



IOOS

Integrated Ocean
Observing System



Manual for Real-Time Quality Control of Dissolved Nutrients Observations

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

Version 1.1
February 2018

<https://doi.org/10.7289/V5TT4P7R>

Document Validation



U.S. IOOS Program Office Validation

A handwritten signature in blue ink, appearing to read 'Carl C. Gouldman', written over a horizontal line.

Carl C. Gouldman, U.S. IOOS Program Director

February 20, 2018

Date

QARTOD Project Manager Validation

A handwritten signature in blue ink, appearing to read 'Kathleen Bailey', written over a horizontal line.

Kathleen Bailey, U.S. IOOS Project Manager

February 20, 2018

Date

QARTOD Board of Advisors Validation

A handwritten signature in blue ink, appearing to read 'Julianna O. Thomas', written over a horizontal line.

Julianna O. Thomas, Southern California Coastal Ocean Observing System

February 20, 2018

Date

Table of Contents

Table of Contents	iii
List of Figures	iv
List of Tables.....	v
Revision History.....	vi
Endorsement Disclaimer	vii
Acknowledgements	viii
Acronyms and Abbreviations	ix
Definitions of Selected Terms.....	x
1.0 Background and Introduction	1
2.0 Purpose/Constraints/Applications	3
2.1 Purpose.....	3
2.2 Temperature/Salinity	5
2.3 Constraints.....	5
2.3.1 Data Processing Methodology	5
2.3.2 Traceability to Accepted Standards.....	6
2.3.3 The Effect of Dynamic Environments on Sensor Data.....	7
2.3.4 Sensor Deployment Considerations and Hardware Limitations	7
2.4 Applications of Dissolved Nutrients Data	15
3.0 Quality Control.....	17
3.1 QC Flags	17
3.2 Test Hierarchy.....	18
3.3 QC Tests	19
3.3.1 Applications of QC Tests to Stationary DN Sensors.....	19
Test 1) Gap Test (Required).....	19
Test 2) Syntax Test (Required).....	20
Test 3) Location Test (Required).....	20
Test 4) Gross Range Test (Required)	21
Test 5) Climatology Test (Strongly Recommended)	21
Test 6) Spike Test (Strongly Recommended)	22
Test 7) Rate of Change Test (Strongly Recommended)	23
Test 8) Flat Line Test (Strongly Recommended).....	24
Test 9) Multi-Variate Test (Suggested)	25
Test 10) Attenuated Signal Test (Suggested)	26
Test 11) Neighbor Test (Suggested).....	27
3.3.2 Applications of QC Tests to DN Sensor Deployments	27
4.0 Summary.....	32
5.0 References	34

Appendix A	Quality Assurance	A-1
A.1	Sensor Calibration Considerations.....	A-1
A.2	Sensor Comparison	A-1
A.3	Bio-fouling and Corrosion Prevention Strategies.....	A-3
A.4	Common QA Considerations.....	A-4
A.5	QA Levels for Best Practices	A-5
A.6	Additional Sources of QA Information.....	A-6
A.7	Sample Checklists	A-6
	General QA Checklist:	A-6
	Deployment Checklist.....	A-7
	Post-deployment Checklist.....	A-7
Appendix B	Dissolved Nutrients Manual Team and Reviewers	Error!
Bookmark not defined.		

List of Figures

Figure 2-1.	Nitrate spikes observed during the passage of a tropical storm are associated with an increase in the standard deviation of the measurements, perhaps attributable to interference such as an increase in turbidity. Close scrutiny would be possible if the high-frequency measurements were available in real time. (Graphic courtesy of Jeff Scudder/University of South Florida)	6
Figure 2-2.	(L) shows a Sea-Bird Scientific SUNA V2 (Submersible Ultraviolet Nitrate Analyzer) mounted on a fixed structure on the Mississippi River at Baton Rouge, where the instrument cage is lowered and raised. (R) shows a NexSens buoy supporting a Sea-Bird Scientific SUNA nitrate sensor and WET Labs Cycle Phosphate sensor (in addition to a YSI EXO multi-parameter sonde measuring algal pigments, turbidity, and dissolved organic matter). (Photos courtesy of Brian Pellerin/USGS)	8
Figure 2-3.	A cage for a boat deployment in the Bay Delta with several instruments (fluorometers, nitrate sensors, phosphate sensors, etc.). (Photo courtesy of Brian Pellerin/USGS)	9
Figure 2-4.	WebbGlider Profiler 3-D (L) (photo courtesy of Dr. Grace Saba) and Liquid Robotics Wave Glider Mobile Surface (R) (Photo courtesy of Liquid Robotics).	9
Figure 2-5.	WET Labs AMP C100 In-Situ Profiler. (Photo courtesy of WET Labs)	10
Figure 2-6.	Commonly used DN sensors. (Photos courtesy of Corey Koch/WET Labs, Pompeo Moscetta/SYSTEA, Vince Kelly/Green Eyes LLC)	12
Figure 2-7.	These Sea-Bird Scientific Cycle PO4 phosphate sensors have accumulated an external bio-fouling coating during deployment (top). A Sea-Bird Scientific SUNA nitrate sensor uses a rotating, motorized brush to keep the optical lenses free of bio-fouling. (Photos courtesy of Corey Koch/WET Labs)	12
Figure 2-8A-F.	Time-series of nitrate concentrations at instrument depth determined optically by the ISUS and standard method chemical assays of total nitrates (nitrate plus nitrite). Burst optical data were collected hourly and data was binned to 10 seconds average calls of nitrate concentration at a sampling rate of 1 Hz. (Photo courtesy of Dr. Eric Milbrandt/Sanibel-Captiva Conservation Foundation)	14

