QUALITY ASSURANCE OF REAL-TIME OCEANOGRAPHIC DATA

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



December 2012

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INTEGRATED OCEAN OBSERVING SYSTEM

The procedures recommended in this manual, 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, are hereby approved for broad use and adoption.

Zdenka S. Willis, Director, U.S. IOOS Program

Date

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

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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		
DAC	Data Assembly Center		
DCP	Data Collection Platform		
DMAC	Data Management and Communications		
DO	Dissolved Oxygen		
EPA	Environmental Protection Agency		
FWC	Florida Wildlife Conservation Commission		
FWRI	Fish and Wildlife Research Institute		
GCOOS	Gulf of Mexico Coastal Ocean Observing System		
GLOS	Great Lakes Observing System		
GOOS	Global Ocean Observing System		
GPS	Global Positioning System		
IMOS	Integrated Marine Observing System		
IOOS	Integrated Ocean Observing System		
MARACOOS	Mid-Atlantic Regional Association Coastal Ocean Observing System		
MBARI	Monterey Bay Aquarium Research Institute		
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	
PaclOOS	Pacific Islands Ocean Observing System	
QARTOD	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	
URL	Uniform Resource Locator	
USGS	United States Geological Survey	
VIMS	Virginia Institute of Marine Science	
WOCE	World Ocean Circulation Experiment	

Preface

On March 30, 2009, President Barack Obama signed the Integrated Coastal and Ocean Observation System (ICOOS) Act of 2009 (Act) 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 10 QC tests; some are required, others are strongly recommended or suggested. Each test contains the codeable instructions for implementation and assumes the involvement of highly knowledgeable scientists, engineers, programmers, and technicians. Suggestions for QA best practices are provided in the appendix 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).

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, insitu currents, CTD (conductivity, temperature and depth), and water quality (biogeophysical 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 realtime quality test.
- 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 realtime 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 Dissolved Oxygen (DO) observations.

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 CO2 Pathogens Phytoplankton Species Salinity Sea Level Stream Flow Surface Currents Surface Waves Temperature Total Suspended Matter Wind Speed and Direction Zooplankton Abundance Zooplankton Species

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 (<u>www.ioos.gov/QARTOD/</u>). 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).

For each variable, a manual will be published describing the individual QC tests to be applied to the data stream prior to data dissemination. The manual will also specify the *set* of QC tests to be applied before data dissemination. For DO data, the manual describes 10 tests that are divided into three bins that are either required (bin 1), strongly recommended (bin 2), or suggested (bin 3) for application prior to dissemination of data entered into the IOOS Data Assembly Centers (DACs). 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 Nth data point might be that the N+1st 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 (<u>www.ioos.gov/QARTOD/</u>) so that they are easily accessible, citable, and dynamic, thus allowing for updates with the appropriate version control procedures in place. The website enables conversations between users and includes items such as code libraries, procedures for testing data, and interactive graphic.

2.0 Purpose/Constraints/Applications

This manual documents suggested standard test procedures for data QC from automated, in-situ dissolved oxygen (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 coasts¹ 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 *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* is a deliverable to the U.S. IOOS RAs and may be useful to the ocean observing community at large. It represents the beginning of a series of QC manuals for U.S. IOOS core variables that will 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. The manual presents a battery of 10 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 for the data were developed by operators with experience using the following sensors:

- Aanderaa Oxygen Optodes
- YSI Reliable Oxygen Sensor (ROX)
- Sea-Bird SBE 43 (Electrochemical)

The practices may also apply to the following sensors, which are believed to behave similarly to the instruments above. However, the operator makes the final determination of the applicability to the specific sensor:

- Hach HydroLab LDO
- Greenspan Galvanic DO 300/350 series
- ALEC Rinko Optical Fast Dissolved Oxygen

¹The coast means coasts of the U.S. Exclusive Economic Zone (EEZ) and territorial sea (<u>http://chartermaker.ncd.noaa.gov/csdl/eez/htm</u>), Great Lakes, and semi-enclosed bodies of water and tidal wetlands connected to the coastal ocean (U.S. IOOS 2006).

