which are determined at the local level and may require trial and error/iteration before final selections are made. This manual does not provide overly generic guidance for selecting thresholds because doing so may not yield a good starting point at the local level. Although more tests imply a more robust QC effort, valid reasons may exist for not invoking a particular test in some instances. Where a test from group 2 or group 3 cannot be implemented, the operator should document the reason it does not apply. The number of tests conducted, together with the justification for not applying some tests, can be used for the development of operator certification levels.

## 3.4 QC Tests

A variety of tests can be performed on the data to indicate data quality. Testing the integrity of the data transmission itself using a Gap Test and Syntax Test is a first step. If the data transmission is not sound, further testing is irrelevant. Additional checks evaluate the DO core variable values themselves through various comparisons to the data stream and to the expected conditions in the given environment. The tests listed in the following section presume a time ordered series of observations and denote the most recent observation as $DO_n$, preceded by a value at $DO_{n-1}$, and so on backwards in time. The focus is primarily on the real-time QC of observation $DO_n$, $DO_{n-1}$, and $DO_{n-2}$. There are several instances when tests are closely related, e.g., the climatology test is similar to the gross range test, the multi-variate test can be similar to the rate of change test, etc. As such, there are opportunities for savvy coding, which are left to the coders.

### 3.4.1 Applications of QC Tests to Stationary DO Sensors

These eleven tests require operators to select a variety of thresholds. These thresholds should not be determined arbitrarily but can be based on historical knowledge or statistics derived from more recently acquired data. Operators must document the reasons and methods used to determine the thresholds. Examples are provided in the following test tables; however, operators are in the best position to determine the appropriate thresholds for their operations. Some tests rely on multiple data points most recently received to determine the quality of the current data point. When this series of data points reveals that the entire group fails, the current data point is flagged, but the previous flags are not changed. This action supports the view that historical flags are not altered. The first example is in Test 8, the Flat Line Test, where this scenario will become clearer.

### Test 1) Gap Test (Required)

| Check for arrival of data | | |
|---|---|---|
| Test determines that the most recent data point has been received within the expected time window (TIM_INC) and has the correct time stamp (TIM_STMP).<br>**Note:** For those systems that don't update at regular intervals, a large value for TIM_STMP can be assigned. The gap check is not a panacea for all timing errors. Data could arrive earlier than expected. This test does not address all clock drift/jump issues. | | |
| **Flags** | **Condition** | **Codable Instructions** |
| Fail=4 | Data have not arrived as expected | NOW – TIM_STMP > TIM_INC |
| Suspect=3 | N/A | |
| Pass=1 | Applies for test pass condition | |
| **Test Exception**: None | | |
| **Test specifications to be established locally by operator**<br>**Example:** TIM_INC= 1 hour | | |

### Test 2) Syntax Test (Required)

| | | |
|---|---|---|
| Received data record (full message) contains the proper structure without any indicators of flawed transmission such as parity errors. Possible tests are: a) the expected number of characters (NCHAR) for fixed length messages equals the number of characters received (REC_CHAR), or b) passes a standard parity bit check, CRC check, etc. Many such syntax tests exist, and the user should select the best criteria for one or more syntax tests.<br>**Note:** Capabilities for dealing with flawed messages vary among operators; some may have the ability to parse messages to extract data within the flawed message sentence before the flaw. Syntax check is performed only at the message level and not at the sub-message level. | | |
| **Flags** | **Condition** | **Codable Instructions** |
| Fail=4 | Data record cannot be parsed to provide a valid observation. | REC_CHAR ≠NCHAR |
| Suspect =3 | N/A | N/A |
| Pass=1 | Expected data record received; absence of parity errors | |
| **Test Exception**: None. | | |
| **Test specifications to be established locally by operator**<br>**Example:** NCHAR = 128 | | |

### Test 3) Location Test (Required)

| Check for reasonable geographic location. | | |
|---|---|---|
| Test checks that the reported present physical location (latitude/longitude) is within operator-determined limits. The location test(s) can vary from a simple invalid location to a more complex check for displacement (DISP) exceeding a distance limit RANGEMAX based upon a previous location and platform speed. Operators may also check for erroneous locations based upon other criteria, such as reported positions over land, as appropriate. | | |
| **Flags** | **Condition** | **Codable Instructions** |
| Fail=4 | Invalid location | If LAT > \| 90 \| or LONG >\| 180 \|, flag = 4 |
| Suspect=3 | Unlikely platform displacement | If DISP > RANGEMAX, flag = 3 |
| Pass=1 | Applies for test pass condition. | N/A |
| **Test Exception**: Test does not apply to fixed deployments when no location is transmitted. | | |
| **Test specifications to be established locally by the operator.**<br>**Example:** Displacement DISP calculated between sequential position reports, RANGEMAX = 20 km | | |

### Test 4) Gross Range Test (Required)

| Data point exceeds sensor or operator selected min/max | | |
|---|---|---|
| All sensors have a limited output range, and this can form the most rudimentary gross range check. No values less than a minimum value or greater than the maximum value the sensor can output (DO_SENSOR_MIN, DO_SENSOR_MAX) are acceptable. Additionally, the operator can select a smaller span (DO_USER_MIN, DO_USER_MAX) based upon local knowledge or a desire to draw attention to extreme values. | | |
| **Flags** | **Condition** | **Codable Instructions** |
| Fail=4 | Reported value is outside of sensor span. | $DO_n$ < DO_SENSOR_MIN, or<br>$DO_n$ > DO_SENSOR_MAX |
| Suspect=3 | Reported value is outside of user-selected span. | $DO_n$ < DO_USER_MIN, or<br>$DO_n$ > DO_USER_MAX |
| Pass=1 | Applies for test pass condition | |
| **Test Exception:** None. | | |
| **Test specifications to be established locally by operator**<br>**Examples:** DO_SENSOR_MAX = 99.9 mg/L (limited by the character output field, for example)<br>DO_USER_MAX = 16 mg/L<br>DO_USER_MIN = 0 mg/L | | |