List of Tables

Table 2-1. Types of platforms and areas included and excluded in this manual.....	4
Table 2-2. DN variables that are included or excluded from this manual.....	5
Table 2-3. Commonly used sensors for DN observations.....	11
Table 3-1. Flags for real-time data (UNESCO 2013)	18
Table 3-2. QC Tests in order of implementation	18
Table 3-3 Application of Required QC Tests for Sensor Deployments. Note: The ‘s’ axis means “along path.”	28
Table 3-4. Application of Strongly Recommended QC Tests for Sensor Deployments	29
Table 3-5. Application Suggested QC Tests for Sensor Deployments	31

Revision History

Date	Revision Description	Notes
September 2015	Original Document Published	
February 2018	<p>Revise cover to reflect correct version and publication date.</p> <p>Revise names and dates on <i>Document Validation</i> page (page ii).</p> <p>Update <i>Table of Contents</i> (pages iii-iv).</p> <p>Update <i>Revision History</i> (page v).</p> <p>Update email address in <i>Request to Manual Users</i> (page vi).</p> <p>Update <i>Acknowledgements</i> to include manual update version 1.1 team members (page vii).</p> <p>Update <i>Acronyms and Abbreviations</i> (pages viii).</p> <p>Add interoperable, sensor, variable to <i>Definitions of Selected Terms</i>. Update format of definitions. (page ix).</p> <p>Update section 1.0 to reflect QARTOD publications completed since original dissolved nutrients manual; added digital object identifiers for each manual (pages 1-2).</p> <p>Update sections 2.1, 2.2 and 2.3 to clarify and enhance existing content. Add definition of conservative variable and reference (section 2.3.3) and revise table 2-1, 2-3, and figure 2-6.</p> <p>Update section 3.3 to reflect more recent references and to make minor editing adjustments to Tests 4, 5, 6, 7, 8, 9, 10, 11, 12, and 13.</p> <p>Add examples to section 3.3.2, table 3-4, Test 7; minor revision to table 3-4, Tests 7 and 8.</p> <p>Update <i>References</i> to include JCGM 2012 added for sensor definition.</p> <p>Update QARTOD Board of Advisor and Regional Association Director listings in appendix B (B-1 through B-3).</p> <p>Perform general editing for consistency in style and terminology; update Web links.</p> <p>Update formatting to ensure compliance to Section 508 requirements.</p>	Version 1.1

Endorsement Disclaimer

Mention of a commercial company or product does not constitute an endorsement by NOAA. Use of information from this publication for publicity or advertising purposes concerning proprietary products or the tests of such products is not authorized.

Request to Manual Users

To gauge the success of the QARTOD project, it helps to be aware of groups working to utilize these QC tests. Please notify us of your efforts or intentions to implement QARTOD processes by sending a brief email to qartod.board@noaa.gov or posting a notice at <http://www.linkedin.com/groups?gid=2521409>.

Acknowledgements

In addition to acknowledging support for the original version of this manual in the paragraphs below, we wish to thank those who assisted in creating this updated version (appendix B). We appreciate the review and comments provided by Robert Maxfield, Senior Science Advisor for Advanced Monitoring Technology (U.S. Environmental Protection Agency/New England). We thank Dr. Brian Pellerin (U.S. Geological Survey) once again, and Brett Johnston from the USGS Florida-Caribbean Water Science Center for their reviews and comments. We are especially thankful for the extensive reviews provided by Dr. Matthias Lankhorst at UCSD Scripps Institution of Oceanography and Vince Kelly at Green Eyes LLC.

We are grateful to our entire dissolved nutrients team (appendix B), especially to those who served on the dissolved nutrients manual committee and provided content and suggestions for the initial draft, as well as all who reviewed each draft and provided valuable feedback.

Much appreciation goes to Dr. Emilio Mayorga (University of Washington/NANOOS) and Daniel Schar (Alliance for Coastal Technologies/University of Hawaii) for their time and enthusiasm while serving as co-editors.

The manual was greatly improved thanks to the extensive feedback provided by Corey Koch (WET Labs) and Dr. Brian Pellerin (USGS). We also benefited from the wisdom of Dr. Carol Janzen (formerly at Sea-Bird Scientific and now at AOOS). Many thanks for early input and support go to Dr. Eric Milbrandt (Sanibel-Captiva Conservation Foundation), to Eric Breuer and Nathan Holcomb (NOS/CO-OPS), and to Dr. Brian Lapointe (Florida Atlantic University). We also appreciate the suggestions related to low nutrient, open-ocean regions provided by Dr. Jia-Zhong Zhang (NOAA/AOML).

Finally, thanks to the QARTOD Board of Advisors (listed in appendix B) and to Carl Gouldman, Derrick Snowden, Kathleen Bailey, and Kate Culpepper (U.S. IOOS) for their support of the QARTOD project.

Acronyms and Abbreviations

AOOS	Alaska Ocean Observing System
AUV	Autonomous Underwater Vehicle
CDIP	Coastal Data Information Program
CeNCOOS	Central and Northern California Ocean Observing System
CO-OPS	Center for Operational Oceanographic Products and Services
CRC	Cyclic Redundancy Check
DIW	De-ionized Water
DMAC	Data Management and Communications
DN	Dissolved Nutrients
GCOOS	Gulf of Mexico Coastal Ocean Observing System
GLOS	Great Lakes Observing System
GOOS	Global Ocean Observing System
IOOS	Integrated Ocean Observing System
ISUS	In-situ Ultraviolet Spectrophotometer
MARACOOS	Mid-Atlantic Regional Association Coastal Ocean Observing System
mg/L	Milligrams per Liter
μM	Micromoles (also called micromolar = 10^{-6} mol/liter)
NANOOS	Northwest Association of Networked Ocean Observing Systems
NERACOOS	North Eastern Regional Association of Coastal Ocean Observing Systems
NIST	National Institute of Standards and Technology
NOAA	National Oceanic and Atmospheric Administration
PacIOOS	Pacific Islands Ocean Observing System
QARTOD	Quality Control/Quality-Assurance of Real-Time Oceanographic Data
QA	Quality Assurance
QC	Quality Control
RCOOS	Regional Coastal Ocean Observing System
SCCOOS	Southern California Coastal Ocean Observing System
SD	Standard Deviation
SECOORA	Southeast Coastal Ocean Observing Regional Association
UNESCO	United Nations Educational, Scientific, and Cultural Organization
USGS	United States Geological Survey