- RBR Global Optical Oxygard
- Eureka Manta 2 Dissolved Oxygen
- YSI Clark Membrane
- Sea-Bird 63 Optical Oxygen

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.

2.2 The Effect of Dynamic Environments on Sensor Data

In addition to DO being a non-conservative² variable, dynamic coastal regions impose a significant challenge through 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.

²A non-conservative variable means that it can be generated or depleted in-situ by both physical and biogeochemical processes, in contrast to conservative variables where concentrations only change through physical processes (e.g., salinity, see <u>http://www.braininajamjar.co.uk/s3302.html</u> Chapter 4).

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.

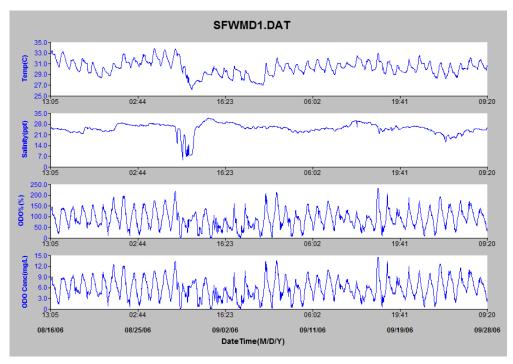


Figure 2-1. Panels 1-4 show temperature, salinity, DO percent, and DO concentration, respectively. The series tracks the passage of a hurricane and the effect it has on the time series before, during, and after the storm front passes (courtesy of Mike Lizotte, YSI).

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-

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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.

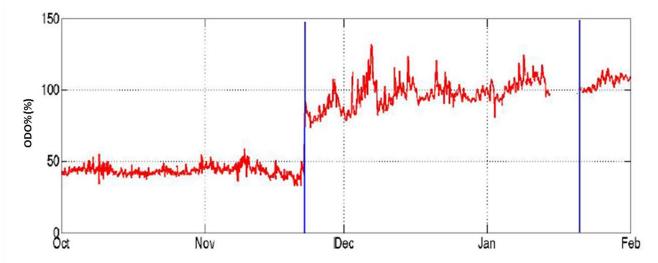


Figure 2-2. Note the abrupt shift in late November 2011 when the badly fouled sensor was replaced. The blue lines indicate the time of sensor replacement. Sensor replacement immediately shows higher saturation percentage. Note also apparent lack of a shift in January 2012 (courtesy of Doug Wilson, NOAA/CBIBS).

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.

Flag	Description
Fail=3	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.
Suspect or Of High Interest=2	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.
Pass=1	Data have passed critical real-time quality control tests and are deemed adequate for use as preliminary data.

 Table 3-1 Flags for real-time data

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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 AUVs). Figures 3-1 and 3-2 provide examples of mobile platforms.



Figure 3-1. WebbGlider Profiler 3-D (L) and Waveglider Mobile Surface (R)



Figure 3-2. WET Labs AMP C100 In-Situ Profiler

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 Wavegliders 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 10 tests described in sections 3.3 and 3.4 can be applied with little modification.

3.3 Test Hierarchy

This section outlines the 10 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 bin 1 are required for all DO data measurements collected for U.S. IOOS. Operators must consider each test in bin 2 and bin 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, 4 of the 10 tests do not apply. Table 3-2 shows the test hierarchy.

Bin 1	Test 1)	Gap Test
Required	Test 2)	Syntax Test
	Test 3)	Gross Range Test
	Test 4)	Climatological Test
Bin 2	Test 5)	Spike Test
Strongly	Test 6)	Rate of Change Test
Recommended	Test 7)	Flat Line Test
Bin 3	Test 8)	Multi-Variate Test
Suggested	Test 9)	Attenuated Signal Test
	Test 10)	Neighbor Test

Table 3-2. QC Tests in order of implementation

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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 bin 2 or bin 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 10 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 7, 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).

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	Codeable Instructions
Fail=3	Data have not arrived as expected	NOW – TIM_STMP > TIM_INC
Suspect=2	N/A	
Pass=1	Applies for test pass condition	
Test Exception: None		

Test specifications to be established locally by operator Example: TIM_INC= 1 hour

Test 2) Syntax Test (Required)

Received data message (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.