### Test 5) Climatology Test (Required)

| Test that data point falls within seasonal expectations. | | |
|---|---|---|
| This test is a variation on the gross range check, where the gross range DO_Season_MAX and DO_Season_MIN are adjusted monthly, seasonally, or at some other operator-selected time period (TIM_TST). Expertise of the local user is required to determine reasonable seasonal averages. Longer time series permit more refined identification of appropriate thresholds. | | |
| **Flags** | **Condition** | **Codable Instructions** |
| Fail=4 | Because of the dynamic nature of DO, no red flag is identified for this test. | |
| Suspect=3 | Reported value is outside of user-identified climatology window. | $DO_n$ < DO_Season_MIN or<br>$DO_n$ > DO_Season_MAX |
| Pass=1 | Applies for test pass condition | |
| **Test Exception:** None. | | |
| **Test specifications to be established locally by operator:** A seasonal matrix of $DO_{max}$ and $DO_{min}$ values at all TIM_TST intervals<br>**Examples:** DO_SPRING_MIN = 1.0 mg/L DO_SPRING_MAX = 16.0 mg/L | | |

### Test 6) Spike Test (Strongly Recommended)

| Data point n-1 exceeds a selected threshold relative to adjacent data points | | |
|---|---|---|
| This check is for single value spikes, specifically the DO value at point n-1 ($DO_{n-1}$). Spikes consisting of more than one data point are notoriously difficult to capture, but their onset may be flagged by the rate of change test. The spike test consists of two user-selected thresholds, THRSHLD_LOW and THRSHLD_HIGH. Adjacent data points ($DO_{n-2}$ and $DO_n$) are averaged to form a spike reference (SPK_REF). The absolute value of the spike is tested to capture positive and negative going spikes. Large spikes are easier to identify as outliers and flag as failures. Smaller spikes may be real and are only flagged suspect. | | |
| **Flags** | **Condition** | **Codable Instructions** |
| Fail=4 | High spike threshold exceeded. | $\| DO_{n-1}$ - SPK_REF$\|$ > THRSHLD_HIGH |
| Suspect=3 | Low spike threshold exceeded. | $\| DO_{n-1}$ - SPK_REF$\|$ > THRSHLD_LOW<br>$\| DO_{n-1}$ - SPK_REF$\|$ < THRSHLD_HIGH |
| Pass=1 | Applies for test pass condition | |
| **Test Exception:** None. | | |
| **Test specifications to be established locally by operator**<br>**Examples:**THRSHLD_LOW = 4 mg/L, THRSHLD_HIGH = 8 mg/L | | |

### Test 7) Rate of Change Test (Strongly Recommended)

Excessive rise/fall test

This test inspects the time series for a time rate of change that exceeds a threshold value identified by the operator. DO values can change dramatically over short periods, hindering the value of this test. A balance must be found between a threshold set too low, which triggers too many false alarms, and one set too high, making the test ineffective. Determining the excessive rate of change is left to the local operator. The following are two different examples provided by QARTOD VI participants used to select the thresholds. Implementation of this test can be challenging. Upon failure, it is unknown which of the points is bad. Further, upon failing a data point, it remains to be determined how the next iteration can be handled.

- The rate of change between $DO_{n-1}$ and $DO_n$ must be less than three standard deviations (3*SD). The SD of the DO time series is computed over the previous 25-hour period (user-selected value) to accommodate cyclical diurnal and tidal fluctuations. Both the number of SDs (N_DEV) and the period over which the SDs (TIM_DEV) are calculated are determined by the local operator.
- The rate of change between $DO_{n-1}$ and $DO_n$ must be less than 1mg/L +2SD.

| Flags | Condition | Codable Instructions |
|---|---|---|
| Fail=4 | Because of the dynamic nature of DO, no red flag is identified for this test. | N/A |
| Suspect=3 | The rate of change exceeds the selected threshold. | $\lvert DO_n - DO_{n-1} \rvert > N\_DEV * SD$ |
| Pass=1 | Applies for test pass condition | |

**Test Exception:** Anoxic conditions introduce the possibility of repeated zero values, challenging the calculation of time-local thresholds. The rate of change check does not apply to zero-valued DO observations.

**Test specifications to be established locally by operator.**
**Example:** N_DEV = 3, TIM_DEV = 25

## Test 8) Flat Line Test (Strongly Recommended)

Invariate DO value

When some sensors and/or data collection platforms (DCPs) fail, the result can be a continuously repeated observation of the same value. This test compares the present observation ($DO_n$) to a number (REP_CNT_FAIL or REP_CNT_SUSPECT) of previous observations. $DO_n$ is flagged if it has the same value as previous observations within a tolerance value EPS to allow for numerical round-off error. Note that historical flags are not changed.

| Flags | Condition | Codable Instructions |
|---|---|---|
| Fail=4 | When the five most recent observations are equal, $DO_n$ is flagged fail. An exception is made for anoxic conditions. | $DO_n \neq 0$<br>AND<br>For i=1,REP_CNT_FAIL $DO_n - DO_{n-i}$ <EPS |
| Suspect=3 | It is possible but unlikely that the present observation and the two previous observations would be equal. When the three most recent observations are equal, $DO_n$ is flagged suspect. | For i=1,REP_CNT_SUSPECT $DO_n - DO_{n-i}$ <EPS |
| Pass=1 | Applies for test pass condition | |

**Test Exception**: Anoxic conditions or sensor failure introduce the possibility of repeated zero values. These are flagged suspect/high interest.