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	Codable instructions are 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	Data record is one or more messages that form a coherent, logical, and complete observation.
Dissolved Nutrients (DN) Sensor	DN sensor is a generic reference to a sensor used to measure one or more specific dissolved nutrients such as NO_3^- , NO_2^- , NH_4^+ , PO_4^{3-} , SiO_4^{3-} , P_{tot} , or N_{tot} . No single sensor is capable of measuring all dissolved nutrients; for a number of dissolved nutrients, no sensors are available.
Interoperable	Interoperable means the ability of two or more systems to exchange and mutually use data, metadata, information, or system parameters using established protocols or standards.
Message	Message means a standalone data transmission. A data record can be composed of multiple messages.
Operator	Operators are individuals or entities responsible for collecting and providing data.
Quality Assurance (QA)	QA means processes that are employed with hardware to support the generation of high quality data. (section 2.0 and appendix A)
Quality Control (QC)	QC means follow-on steps that support the delivery of high-quality data, requiring both automation and human intervention. (section 3.0)
Real Time	Real time means that: data are delivered without delay for immediate use; time series extends only backwards in time, where the next data point is not available; and sample intervals may range from a few seconds to a few hours or even days, depending upon the sensor configuration (section 1.0).
Sensor	A sensor is a device that detects or measures a physical property and provides the result without delay. A sensor is an element of a measuring system that is directly affected by a phenomenon, body, or substance carrying a quantity to be measured. (JCGM 2012)
Thresholds	Thresholds are limits that are defined by the operator.
Variable	A variable is an observation (or measurement) of biogeochemical properties within oceanographic and/or meteorological environments.

1.0 Background and Introduction

The U.S. Integrated Ocean Observing System (IOOS®) has a vested interest in collecting high-quality data for the 26 core variables (U.S. IOOS 2010) measured on a national scale. In response to this interest, 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) Project, addressing each variable as funding permits. This dissolved nutrients (DN) data manual is the eighth in a series of guidance documents that address the QC of real-time data for each core variable and the eighth manual to be updated.

Please refer to <https://ioos.noaa.gov/project/qartod/> for the following documents:

- 1) U.S. Integrated Ocean Observing System, 2015. U.S IOOS QARTOD Project Plan - Accomplishments for 2012–2016 and Update for 2017–2021. 47 pp. <https://doi.org/10.7289/V5JQ0Z71>
- 2) 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. 48 pp. <https://doi.org/10.7289/V5ZW1J4J>
- 3) U.S. Integrated Ocean Observing System, 2015. Manual for Real-Time Quality Control of In-Situ Current Observations Version 2.0: A Guide to Quality Control and Quality Assurance of Acoustic Doppler Current Profiler Observations. 51 pp. <https://doi.org/10.7289/V5WM1BMZ>
- 4) U.S. Integrated Ocean Observing System, 2015. Manual for Real-Time Quality Control of In-Situ Surface Wave Data Version 2.0: A Guide to Quality Control and Quality Assurance of In-Situ Surface Wave Observations. 64 pp. <https://doi.org/10.7289/V5KK991T>
- 5) U.S. Integrated Ocean Observing System, 2015. Manual for Real-Time Quality Control of In-Situ Temperature and Salinity Data Version 2.0: A Guide to Quality Control and Quality Assurance of In-Situ Temperature and Salinity Observations. 56 pp. <https://doi.org/10.7289/V5V40SD4>
- 6) U.S. Integrated Ocean Observing System, 2014. Manual for Real-Time Quality Control of Water Level Data Version 2.0: A Guide to Quality Control and Quality Assurance of Water Level Observations. 43 pp. <https://doi.org/10.7289/V5QC01Q7>
- 7) U.S. Integrated Ocean Observing System, 2017. Manual for Real-Time Quality Control of Wind Data Version 1.1: A Guide to Quality Control and Quality Assurance of Coastal and Oceanic Wind Observations. 47 pp. <https://doi.org/10.7289/V5FX77NH>
- 8) U.S. Integrated Ocean Observing System, 2017. Manual for Real-Time Quality Control of Ocean Optics Data Version 1.1: A Guide to Quality Control and Quality Assurance of Coastal and Oceanic Optics Observations. 49 pp. <https://doi.org/10.7289/V5XW4H05>
- 9) U.S. Integrated Ocean Observing System, 2016. Manual for Real-Time Quality Control of High Frequency Radar Surface Currents Data Version 1.0: A Guide to Quality Control and Quality Assurance of High Frequency Radar Surface Currents Data Observations. 58 pp. <https://doi.org/10.7289/V5T43R96>

- 10) U.S. Integrated Ocean Observing System, 2017. Manual for Real-Time Quality Control of Phytoplankton Data Version 1.0: A Guide to Quality Control and Quality Assurance of Phytoplankton Data Observations. 67 pp. <https://doi.org/10.7289/V56D5R6S>
- 11) U.S. Integrated Ocean Observing System, 2017. Manual for Real-Time Quality Control of Passive Acoustics Data Version 1.0: A Guide to Quality Control and Quality Assurance of Passive Acoustics Observations. 45 pp. <https://doi.org/10.7289/V5PC30M9>

Please reference this document as:

U.S. Integrated Ocean Observing System, 2018. Manual for Real-Time Quality Control of Dissolved Nutrients Data Version 1.1: A Guide to Quality Control and Quality Assurance of Coastal and Dissolved Nutrients Observations. 56 pp. <https://doi.org/10.7289/V5TT4P7R>

This manual is a living document that reflects the state-of-the-art QC testing procedures for DN observations. It is written for the experienced operator but also provides examples for those who are just entering the field.