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	Codeable Instructions	
Fail=3	Data sentence cannot be parsed to provide a valid observation.	REC_CHAR ≠NCHAR	
Suspect =2	N/A	N/A	
Pass=1	Expected data sentence received; absence of parity errors		
Test Exception: None.			
Test specifications to be established locally by operator			
Example:	Example: NCHAR = 128		

Test 3) 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	Codeable Instructions	
Fail=3	Reported value is outside of sensor span.	DO _n < DO_SENSOR_MIN, or DO _n > DO_SENSOR_MAX	
Suspect=2	Reported value is outside of user- selected span.	DO _n < DO_USER_MIN, or DO _n > DO_USER_MAX	
Pass=1	Applies for test pass condition		
Test Exception: None.			
Test specifications to be established locally by operator			
Examples:	DO_SENSOR_MAX = 99.9 mg/L (limited by the character output field, for example)		
	DO_USER_MAX = 16 mg/L		
	DO_USER_MIN = 0 mg.L		

Test 4) 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 Codeable Instructions			
Fail=3	Because of the dynamic nature of DO, no red flag is identified for this test.			
Suspect=2	Reported value is outside of user- identified climatology window.	DO _n < DO_Season_MIN or 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 Examples: DO SPRING MIN = 1.0 mg/L DO SPRING MAX = 16.0 mg/L				

Test 5) 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	Codeable Instructions
Fail=3	High spike threshold exceeded.	DO _{n-1} - SPK_REF > THRSHLD_HIGH
Suspect=2	Low spike threshold exceeded.	DO _{n-1} - SPK_REF > THRSHLD_LOW 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 Examples:THRSHLD_LOW = 4 mg/L, THRSHLD_HIGH = 8 mg/L

Test 6) 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	Codeable Instructions	
Fail=3	Because of the dynamic nature of DO, no red flag is identified for this test.	N/A	
Suspect=2	The rate of change exceeds the selected threshold.	$ DO_n - DO_{n-1} > 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	1_DEV = 3, TIM_DEV = 25		

Test 7) 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	Codeable Instructions	
Fail=3	When the five most recent observations are equal, DO _n is flagged fail. An exception is made for anoxic conditions.	DO _n ≠ 0 AND For i=1,REP_CNT_FAIL DO _n -DO _{n·i} <eps< td=""></eps<>	
Suspect=2	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< td=""></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 8) 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	Codeable Instructions			
Fail=3	Because of the dynamic nature of DO, no red flag is identified for this test.	N/A			
Suspect=2	<i>DO_n</i> 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 AND TEMP _n - TEMP _{n-1} <n_temp_dev*sd_t< td=""></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 9) 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	Codeable Instructions
Fail=3	Variation fails to meet the minimum threshold MIN_VAR_FAIL	During TST_TIM, SD <min_var_fail, or<br="">During TST_TIM, MAX-MIN <min_var_fail< td=""></min_var_fail<></min_var_fail,>
Suspect=2	Variation fails to meet the minimum threshold MIN_VAR_WARN	During TST_TIM, SD <min_var_warn, or<br="">During TST_TIM, MAX-MIN <min_var_warn< td=""></min_var_warn<></min_var_warn,>
Pass=1	Applies for test pass condition	
Test Exception: Anoxic conditions introduce the possibility of repeated zero values. The attenuated signal		

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 10) 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	Codeable Instructions	
Fail=3	Because of the dynamic nature of DO, no red flag is identified for this test.	N/A	
Suspect=2	DO _n fails the DO rate of change and the second DO sensor does not exceed the rate of change.	$ DO1_{n} - DO1_{n-1} > N_DO1_DEV*SD1$ AND $ DO2_{n} - DO2_{n-1} < 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.