**Test specifications to be established locally by operator**
**Examples:** REP_CNT_FAIL = 5, REP_CNT_SUSPECT= 3

### Test 9) Multi-Variate Test (Suggested)

Comparison to other variables

This is an advanced family of tests, starting with the simpler test described here and anticipating growth towards full co-variance testing in the future. To our knowledge, no one is conducting tests such as these in real time. As these tests are developed and implemented, they should indeed be documented and standardized in later versions of this living DO manual.

In this simple example, it is a pair of rate of change tests as described in test 7. The DO rate of change test is conducted with a more restrictive threshold (N_DO_DEV). If this test fails, a second rate of change test operating on a second variable (temperature or conductivity would be the most probable) is conducted. The absolute valued rate of change should be tested since the relationship between DO and variable two is indeterminate. If the rate of change test on the second variable *fails* to exceed a threshold (e.g., an anomalous step is found in DO and is lacking in temperature), then the $DO_n$ value is flagged.

| Flags | Condition | Codable Instructions |
|---|---|---|
| Fail=4 | Because of the dynamic nature of DO, no red flag is identified for this test. | N/A |
| Suspect=3 | $DO_n$ fails the DO rate of change and the second variable does not exceed the rate of change. | $\|DO_n - DO_{n-1}\|$>N_DO_DEV*SD_DO<br>AND<br>$\|TEMP_n - TEMP_{n-1}\|$<N_TEMP_DEV*SD_T |
| Pass=1 | | |

**Test Exception:** Anoxic conditions introduce the possibility of repeated zero values, challenging the calculation of time-local thresholds. The multi-variate check does not apply to zero valued DO observations.

**Test specifications to be established locally by operator**
**Examples:** N_DO_DEV = 2, N_TEMP_DEV=2, TIM_DEV = 25 hours

**NOTE:** In a more complex case, more than one secondary rate of change test can be conducted. Temperature, salinity, turbidity, nutrients, and chlorophyll are all possible secondary candidates, and they all could be checked for anomalous rate of change values. In this case, a knowledgeable operator may elect to green flag a high rate of change DO observation when any one of the secondary variables also exhibits a high rate of change. Such tests border on modeling, should be carefully considered, and may be beyond the scope of this effort.

QARTOD VI participants recognized the high value in full co-variance testing but also noted the challenges. Such testing remains to be a research project not yet ready for operational implementation.

## Test 10) Attenuated Signal Test (Suggested)

A test for inadequate variation of the time series

A DO sensor failure can provide a data series that is nearly but not exactly a flat line (for example, if the sensor head was to become wrapped in debris). This test inspects for a standard deviation (SD) value or a range variation (MAX-MIN) value that fails to exceed threshold values (MIN_VAR_WARN, MIN_VAR_FAIL) over a selected time period (TST_TIM).

| Flags | Condition | Codable Instructions |
|---|---|---|
| Fail=4 | Variation fails to meet the minimum threshold MIN_VAR_FAIL | During TST_TIM, SD <MIN_VAR_FAIL, or During TST_TIM, MAX-MIN <MIN_VAR_FAIL |
| Suspect=3 | Variation fails to meet the minimum threshold MIN_VAR_WARN | During TST_TIM, SD <MIN_VAR_WARN, or During TST_TIM, MAX-MIN <MIN_VAR_WARN |
| Pass=1 | Applies for test pass condition | |

**Test Exception:** Anoxic conditions introduce the possibility of repeated zero values. The attenuated signal check does not apply to zero values.

**Test specifications to be established locally by operator**
**Examples:** TST_TIM = 12 hours
MIN_VAR = 0.1 mg/L, MIN_VAR_WARN=0.5 mg/L, MIN_VAR_FAIL=0.1 mg/L

### Test 11) Neighbor Test (Suggested)

Comparison to nearby DO sensors

The check has the potential to be the most useful test when a nearby second sensor is determined to have a similar response.

In a perfect world, redundant DO sensors utilizing different technology would be co-located and alternately serviced at different intervals. This close neighbor would provide the ultimate QC check, but cost prohibits such a deployment in most cases.

In the real world, there are very few instances where a second DO sensor is sufficiently proximate to provide a useful QC check. Just a few hundred meters in the horizontal and less than 10 meters vertical separation yield greatly different results. Nevertheless, the test should not be overlooked where it may have application.

This test is the same as *9) Multi-variate Check – comparison to other variables* where the second variable is the second DO sensor. The selected thresholds depend entirely upon the relationship between the two sensors as determined by the local knowledge of the operator.