2.0 Purpose/Constraints/Applications

The following sections describe the purpose of this manual, as well as the constraints that operators may encounter when performing QC of DN data and specific applications of those data.

2.1 Purpose

The purpose of this manual is to provide guidance to the U.S. IOOS and the dissolved nutrients community at large for the real-time QC of DN measurements using an agreed-upon, documented, and implemented standard process. This manual is also a deliverable to the U.S. IOOS Regional Associations and the ocean observing community and represents a contribution to a collection of core variable QC documents.

Most operators provide real-time data on a provisional basis, alerting users that post-processing is required to validate their data. However, even this provisional data should be quality controlled. Data released in real time should be subjected to automated QC processes, which: 1) provide a quality-control indicator, 2) alert the operator when questionable or interesting data are presented, and 3) prevent the dissemination of bad data.

These practices for sensor QC of DN data were developed by operators with experience using a variety of sensors and technologies. In-situ, real-time detection of DN can be accomplished using direct spectroscopy methods, ion-specific electrodes, or more traditional wet chemistry. Systems using wet chemistry draw water samples into a reagent mixing chamber, where the chemical reaction is measured and quantified. This process is controlled by micro-pumps, injection valves, and small reactor cells combined with absorption or fluorescence detectors. Using these miniaturized colorimetric or fluorometric methods leads to sensitive in-situ measurements of any dissolved chemical species that can form a color complex. Some of these systems may require frequent maintenance due to the complexity associated with pumps, chambers, mixing, and detection components. They may require frequent calibration of fluid delivery devices (pumps) and replenishment of multiple reagent and standard solutions, some of which are not stable unless kept at low temperature and shielded from light. Some systems can operate from four to eight weeks without replacing reagents, depending on sample frequency and other environmental circumstances. Spectroscopic and ion-specific electrode technologies are equally subject to drift, which requires quality assurance (QA) and QC.

DN 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. These tests draw from existing expertise in programs such as the Studies of Ecological and Chemical Responses to Environmental Trends, a joint effort by the California Cooperative Oceanic Fisheries Investigations and the Monterey Bay Aquarium Research Institute.

This manual differs from existing QC procedures for DN measurements in that its focus is on real-time data. It presents a series of eleven tests that operators can incorporate into practices and procedures for QC of DN measurements. These tests apply only to the in-situ, real-time measurement of DN as observed by sensors deployed on fixed or mobile platforms and not to remotely sensed DN measurements (e.g., satellite observations). Table 2-1 shows types of platforms and areas that are included and excluded in this manual. Those excluded are deemed to require substantially different QC tests, a different observational community,

¹The 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.

substantially greater resources, or they presently lack a real-time data delivery capability. Whenever possible, they will be included in later manual updates.

Table 2-1. Types of platforms and areas included and excluded in this manual.

Platforms Included	Platforms Excluded
Coastal and offshore buoys Oil platforms C-MAN (Coastal-Marine Automated Network) Surface fixed and mobile platforms Autonomous surface vessels and ships	Satellite Aircraft

These test procedures are written as a high-level narrative from which a computer programmer can develop code to execute specific tests and set data flags (data quality indicators) within a software program. Those implementing QARTOD tests have created a code repository (<https://github.com/ioos/qartod>) where operators may find or post examples of code in use. Although certain tests are recommended, thresholds can vary among data providers. The tests described here are designed to support a range of DN sensors and operator capabilities. Some well-established programs, such as the U.S. Geological Survey (USGS) National Real-Time Water Quality program (<http://nrtwq.usgs.gov>), with the highest standards have implemented very rigorous QC processes. Others, with different requirements, may utilize sensors with data streams that cannot support as many QC checks—all have value when used prudently. It is the responsibility of the users to understand and appropriately utilize data of varying quality, and operators must provide support by documenting and publishing their QC processes. A balance must be struck between the time-sensitive needs of real-time observing systems and the degree of rigor that has been applied to non-real-time systems by operators with decades of QC experience.

High-quality marine observations require sustained QA and QC practices to ensure credibility and value to operators and data 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. Other QA practices include: 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. Post-deployment calibration (instrument verification after recovery) issues are not part of the scope of this manual. However, QC and QA are interrelated, and both are important to the process; therefore, QA considerations are briefly addressed in appendix A.

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).

The process of ensuring data quality is not always straightforward. QA/QC procedures may be specific to a sensor technology or even to a particular manufacturer's model, so the establishment of a methodology that is applicable to every sensor is challenging.

2.2 Temperature/Salinity

The DN sensor detects a measure of dissolved nutrient concentration, but the sensor response and DN concentration calculations may also depend upon the quality of the temperature and salinity data (Martini et al. 2017). Corrections to the sensor output may be required to account for the effects of temperature and salinity. These corrections might occur internally in many instruments, and in these cases, failure of the instrument to collect accurate temperature and/or salinity data necessitates that the DN 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 salinity. Some DN sensors require the operator to input a fixed salinity that represents the likely value. Often these temperature and salinity corrections are applied during post-processing. Other interferences can be important as well. For example, high turbidity and colored dissolved organic matter values can cause measurement errors, especially in lakes and coastal regions.

2.3 Constraints

Many measurements of the 26 U.S. IOOS core variables of interest utilize similar sensing technologies but require substantially different QC methods. However, QC tests should not be overly generic, so these variables must be divided and grouped so that specific meaningful tests are appropriate to the variables included in the group. In this manual, DN that are sufficiently common in nature to have similar QC checks are identified. Table 2-2 shows the variables to be addressed in this manual, as well as those that are excluded.