Test	Condition	Platform	Codeable Instructions
1) Gap Test (Required) 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 Fixed Vertical Mobile 3D	No change
2) Syntax Test (Required) Received data 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.	Expected data sentence received, absence of parity errors	Stationary Fixed Vertical Mobile 3D	No change
3) Gross Range Test (Required) 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 Fixed Vertical Mobile 3D	No change
4) Climatology Test (Required) 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 Fixed Vertical Mobile 3D	No changeTest is conducted along z axisTest is conducted along s, x, or y axisTest is conducted along s, x, or y axisTest is conducted along s, x, y, or z axis

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

Test	Condition	Platform	Codeable Instructions
5) Spike Test (Strongly Recommended)	Data point n-1 exceeds a selected threshold relative to adjacent data points.	Stationary	No change
This check is for single value spikes, specifically the DO value at point n-1 (DO_{n-1}). Spikes		Fixed Vertical	Test is conducted along z axis
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		Mobile	No change, or test is conducted along s, x, or y axis
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.		3D	No change, or test is conducted along s, x, y, or z axis
6) Rate of Change Test (Strongly Recommended)	Excessive	Stationary	No change
This test inspects the time series for time rate of change in that exceed a threshold value	rise/fall test	Fixed Vertical	Test is conducted along z axis
identified by the operator. DO values can change dramatically over short periods, hindering the value of this test. A balance must be found		Mobile	No change, or test is conducted along s, x, or y axis
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.		3D	No change, or test is conducted along s, x, y, or z axis
7) Flat Line Test (Strongly Recommended)	Invariate DO	Stationary	No change
When some sensors and/or data collection platforms (DCPs) fail, the result can be a	value	Vertical	Test is conducted along z axis
continuously repeated observation of exactly the same value. This test compares the present observation (DOn) to a number (REP_CNT_FAIL		Mobile	No change, or test is conducted along s, x, or y axis
or REP_CNT_SUSPECT) of previous observations. DOn 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.		3D	No change, or test is conducted along s, x, y, or z axis

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

Condition	Platform	Codeable Instructions
Comparison to	Stationary	No change
other variables	Fixed Vertical	Test is conducted along z axis
	Mobile	Test is conducted along s, x, or y axis
	3D	Test is conducted along s, x, y, or z axis
Inadequate	Stationary	No change
variation test	Fixed Vertical	Test is conducted along z axis
	Mobile	No change, or test is conducted along s, x, or y axis
	3D	No change, or test is conducted along s, x, y, or z axis
Comparison to	Stationary	No change
nearby DO sensors	Fixed Vertical	Test is conducted along z axis
	Mobile	No change
	3D	No change
	Comparison to other variables	Comparison to other variablesStationary Fixed VerticalMobile3D3D3DInadequate variation testStationary Fixed VerticalInadequate variation testStationary Fixed VerticalMobile3DStationary Fixed Vertical3DStationary Fixed VerticalStationary Fixed VerticalMobile3DStationary Fixed VerticalStationary Fixed VerticalMobile3DSensorsStationary Fixed VerticalMobileStationary Fixed VerticalMobileStationary Fixed VerticalMobileStationary Fixed VerticalMobileStationary Fixed VerticalMobileStationary Fixed VerticalMobileStationary Fixed VerticalMobileStationary Fixed VerticalMobileStationary Fixed VerticalMobileMobile

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

4.0 Conclusion

This DO manual has been developed 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 codeable 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 vendors can play a huge role in this area. The vendors have spent enormous efforts helping customers use these sensors successfully. Most vendors have instructions for best practices, and those practices should be used as a first-order QA for all measurements. The vendor-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, either with water samples periodically, a known calibrated and maintained reference instrument, or 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. Separate manuals will be used to discriminate between near real-time data, which might be used for ecosystem-based management, and delayed-mode data, which might be suitable for climate studies.