In the instructions and examples below, data from one site (D01) are compared to a second site (D02). The standard deviation for each site (SD1, SD2) is calculated over the period (TIM_DEV) and multiplied as appropriate (N_DO1_DEV for site DO1) to calculate the rate of change threshold. Note that an operator could also choose to use the same threshold for each site since they are presumed to be similar.

| Flags | Condition | Codable Instructions |
|---|---|---|
| Fail=4 | Because of the dynamic nature of DO, no red flag is identified for this test. | N/A |
| Suspect=3 | $DO_n$ fails the DO rate of change and the second DO sensor does not exceed the rate of change. | $\vert DO1_n - DO1_{n-1}\vert >$ N_DO1_DEV*SD1<br>AND<br>$\vert DO2_n - DO2_{n-1}\vert <$ N_DO2_DEV*SD2 |
| Fail=1 | | |

**Test Exception:** Anoxic conditions introduce the possibility of repeated zero values, challenging the calculation of time-local thresholds. The neighbor check would only apply to co-located DO sensors in the presence of anoxic conditions.

**Test specifications to be established locally by operator**
**Examples:** N_DO1_DEV = 2, N_DO2_DEV=2, TIM_DEV = 25 hours

### 3.4.2 Applications of QC Tests to DO Sensor Deployments

The specific application of the QC tests can be dependent on the way the sensor is deployed. Table 3-3 provides a summary of each QC test described in section 3.4 and indicates any changes necessary for the test to be applied to different deployment scenarios. Note that the "s" axis indicates "along path" for mobile platforms.

**Table 3-3** Application of Required QC Tests for Sensor Deployments. **Note:** The 's' axis means "along path."

| Test | Condition | Platform | Codable Instructions |
|---|---|---|---|
| **1) Gap Test (Required)**<br>Test determines that the most recent data point has been received within the expected time window (TIM_INC) and has the correct time stamp (TIM_STMP). Note: For those systems that don't update at regular intervals, a large value for TIM_STMP can be assigned. The gap check is not a panacea for all timing errors. Data could arrive earlier than expected. This test does not address all clock drift/jump issues. | Check for arrival of data. | Stationary<br>Fixed Vertical<br>Mobile<br>3-D | No change |
| **2) Syntax Test (Required)**<br>Received data record contains the proper structure without any indicators of flawed transmission such as parity errors. Possible tests are: a) the expected number of characters (NCHAR) for fixed length messages equals the number of characters received (REC_CHAR), or b) passes a standard parity bit check, CRC check, etc. Many such syntax tests exist, and the user should select the best criteria for one or more syntax tests. | Expected data record received, absence of parity errors. | Stationary<br>Fixed Vertical<br>Mobile<br>3-D | No change |
| **3) Location Test (Required)**<br>Test checks that the reported present physical location (latitude/longitude) is within operator-determined limits. The location test(s) can vary from a simple invalid location to a more complex check for displacement (DISP) exceeding a distance limit RANGEMAX based upon a previous location and platform speed. Operators may also check for erroneous locations based upon other criteria, such as reported positions over land, as appropriate. | Check for reasonable geographic location. | Stationary<br>Fixed Vertical<br>Mobile<br>3-D | No change |
| **4) Gross Range Test (Required)**<br>All sensors have a limited output range, and this can form the most rudimentary gross range check. No values less than a minimum value or greater than the maximum value the sensor can output (DO_SENSOR_MIN, DO_SENSOR_MAX) are acceptable. Additionally, the operator can select a smaller span (DO_USER_MIN, DO_USER_MAX) based upon local knowledge or a desire to draw attention to extreme values. | Data point exceeds sensor or operator selected min/max. | Stationary<br>Fixed Vertical<br>Mobile<br>3-D | No change |
| **5) Climatology Test (Required)**<br>This test is a variation on the gross range check, where the gross range DO_Season_MAX and DO_Season_MIN are adjusted monthly, seasonally, or at some other operator-selected time period (TIM_TST). Expertise of the local user is required to determine reasonable seasonal averages. Longer time series permit more refined identification of appropriate thresholds. | Test that data point falls within seasonal expectations. | Stationary | No change |
| | | Fixed Vertical | Test conducted along z axis |
| | | Mobile | Test conducted along s, x, or y axis |
| | | 3-D | Test conducted along s, x, y, or z axis |

**Table 3-4.** Application of Strongly Recommended QC Tests for Sensor Deployments

| Test | Condition | Platform | Codable Instructions |
|---|---|---|---|
| **6) Spike Test (Strongly Recommended)**<br>This check is for single value spikes, specifically the DO value at point n-1 ($DO_{n-1}$). Spikes consisting of more than one data point are notoriously difficult to capture, but their onset may be flagged by the rate of change test. The spike test consists of two user-selected thresholds above or below adjacent data points, THRSHLD_LOW and THRSHLD_HIGH. Adjacent data points ($DO_{n-2}$ and $DO_n$) are averaged to form a spike reference (SPK_REF). The absolute value of the spike is tested to capture positive and negative going spikes. Large spikes are easier to identify as outliers and flag as failures. Smaller spikes may be real and are only flagged suspect. | Data point n-1 exceeds a selected threshold relative to adjacent data points. | Stationary | No change |
| | | Fixed Vertical | Test is conducted along z axis |
| | | Mobile | No change, or test is conducted along s, x, or y axis |
| | | 3-D | No change, or test is conducted along s, x, y, or z axis |
| **7) Rate of Change Test (Strongly Recommended)**<br>This test inspects the time series for time rate of change in that exceed a threshold value identified by the operator. DO values can change dramatically over short periods, hindering the value of this test. A balance must be found between a threshold set too low, which triggers too many false alarms, and one set too high, making the test ineffective. Determining the excessive rate of change is left to the local operator. The following are two different examples provided by QARTOD VI participants used to select the thresholds. Implementation of this test can be challenging. Upon failure, it is unknown which of the points is bad. Further, upon failing a data point, it remains to be determined how the next iteration can be handled. | Excessive rise/fall test. | Stationary | No change |
| | | Fixed Vertical | Test is conducted along z axis |
| | | Mobile | No change, or test is conducted along s, x, or y axis |
| | | 3-D | No change, or test is conducted along s, x, y, or z axis |
| **8) Flat Line Test (Strongly Recommended)**<br>When some sensors and/or data collection platforms (DCPs) fail, the result can be a continuously repeated observation of exactly the same value. This test compares the present observation ($DO_n$) to a number (REP_CNT_FAIL or REP_CNT_SUSPECT) of previous observations. $DO_n$ is flagged if it has the same value as previous observations within a tolerance value EPS to allow for numerical round-off error. Note that historical flags are not changed. | Invariate DO value. | Stationary | No change |
| | | Vertical | Test is conducted along z axis |
| | | Mobile | No change, or test is conducted along s, x, or y axis |
| | | 3-D | No change, or test is conducted along s, x, y, or z axis |