Table 2-2. DN variables that are included or excluded from this manual.

Variables Included	Variables Excluded
Nitrogen (NO ₃ , NO ₂ , and NH ₄)	Dissolved Organic Carbon Sulfur/Sulphates
Phosphate (PO ₄)	Dissolved Organic Nitrogen
Silicate (SiO ₄)	Dissolved Organic Phosphorus

2.3.1 Data Processing Methodology

The type of sensor system used to collect DN data and the system used to process and transmit the measurements determine which QC algorithms are used. In-situ systems with sufficient onboard processing power within the sensor may substantially process the data to produce derived products, such as temperature and salinity corrections to DN observations. Some sensors may sample at high-rate or burst mode (e.g., 1 Hz). These samples are used to produce the actual, real-time value transmitted (e.g., hourly value). Statistical information about the high-rate sample distributions can also be used and transmitted as real-time QC parameters (e.g., sample standard deviations and outliers). If ample transmission capability is available, expanded data streams may be transmitted ashore and subsequently quality controlled from there. To accommodate a range of different operator methodologies, three levels of QC are proposed: required, strongly recommended, and suggested.

When onboard processing is used to reduce high-frequency sampling, apply associated corrections, and generate the resultant observation to be transmitted, operators should have a full understanding of the algorithms employed. These processes are often proprietary, and when not fully revealed by the vendor or manufacturer, the operator should sufficiently test the system to gain the needed understanding. In the example provided in fig. 2-1, nitrate data obtained during the passage of Tropical Storm Debbie are shown. The 1 Hz data samples were processed by a data logger for 30 seconds. There is a clear nitrate signal, but the associated standard deviation values show that the data quality is poor, perhaps due to an increase in turbidity.

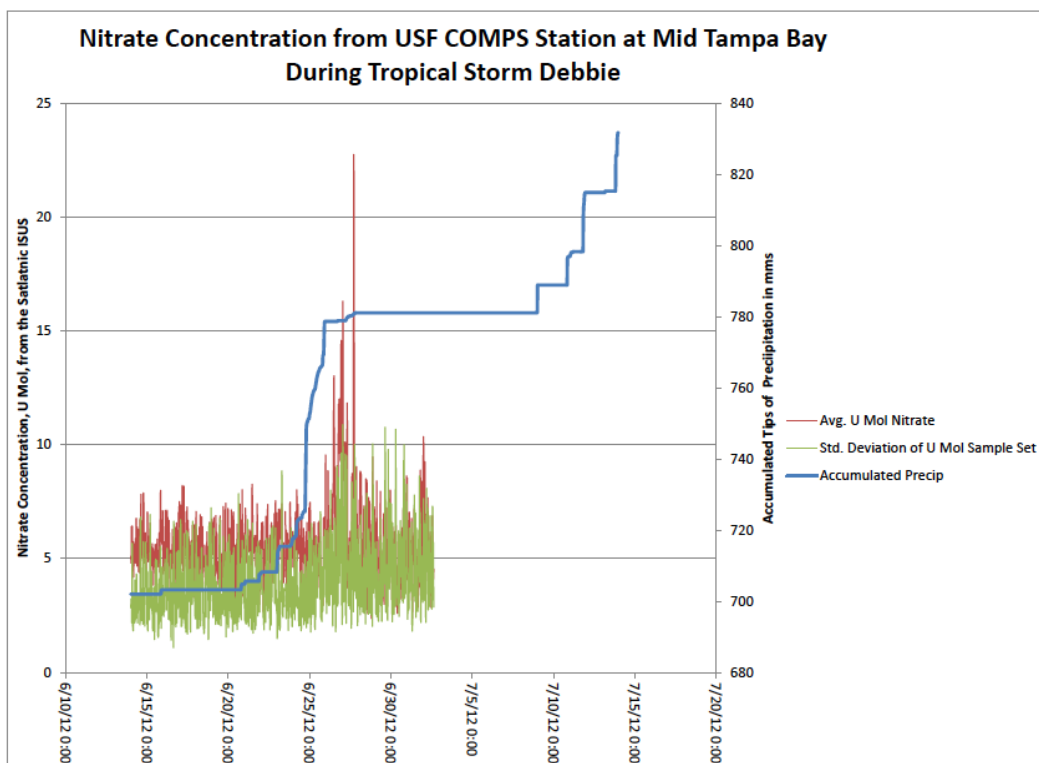


Figure 2-1. Nitrate spikes observed during the passage of a tropical storm are associated with an increase in the standard deviation of the measurements, perhaps attributable to interference such as an increase in turbidity. Close scrutiny would be possible if the high-frequency measurements were available in real time. (Graphic courtesy of Jeff Scudder/University of South Florida)

2.3.2 Traceability to Accepted Standards

To ensure that DN sensors produce accurate data, rigorous calibrations and calibration checks must be performed in addition to QC checks. Most operators rely upon manufacturer calibrations and conduct calibration checks only before deployment. These calibration checks are critical to ensuring that the manufacturer calibration is still valid. Manufacturers describe how to conduct these calibration checks in their user manuals, which are currently considered QA and further addressed in appendix A. Calibration for nutrients should be done using either approved Environmental Protection Agency methods or standard oceanographic techniques, such as those provided by SEAL Analytics.

Calibrations and calibration checks must be traceable to accepted standards. The National Institute of Standards and Technology (NIST) (<http://www.nist.gov/index.html>), a provider of internationally accepted standards, is often the source for these standards. Calibration activities must be tailored to match data use and resources. Calibration cost and effort increase dramatically as accuracy requirements increase. Fundamental NIST standards such as mass and volume may be required when conducting calibration checks on DN sensors, and DN-specific standards are usually procured from chemical manufacturers such as Hach®. Where NIST standards are not available, an active research effort generally exists among operators and manufacturers regarding the use of primary and secondary standards for instrument calibration and calibration checks (Pellerin et al. 2013). For example, for some DN sensors deployed in the ocean, a low nutrient seawater is needed to prepare the calibration standards, and the background nutrients in the low nutrient seawater need to be accurately quantified. However, many labs have no capability to measure low

background nutrients in the low nutrient seawaters. Seawater nutrient consensus reference material for total dissolved nitrogen from the International GO-SHIP community is available at <http://yyy.rsmas.miami.edu/groups/biogeochem/CRM.html>.