Each QC manual is envisioned to be a dynamic document and will be posted on the QARTOD website at <u>www.ioos.gov/QARTOD/</u>. This will allow for updating of 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. The website also accommodates conversations between users and interaction amongst peers via a chat room, allowing questions and answers to be posted. The website includes such items as code libraries, procedures for testing data, and interactive graphics, and makes it possible for 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 vendors 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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- Specifics about discrete sample oxygen methods can be viewed at: <u>http://calcofi.org/references/ccmethods/294-dissolved-oxygen.html</u> <u>http://calcofi.org/references/clhandbook/80-o2samples.html</u>
- 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. <u>http://www.oceandatastandards.org/index.php?option=com_content&task=view&id=46&Itemid=0</u>
- The ocean data standards resource pool can be found at: <u>http://www.oceandatastandards.org/index.php?option=com_content&task=view&id=22&Itemid=28</u>
- <u>http://www.oceandatastandards.org/index.php?option=com_content&task=view&id=5&Itemid=7</u> is the higher level page (see menu to the right for sub pages). There is a sub page 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:

(http://www.ioos.gov/qartod/)

Quality Control of Profiling Float Oxygen Data (file name: AGU_2010_Float_Oxy_Final) Report from the COL-NASA Data QA/QC Workshop (file name: Data_QC_Workshop_Final_Report_2012-08-07) **U.S. IOOS Development Plan** (file name: ioos_devplan) NDBC Handbook of Automated Data Quality Control (file name: NDBCHandbookofAutomatedDataQualityControl2009) YSI Environmental Dissolved Oxygen Values above 100% Air Saturation (file name: Super Saturation) WHP Operations and Methods – July 1991 Dissolved Oxygen (file name: WOCE 02 recommendations) Argo Quality Control Manual, V 2.7 3 January 2012 (file name: argo-quality-control-manual-V2.7) Data Quality Control in the U.S. IOOS (file name: IOOS CWP_Lankhorst_Data_QC.doc) Ocean Deoxygenation in a Warming World (file name: Keeling et al 2010. 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 (file name: QAPP_CoastalGlider_Final_revised_signed) In-situ Calibration of Optode-Based Oxygen Sensors (file name: Uchida et al., 2008, In-situ calib) National Water Quality Monitoring Council Water Quality Data Elements: A User Guide (file name: wqde_trno3) Requirements for Global Implementation of the Strategic Plan for Coastal GOOS - Panel for Integrated Coastal Observation (PICO-I) (file name: Requirements_for_Global_Implementation_of_the_Strategic_Plan_for) Coastal) GOOS_GOOS-193) Integrating Standards in Data QA/QC Into OpenGeospatial Consortium Sensor Observation Services (file name: IEEE Ocean09Bremen) **UHM Stormwater Monitoring System Servicing Checklist** (file name: UHM Stormwater Monitoring System Servicing Checklist PDF) One Man's Advice on the Determination of Dissolved Oxygen in Seawater (file name: Codispoti1988_OxygenProtocol-a)

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 sensor calibration, sensor handling and service, 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 vendors, preferably utilizing several different technologies, constitutes an acceptable check. Because of the trend towards corporate conglomeration, those wishing to employ a consensus standard should ensure that the different vendors are truly independent.

A.2 Sensor Comparison

An effective QA effort continuously 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 vendor for similar inhouse 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, and they must be understood in order to properly report results. For those who succeed, the additional sensors provide a highly robust demonstration of capability. Such efforts form the basis of a strong QA/QC effort. Further, it provides the operator with an expanded supply source, permitting less reliance upon a single vendor 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 (not on aluminum).
- Tributyltin oxide (TBTO) anti-foulant device such as SBE often used in conjunction with a pumped system.
- Wrap body of sensor with clear packing tape for a small probe or plastic wrap for a large instrument. This keeps the PVC tape from leaving residue on the sensor. Heavy PVC underground cable tape is the best for bad biofouling.
- Wrap 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 power (battery).
- 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 S. Florida during the summer. Sediment and particles that become embedded in the wipers can scratch the surface of the membrane on optical DO sensors.
- Put the sensor in the dark.
- Avoid or isolate dissimilar metals.
- Maintain sacrificial anodes and ensure they are properly installed (good electrical contact).
- Maximize use of non-metallic components.
- Use UV-stabilized components that are not subject to sunlight degradation.
- Mount sensors vertically to minimize sediment buildup mesh and cone –especially useful for sensors with flow-through tubes.
- Where applicable, maintain sensor surfaces by gentle cleaning (e.g., using a baby toothbrush)
- Store the device in the air inside a housing (or barn) between measurements
- Make use of a pumped system where the sensor is kept above water and [water only] pumped through a flow chamber just before a reading is required.
- Avoid use of stilling wells. Ziplines are better.
- 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:

- Pre-deployment calibrations on every sensor
- Post-deployment calibrations on every sensor, plus in-situ comparison before recovery
- Periodic calibration of ready-to-use spares
- Monitor with redundant sensors whenever possible
- 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 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 previous deployed sensor can determine if it is the source of the discontinuity in readings. If the newly deployed sensor is suspected to have problems then an initial adjustment can be made in the values based on the offset from the previously deployed sensor 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)
 - o Lowest and highest possible readings
- Operating range (i.e., some instruments won't operate at certain temperatures)
 - Could be depth or pressure range
 - o Salinity correction
- Resolution/precision required
- Sampling frequency how fast sensor can take measurements
- Reporting frequency how often the sensor reports the data
- Response time of the sensor sensor lag time response
- Instrument check visual inspection for defects, bio-fouling, etc.
- Power check master clock, battery, etc. variability in these among sensors
- Standardize sensor clock to a reference such as GPS timing]
- Capability to reveal a problem with data

When evaluating which specifications must be met:

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

General comments regarding QA procedures:

- A diagram (<u>http://www.ldeo.columbia.edu/~dale/dataflow/</u>), contributed by Dale Chayes (LDEO) provides a visual representation of proper QA procedures.
- Require serial numbers and model ID from the supplier.
- Do not make the checklist so detailed that it will not be used. (e.g., Codispoti1988 OxygenProtocol)
- 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 thermometers and barometers when conducting calibrations or calibration checks.
- Keep maintenance records, including when membranes and optical caps are replaced. Servicing by OEM. Calibration checks of temperatures. Calibration checks of salinity, along with age of these sensors and servicing.
- A sensor that maintains an internal file of past calibration constants is very useful since it can be downloaded instead of transcribed manually introducing human error.
- The calibration constants or deviations from a standard should be plotted 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.
- Never assume that anomalous values are problems with a sensor. Always compare measurements with other sensors (e.g. chlorophyll fluorescence) to help determine is the reading is real then examine the possibility of problems with a sensor.
- If 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 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 target data reproducibility requirements, if accuracy cannot be determined. 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.

QA Best Practices Indicator	Description
Good Process	DO sensors are swapped and/or serviced at sufficient 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	Good process, plus pre- and post-deployment calibration checks using either titrations or alternative sensors to confirm performance.
Best Process	Better process, plus use of high-quality Winkler titrations following a well- documented protocol or alternative sensors to validate in-situ deployments. Or, the better process employing manufacturer conducted pre- and post-calibrations.

Table A-1. Best practices indicator for QA

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

QARTOD

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

Pre-deployment QA Checklist:

- \Box 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). Control chart calibrations.
- Check the sensor history for past repairs, maintenance, and calibration.
- Consider storing and shipping information before deploying.
 - Heat, cold, vibration, etc.
- Provide detailed documentation.
- **D** Record operator/user experiences with this sensor after reading the manual.
- 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 visual tracking system for training to identify those technicians who are highly trained and then pair them with inexperienced technicians. Have data quality review chain.

Deployment Checklist

- □ Scrape bio-fouling off platform.
- □ Verify sensor serial numbers.
- Deploy and co-locate multiple sensors (attention to interference if too close).
- Perform visual inspection; take photos if possible (verify position of sensors, connectors, fouling, cable problems).
- Verify instrument function at deployment site prior to site departure. Allot sufficient time for temperature equilibration.
- □ Monitor sensors for issues (freezing, fouling).
- Automate processing so you can monitor the initial deployment and confirm the sensor is working while still on-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

- **D** Take pictures of recovered sensor as is for metadata
- □ Check to make sure all clocks agree or, if they do not agree, record all times and compare with NIST.
- D Post-calibrate sensor and document before and after cleaning readings.
- D Perform in-situ side by side check using another sensor.
- **D** Provide a mechanism for feedback on 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;
 - 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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