**Table 3-5.** Application Suggested QC Tests for Sensor Deployments

| Test | Condition | Platform | Codable Instructions |
|---|---|---|---|
| **9) Multi-Variate Test (Suggested)**<br>This is an advanced family of tests, starting with the simpler test described here and anticipating growth towards full co-variance testing in the future.<br>In the simplest case, it is a pair of rate of change tests as described in test 7. The DO rate of change test is conducted with a more restrictive threshold (N_DO_DEV). If this test fails, a second rate of change test operating on a second variable (temperature or conductivity would be the most probable) is conducted. The absolute valued rate of change should be tested since the relationship between DO and variable two is indeterminate. If the rate of change test on the second variable *fails* to exceed a threshold (e.g., an anomalous step is found in DO and is lacking in temperature), then the DO value $n_0$ is flagged. | Comparison to other variables. | Stationary | No change |
| | | Fixed Vertical | Test is conducted along z axis |
| | | Mobile | Test is conducted along s, x, or y axis |
| | | 3-D | Test is conducted along s, x, y, or z axis |
| **10) Attenuated Signal Test (Suggested)**<br>A DO sensor failure can provide a data series that is nearly but not exactly a flat line (for example, if the sensor head was to become wrapped in debris). This test inspects for a standard deviation (SD) value or a range variation (MAX-MIN) value that fails to exceed a threshold value (MIN_VAR) over a selected time period (TST_TIM). | Inadequate variation test. | Stationary | No change |
| | | Fixed Vertical | Test is conducted along z axis |
| | | Mobile | No change, or test is conducted along s, x, or y axis |
| | | 3-D | No change, or test is conducted along s, x, y, or z axis |
| **11) Neighbor Test (Suggested)**<br>The check has the potential to be the most useful test when a nearby second sensor is determined to have a similar response.<br>This test is the same as test *9) Multi-variate Check – comparison to other variables* where the second variable is the second DO sensor. The selected thresholds depend entirely upon the relationship between the two sensors as determined by the local knowledge of the operator. | Comparison to nearby DO sensors. | Stationary | No change |
| | | Fixed Vertical | Test is conducted along z axis |
| | | Mobile | No change |
| | | 3-D | No change |

## 4.0 Conclusion

This DO manual was developed and updated to create a framework for QC tests of DO and serves as a template for the other 25 IOOS core variables. The proposed minimum set of tests for certification (compliance) and suggested hierarchy of those tests is included, and suggestions for QA best practices have been added in appendix A.

This QC DO manual is meant to advise the RA data providers, without being overly prescriptive, by providing meaningful guidance and thresholds that everyone can accomplish within a National framework. Certain tests have been recommended, but thresholds can vary among and within each RA. The goal is to improve QC through agreed-upon, documented, implementable, and codable standard processes and procedures

The QC tests have been described in detail sufficient for generation of software that can be implemented for real-time collection and processing of DO. The problem of real-time QC of DO has been constrained to specific sensor types in coastal areas.

The RAs and the ocean observing community at large should adopt and deploy these DO QC procedures developed by the U.S. IOOS QARTOD Project. The QC tests (and QA best practices in appendix A) have been developed or evolved from practices in the ocean observing community and in operational centers such as NDBC. Thus, the same practices are recommended for the observing systems of both the non-federal and federal backbone. Quality flags and metadata will be transmitted without loss of data through the U.S. IOOS DMAC subsystem for use by various end users.

Training and education are of paramount importance to ensuring that both QA and QC practices are in place. The sensor manufacturers can play a huge role in this area. The manufacturers have spent enormous efforts helping customers use these sensors successfully. Most manufacturers provide instructions for best practices, and those practices should be used as a first-order QA for all measurements. The manufacturer-supplied user's manual includes these instructions, and following them carefully is critical to knowing how to use the instruments, understanding their limitations and accuracy, knowing how to interpret output, and then having a meaningful way to validate performance. Validation of sensor performance can be done by taking periodic water samples, using a known calibrated and maintained reference instrument, or performing laboratory tests to a given accuracy.

**Knowledgeable human involvement** is required to properly understand the physical, chemical, and biological conditions within which the DO observations are being taken.

Future QARTOD reports will address standard QC procedures and best practices for all types of common as well as uncommon platforms and sensors for all the U.S. IOOS core variables. Some procedures may take place within the sensor package. Significant components of metadata will reside in the instrument and be transmitted either on demand or automatically along with the data stream. Users may also reference metadata through Uniform Resource Locators (URLs) to make it easy to identify which QC steps have been applied to data.