2.3.3 The Effect of Dynamic Environments on Sensor Data

DN measurements can be challenging for two reasons: DNs are non-conservative² variables, and dynamic coastal regions create rapid horizontal and vertical water mass changes. Tidal and meteorological events can create substantial steps in the DN time series. Other variations are induced by such things as seasonal stratification, upwelling, organic loading, increased biological activity (blooms), air-sea exchange, river inputs, spawning aggregations, fish kills, (indeed, all biological activities), sediment-water exchange, groundwater seepage, and springs.

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 acknowledged as substantial if real, and identified as potentially questionable in the absence of causal forces.

2.3.4 Sensor Deployment Considerations and Hardware Limitations

DN 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. They may be lowered from a ship, deployed aboard autonomous surface or submerged vehicles, or installed on moored or drifting buoys. The typical constraints of oceanographic data collection apply—including cost, power, data transmission, bio-fouling, vandalism, and electronics in a marine environment. Examples of these deployment options are shown in figs. 2-2 and 2-3.

Mobile platforms are available in a variety of configurations and require different real-time DN 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 2-4 and 2-5 provide examples of mobile platforms.

Data derived from sensors on moving platforms are limited due to response time of the sensor, i.e., the time it takes for a technology to respond to a step change in the environment or to multiple forces. For example, a nutrient sensor might respond to a change in nutrient concentration, as well as to changes in temperature, salinity, pressure, and other chemical conditions in the water column. Light can also cause interference on optical instruments. Data from a glider or profiling CTD (conductivity/temperature/depth) system on a moving platform will be affected by dynamic errors that, in most cases, have to be corrected in post-processing. These limitations occur in most sensor technology.

^{2c}Conservative constituents are physical, chemical, or biological properties of sea water that are not altered by external or internal processes which may either create or destroy the amount or concentration of such constituents or properties in a given volume of water” (Neumann and Pierson 1966). 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.

Spatial and temporal resolution require a clear understanding of sensor response time, sample rate of the instrument (and in some cases the average period per measurement, if one exists), and the vehicle speed. The response time will often limit the realized resolution of an instrument, and accuracy may be limited relative to the nutrient gradients through which the vehicle is traveling. For example, a sensor with a response time of 60 seconds, sampling at 1 Hz and moving through the water at 25 knots will not yield accurate map conditions. Generally speaking, dynamic errors in moving platform data complicate QA/QC actions for real-time data. Operators must understand the magnitude of these errors before setting QA/QC limits on data.



Figure 2-2. (L) shows a Sea-Bird Scientific SUNA V2 (Submersible Ultraviolet Nitrate Analyzer) mounted on a fixed structure on the Mississippi River at Baton Rouge, where the instrument cage is lowered and raised. (R) shows a NexSens buoy supporting a Sea-Bird Scientific SUNA nitrate sensor and WET Labs Cycle Phosphate sensor (in addition to a YSI EXO multi-parameter sonde measuring algal pigments, turbidity, and dissolved organic matter). (Photos courtesy of Brian Pellerin/USGS)



Figure 2-3. A cage for a boat deployment in the Bay Delta with several instruments (fluorometers, nitrate sensors, phosphate sensors, etc.). (Photo courtesy of Brian Pellerin/USGS)

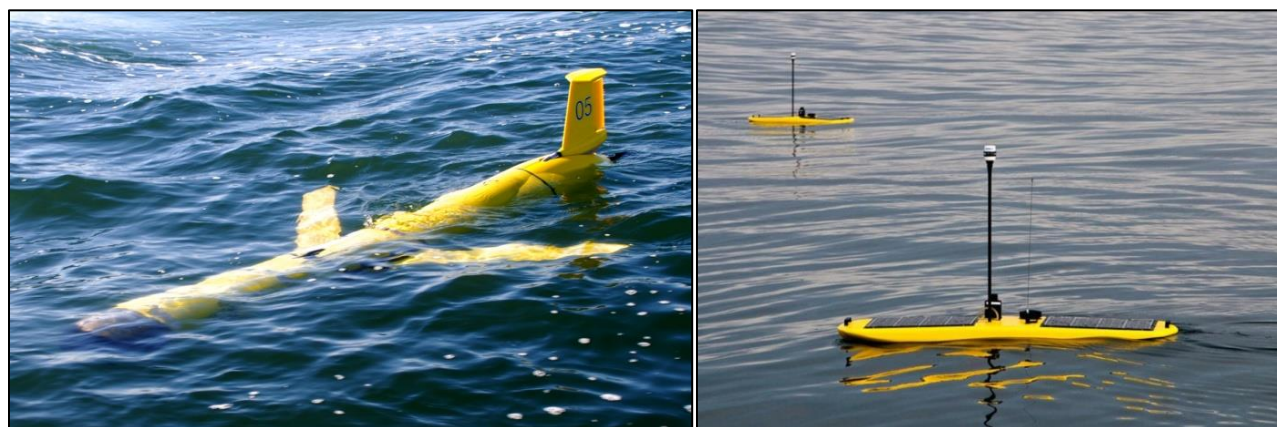


Figure 2-4. WebbGlider Profiler 3-D (L) (photo courtesy of Dr. Grace Saba) and Liquid Robotics Wave Glider Mobile Surface (R) (Photo courtesy of Liquid Robotics).



Figure 2-5. WET Labs AMP C100 In-Situ Profiler. (Photo courtesy of WET Labs)

Fixed, In-Situ Vertical Profilers

Fixed vertical DN 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 section 3.3.1) either remain unchanged or are conducted along the vertical ‘z’ axis, as well as along a time series of observations.

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 DN 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-D Profiler Vessels

Gliders, floats, and powered AUVs can provide DN 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 3.2 and 3.3 can be applied with little modification.

Instrumentation

DN instrumentation can be constructed as a single function device, such as Satlantic’s ISUS (In-Situ Ultraviolet Spectrophotometer) nitrate sensor but can also be housed and commingled with additional sensors to form a multi-parameter package, such as the Sea-Bird Scientific LOBO (Land/Ocean

Biogeochemical Observatory). To make the most meaningful DN observations, operators often co-locate a wide variety of additional sensors such as pressure, temperature, salinity/conductivity, and chlorophyll A.

To make DN observations, operators employ a variety of sensors. Listed below are descriptions of several types of sensors that generate data that could be subjected to the tests described herein. The list is not comprehensive, and operators must determine if these tests apply to their particular DN sensor.

- Nitrate sensors: Modern instruments use ion-specific electrodes or UV absorption techniques, and some apply temperature/salinity compensation to compute nitrate concentration.
- Phosphate sensors: These devices still require the use of wet chemistry.

Table 2-3 provides examples of manufacturers and sensors that are typically used to observe dissolved nutrients, and fig. 2-6 shows several sensors listed in table 2-3. Some manufacturers have changed names, and some sensors are not currently marketed; however, data from these devices may still be generated, and they are included here as valid representatives of the technology.

As with most sensors, the effects of bio-fouling must be considered (fig. 2-7). Bio-fouling varies seasonally and geographically and can often be the limiting factor in determining the deployment duration. DN sensors using optical or ion-specific electrodes have surfaces that must remain free of contamination, or they will drift as growth accumulates. DN sensors that draw in a water sample for chemical analysis must filter the input sample to avoid clogging, and the filter itself must remain free of growth.

Table 2-3. Commonly used sensors for DN observations.

Manufacturer/Sensor	Variables Measured	Measuring Principle
Green Eyes LLC NuLAB, Eco LAB	Nitrate, Phosphate, Silicate, Ammonia	Reagent colorimetric, fluorescence or optical beam attenuation
Hach Nitratax	Nitrate	UV absorption
ProPS-UV	Nitrate, Nitrite	Hyperspectral UV absorption
Satlantic ISUS*	Nitrate	UV absorption
S::CAN Spectrolyzer	Nitrate and others	UV-Vis spectrometry
Sea-Bird Scientific Hydro Cycle PO4	Phosphate	Reagent colorimetric
Sea-Bird Scientific SUNA V2	Nitrate	UV spectroscopy
Subchem APNA (Autonomous Profiling Nutrient Analyzer)	Multi-nutrient	Reagent spectroscopy and fluorometry
SubChem FIN	Nitrate, Nitrite	Reagent spectroscopy and fluorometry
SYSTEA WIZ (Water In-situ Analyzer)	Nitrate, Nitrite, Phosphate, Ammonia, Silicates, Iron, others	Reagent colorimetric
YSI NitraVis	Nitrate	UV-VIS absorbance spectrometry
* No longer manufactured.		



Figure 2-6. Commonly used DN sensors. (Photos courtesy of Corey Koch/WET Labs, Pompeo Moscetta/SYSTEA, and Vince Kelly/Green Eyes LLC)



Figure 2-7. These Sea-Bird Scientific Cycle PO4 phosphate sensors have accumulated an external bio-fouling coating during deployment (top). A Sea-Bird Scientific SUNA nitrate sensor uses a rotating, motorized brush to keep the optical lenses free of bio-fouling. (Photos courtesy of Corey Koch/WET Labs)

The following sections describe the sensor technologies that are most often used, with a brief note about typical observations and associated issues with nitrate sensors. Figure 2-8 shows the time series of nitrate

observations obtained with Satlantic ISUS (now Sea-Bird Scientific) sensors at six locations in south Florida. One problem in the maintenance routines provided by the manufacturer occurs during the 48 hours (sometimes longer or shorter) after the ISUS is cleaned. The problem is particularly visible in figs. 2E and 2F. The ISUS concentrations spike, then exponentially drop over time while the air bubble is worked out of the system.

Field calibration of the ISUS can unpredictably and abruptly change the nitrate concentrations (figs. 2-8A-F). Satlantic recommends updating the instrument calibrations in the field; however, the small volume of the cuvette and the unpredictable nature of field conditions have led to problems. The small volume of the cuvette used is subject to contamination by water containing particles and cells dripping off the bulkhead. Under the current protocol, the probe tip is cleaned with isopropanol, then Type I DIW (de-ionized water). If the DIW test is not within the instrument specifications ($\pm 2 \mu\text{M}$), then a new calibration is applied using fresh Type I DIW. This calibration is done in the field under conditions that are less than ideal and where temperature differences between calibrations and stations may cause large changes in the baseline nitrate concentrations. It may be better to clean the instrument in the field but delay the update to the calibrations until the instrument is in the laboratory under more tightly controlled conditions.