Each QC manual is a dynamic document and is posted on the QARTOD website (www.ioos.noaa.gov/qartod/) upon completion. This practice allows for updating each U.S. IOOS core variable QC manual as technology development occurs, accommodating not only new sensors, but also the upgrades envisioned for the current sensors.

This website permits easy access to all QARTOD material and updates as they are identified. It includes code libraries, procedures for testing data, and links to social media—enabling the growing ocean observing community to stay engaged across the enterprise regionally, nationally, and internationally.

This QARTOD project may be one of the best working examples of private-public partnerships, which is a fundamental tenet of U.S. IOOS. As this DO manual has exemplified, the sensor manufacturers must be fully involved in the creation of most, if not all, QC manuals for the 26 U.S. IOOS core variables.

It is through this kind of uniform QC process that integration can occur across the national ocean enterprise, capitalizing the *I* in U.S. IOOS. Implementing these procedures will accelerate the research-to-operations process to support a real-time, operational, integrated ocean observing system of defined data quality.

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CALCOFI: Seabird dual SBE43 **oxygen** sensors (O2); rated to 7000m used with Seabird CTD in conjunction with temperature and salinity sensors to calculate all pertinent data. http://calcofi.org/references/ccmethods/283-art-ctdatsea.html

Specifics about discrete sample oxygen methods can be viewed at:
http://calcofi.org/references/ccmethods/294-dissolved-oxygen.html
http://calcofi.org/references/clhandbook/80-o2samples.html

Scheme on QC flags, which is a general document that discusses how to write the results of tests, but does not discuss the actual tests.
http://www.oceandatastandards.org/

The ocean data standards resource pool can be found at:
http://www.oceandatastandards.org/index.php?option=com_content&task=view&id=22&Itemid=28

http://www.oceandatastandards.org/index.php?option=com_content&task=view&id=5&Itemid=7 is the higher level page (see menu to the right for subpages). There is a subpage for T and S profiles that contains a lot of good information including names and reference documents. Some of the references under T and S also apply to DO.

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## Supporting Documents Found on the QARTOD Website:

www.ioos.noaa.gov/qartod/

Quality Control of Profiling Float Oxygen Data

Report from the COL-NASA Data QA/QC Workshop

U.S. IOOS Development Plan

NDBC Handbook of Automated Data Quality Control

YSI Environmental Dissolved Oxygen Values above 100% Air Saturation

WHP Operations and Methods – July 1991 Dissolved Oxygen

Argo Quality Control Manual, V 2.7 3 January 2012

Data Quality Control in the U.S. IOOS

Ocean Deoxygenation in a Warming World

Spatial and Temporal Monitoring of Dissolved Oxygen (DO) in New Jersey Coastal Waters using AUVs – Data Quality Assurance Project Plan

In-situ Calibration of Optode-Based Oxygen Sensors

National Water Quality Monitoring Council Water Quality Data Elements: A User Guide)

Requirements for Global Implementation of the Strategic Plan for Coastal GOOS - Panel for Integrated Coastal Observation (PICO-I)

Integrating Standards in Data QA/QC into OpenGeospatial Consortium Sensor Observation Services

UHM Stormwater Monitoring System Servicing Checklist

One Man's Advice on the Determination of Dissolved Oxygen in Seawater

# Appendix A Quality Assurance

A major pre-requisite for establishing data quality for dissolved oxygen observations is having strong QA practices that address all actions related to the sensor during pre-deployment, deployment, and post-deployment. The consensus that emerged from past QARTOD meetings was that good quality data requires good QA, and good QA requires good scientists, engineers, and technicians applying consistent practices. Generally, QA practices relate to observing systems' sensors (the hardware) and include things like appropriate sensor selection, calibration, sensor handling and service, and evaluation of sensor performance.

## A.1 Sensor Calibration Considerations

Observations must be traceable to one or more accepted standards through a calibration performed by the manufacturer and/or the operator (e.g., Carpenter 1965). If the calibration is conducted by the manufacturer, the operator must also conduct some form of an acceptable calibration check, which for DO is the traditional air-saturated water check.

An often overlooked calibration or calibration check can be performed by choosing a consensus standard. For example, deriving the same answer (within acceptable levels of data precision or data uncertainty) from four different sensors of four different manufacturers, preferably utilizing several different technologies, constitutes an acceptable check. Because of the trend toward corporate conglomeration, those wishing to employ a consensus standard should ensure that the different manufacturers are truly independent.

## A.2 Sensor Comparison

An effective QA effort continually strives to ensure that end data products are of high value and to prove they are free of error. Operators should seek out partnering opportunities to inter-compare systems by co-locating differing sensors, thereby demonstrating high quality by both to the extent that there is agreement and providing a robust measure of observation data uncertainty by the level of disagreement. If possible, operators should retain an alternate sensor or technology from a second manufacturer for similar in-house checks. For resource-constrained operators, however, it may not be possible to spend the time and funds needed to procure and maintain two systems. For those who do so and get two different results, the use of alternate sensors or technologies provide several important messages: a) a measure of corporate capabilities; b) a reason to investigate, understand the different results, and take corrective action; and c) increased understanding that, when variables are measured with different technologies, different answers can be correct; they must be understood in order to properly report results. For those who succeed in obtaining similar results, the additional sensors provide a highly robust demonstration of capability. Such efforts form the basis of a strong QA/QC effort. Further, sensor comparison provides the operator with an expanded supply source, permitting less reliance upon a single manufacturer and providing competition that is often required by procurement offices.

## A.3 Bio-fouling and Corrosion Prevention Strategies

Bio-fouling is the most frequent cause of DO sensor failure, so the following strategies may be useful for ameliorating the problem:

- Use anti-fouling paint with the highest copper content available (up to 75%) when possible (but not on aluminum).
- Tributyltin oxide (TBTO) anti-foulant systems, often used in conjunction with a pumped system, are highly effective (e.g., Sea-Bird SBE 43)
- To help with post-deployment clean-up (but not as an anti-foulant), wrap the body of the sensor with clear packing tape for a small probe or plastic wrap for a large instrument, followed by PVC pipe wrap tape. (This keeps the PVC tape from leaving a residue on the sensor.) Wrap the sensor body with copper tape (again, beware of aluminum).
- Coat with zinc oxide (Desitin ointment).
- Use brass door/window screen around opening to sensor. The combination of copper and zinc is a great anti-foulant and is significantly cheaper than copper screen.
- Remember that growth is sensor, depth, location, and season dependent.
- Maintain wipers on optical sensors per manufacturers' recommendation.
- Flush out with chlorine gas pumped through the system. This technique requires a lot of battery power.
- Plan for routine changing or cleaning of sensor as necessary.
- Check with calibration facility on which anti-foulants will be handled (allowed) by the calibrators.
- Use copper plates as shutters, which keep the sensor open for limited time. This is ideal over wipers in oceanic environments with encrusting organisms like barnacles. Wipers do not work well in southern Florida during the summer. Sediment and particles that become embedded in the wipers can scratch the surface of the membrane on optical DO sensors.
- Store the sensor in the dark when not in use.
- Avoid or isolate dissimilar metals.
- Maintain sacrificial anodes and ensure they are properly installed (good electrical contact).
- Maximize the use of non-metallic components.
- Use UV-stabilized components that are not subject to sunlight degradation.
- Mount sensors vertically to minimize sediment buildup – employ filters for sensors with flow-through tubes.
- Where applicable, maintain sensor surfaces by gentle cleaning (e.g., using a baby toothbrush).
- Store the device above the surface between measurements.
- Make use of a pumped system where the sensor is kept above water and the sample is pumped through a flow chamber just before a reading is required.
- Use petroleum-based lubricants as biocides.

## A.4 Common QA Considerations

The following lists suggest ways to ensure QA by using specific procedures and techniques:

- Perform pre-deployment calibrations on every sensor.
- Perform post-deployment calibrations on every sensor, plus in-situ comparison before recovery.
- Calibrate ready-to-use spares periodically.
- Monitor with redundant sensors whenever possible.
- Collect in-situ water samples to compare with the sensor.
- Take photos of sensor fouling for records.
- Record all actions related to sensors – calibration, cleaning, deployment, etc.
- Compare the first day or less of readings from newly deployed sensor to last sensor deployed. Large shifts in median values can indicate a problem with one of the sensors. A post calibration of a previously deployed sensor may help to determine if it is the source of the discontinuity in readings.
- Monitor battery voltage and watch for unexpected fluctuations.

**When evaluating which instrument to use, consider these factors:**

- Selection of a reliable and supportive manufacturer and appropriate model
- Measurable data concentration range (including detection limit)
  - Lowest and highest possible readings
- Operating range (i.e., some instruments won't operate at certain temperatures)
  - Could be depth or pressure range
  - Salinity correction
- Resolution/precision required
- Sampling frequency – how fast the sensor can take measurements
- Reporting frequency – how often the sensor reports the data
- Response time of the sensor – sensor lag – time response
- Power source limitations
- Clock stability and timing issues
- Internal fault detection and error reporting capabilities

**When evaluating which specifications must be met:**

- State the expected accuracy.
- Determine how the sensor compared to the design specifications.
- Determine if sensor met those specifications.
- Determine whether the result is good enough (fit for purpose: data are adequate for nominal use as preliminary data).

**General comments regarding QA procedures:**

- A diagram (http://www.ldeo.columbia.edu/~dale/dataflow/), contributed by Dale Chayes (LDEO) provides a visual representation of proper QA procedures.
- Require serial numbers and model ID from the supplier.
- Develop useful checklists and update them as needed.
- Do not assume the calibration is perfect (could be a calibration problem rather than a sensor problem).
- Keep good records of all related sensor calibrations and checks (e.g., DO, conductivity, temperature).
- Use NIST-traceable standards when conducting calibrations or calibration checks.

- Keep good maintenance records. Favor sensors that maintain an internal file of past calibration constants, which is very useful since it can be downloaded instead of transcribed manually, thus introducing human error.
- Plot calibration constants or deviations from a standard over time to determine if the sensor has a drift in one direction or another. A sudden change can indicate a problem with the sensor or the last calibration.
- Don't presume that anomalous values are always problems with a sensor. Compare measurements with other sensors to help determine if the reading is real; then examine the possibility of problems with a sensor.
- Follow the manufacturer's recommendations and best practices established by knowledgeable users to ensure proper sampling techniques. For example, in a non-pumped sensor in a turbulent environment, bubbles can adhere to the surface of a sensor resulting in anomalous readings. Cycle the wipers or shutter before the reading to brush off the bubbles from the face of the instrument. For a pumped system in a turbulent environment, a degassing "Y" may limit bubbles adhering to the face of the sensor.

## A.5 QA Levels for Best Practices

A wide variety of techniques are used by operators to assure that DO sensors are properly calibrated and operating within specifications. While all operators must conduct some form of validation, there is no need to force operators to adhere to one single method. A balance exists between available resources, level of proficiency of the operator, and accuracy. The various techniques span a range of validation levels and form a natural hierarchy that can be used to establish levels of certification for operators (table A-1). The lists in the following sections suggest ways to ensure QA by using specific procedures and techniques.

Table A-1. Best practices indicator for QA

| QA Best Practices Indicator | Description |
|---|---|
| **Good Process** | DO sensors are swapped and/or serviced at sufficiently regular intervals so as to avoid data steps (unexpected offsets) upon swap/service. Sensors are pre- and post-deployment calibration checked by water saturation tests. |
| **Better Process** | The good processes are employed, plus pre- and post-deployment calibration checks are conducted using either titrations or alternative sensors to confirm performance. |
| **Best Process** | The better processes are employed, plus high-quality Winkler titrations are conducted following a well-documented protocol, or alternative sensors are used to validate in-situ deployments. Or, pre- and post-calibrations are conducted by the manufacturer. |

## A.6 Additional Sources of QA Information

Operators using DO sensors also have access to other sources of QA practices and information about a variety of instruments. For example, the Alliance for Coastal Technologies (ACT) serves as an unbiased, third party testbed for evaluating sensors and platforms for use in coastal and ocean environments. ACT conducts instrument performance demonstrations and verifications so that effective existing technologies can be recognized and promising new technologies can become available to support coastal science, resource management, and ocean observing systems (ACT 2012). The NOAA Ocean Systems Test and Evaluation Program (OSTEP) also conducts independent tests and evaluations on emerging technology as well as new sensor models. Both ACT and OSTEP publish findings that can provide information about QA, calibration, and other aspects of sensor functionality. The following list provides links to additional resources on QA practices.

- Manufacturer specifications and supporting Web pages/documents
- QARTOD - http://nautilus.baruch.sc.edu/twiki/bin/view/Main/WebHome
- ACT - http://www.act-us.info/
- CO-OPS - http://tidesandcurrents.noaa.gov/pub.html under the heading Manuals and Standards
- USGS - http://water.usgs.gov/owq/quality.html
- USGS - http://pubs.usgs.gov/tm/2006/tm1D3/
- USGS http://or.water.usgs.gov/pubs/WRIR01-4273/wri014273.pdf
- WOCE http://woce.nodc.noaa.gov/wdiu/
- NDBC http://www.ndbc.noaa.gov/
- NWQMC http://acwi.gov/monitoring/

## A.7 Sample Checklists

The following samples provide hints for development of deployment checklists taken from QARTOD IV:

### General QA Checklist:

- ❒ Read the manual.
- ❒ Establish, use, and submit (with a reference and version #) a documented sensor preparation procedure (protocol). Should include cleaning sensor according to the manufacturer's procedures.
- ❒ Calibrate sensor against an accepted standard and document (with a reference and version #).
- ❒ Compare the sensor with an identical, calibrated sensor measuring the same thing in the same area (in a calibration lab).
- ❒ View calibration specifications with a critical eye (don't presume the calibration is infallible). Execute detailed review of calibrated data.
- ❒ Check the sensor history for past calibrations, including a plot over time of deviations from the standard for <u>each</u> (this will help identify trends such a progressively poorer performance). Check the sensor history for past repairs, maintenance, and calibration.
- ❒ Consider storing and shipping information before deploying.
    - Heat, cold, vibration, etc.
- ❒ Record operator/user experiences with this sensor.
- ❒ Search the literature for information on your particular sensor(s) to see what experiences other researchers may have had with the sensor(s).

- ❒ Establish and use a formal pre-deployment checklist.
- ❒ Ensure that technicians are well-trained. Use a tracking system to identify those technicians who are highly trained and then pair them with inexperienced technicians for training purposes..

## Deployment Checklist

- ❒ Scrape bio-fouling off platform.
- ❒ Verify sensor serial numbers.
- ❒ Perform visual inspection; take photos if possible (verify position of sensors, connectors, fouling, and cable problems).
- ❒ Verify instrument function at deployment site just prior to site departure. Monitor sensors for issues (freezing, fouling).
- ❒ Use established processes to confirm that the sensor is properly functioning, before departing the deployment site.
- ❒ Specify date/time for all recorded events. Use GMT or UTC.
- ❒ Check software to ensure that the sensor configuration and calibration coefficients are correct. Also check sampling rates and other timed events, like wiping and time averaging.
- ❒ Visually inspect data stream to ensure reasonable values.
- ❒ Compare up and down casts and/or dual sensors (if available).
- ❒ Note weather conditions and members of field crew.

## Post-deployment Checklist

- ❒ Take pictures of recovered sensor prior to cleaning.
- ❒ Check to make sure all clocks agree or, if they do not agree, record all times and compare with NIST.
- ❒ Post-calibrate sensor before and after cleaning, if possible. Perform in-situ side by side check using another sensor, if possible
- ❒ Use standard procedures to provide feedback about possible data problems and/or sensor diagnostics.
- ❒ Clean and store the sensor properly or redeploy.
- ❒ Visually inspect physical state of instrument.
- ❒ Verify sensor performance by:
    - o Checking nearby stations;
    - o Making historical data comparisons (e.g., long-term time-series plots, which are particularly useful for identifying long-term bio-fouling or calibration drift.)

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