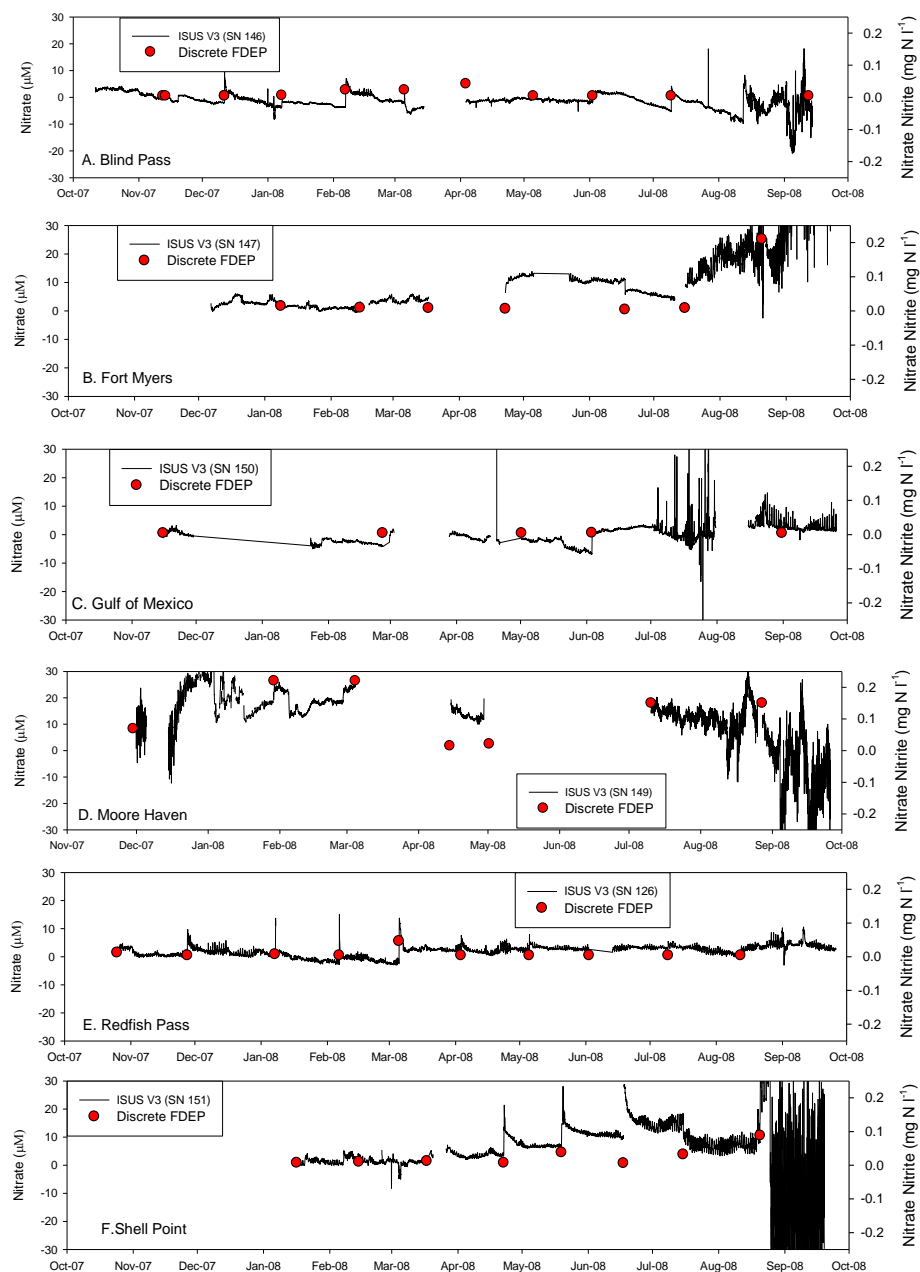


Figure 2-8A-F. Time-series of nitrate concentrations at instrument depth determined optically by the ISUS and standard method chemical assays of total nitrates (nitrate plus nitrite). Burst optical data were collected hourly and data was binned to 10 seconds average calls of nitrate concentration at a sampling rate of 1 Hz. (Photo courtesy of Dr. Eric Milbrandt/Sanibel-Captiva Conservation Foundation)

Such steps in a time series during a calibration, sensor swap, or cleaning provide valuable information for future service intervals, and (if caused by bio-fouling) can be highly dependent on both the site and season. Correcting a data shift like this is extremely difficult, so servicing schedules and the technology used should be carefully considered. Constant improvements in anti-fouling measures and sensor technology stability are being made. Operators should investigate which technology best suits their application, the field service budget, and data quality goals.

Figures 2-8A-F also show increased noise levels toward the end of the record. Additional co-located sensors might help to explain the cause, which could be optical interference by high levels of dissolved organic matter. Test 9, the multi-variate test described herein, is designed with this specific application in mind.

While outside the scope of the real-time tests described in this manual, QA is critical to data quality. Sensors require attention to proper QA measures both before and after the deployment. Operators must follow the manufacturer's recommendations for factory calibration schedules and proper sensor maintenance. Often, operators take field samples during deployment, recovery, or service to validate the performance of an in-situ sensor. As illustrated in figure 2-8, this is a risky time period for ensuring quality sensor data, often due to initial stabilization, sensor/environment disturbance, or high fouling near the end. If resources permit, it is recommended that samples be obtained mid-deployment without disturbing the sensor.

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 bounds 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 bounds. 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.

Sensor redundancy is key to obtaining measurements and ensuring that uncertainties can be assigned to those measurements. DN measurements are not independent, being sensitive primarily to local concentration. Hence, comparing two adjacent instruments can assist in evaluation of data quality, as well as provide two (or more) independent estimates of a variable of interest. Variation in the estimated values can be useful in uncertainty calculations.

2.4 Applications of Dissolved Nutrients Data

Real-time observations of DN are important for a wide variety of applications, including:

- Water quality
 - Monitoring for adherence to regulations
 - Monitoring stormwater runoff and wastewater discharge
 - Monitoring fish farm effluent
 - Making load estimates
 - Establishing nutrient criteria
 - Evaluating nutrient management strategies and technologies

- Ocean biogeochemistry research, e.g., harmful algal blooms prediction models
- Ocean productivity, e.g., fisheries studies
- Freshwater nutrient cycling research
- Agricultural best practices research

Other applications utilizing post-processed data do not require real-time QC but benefit from it through early detection of DN sensors' issues. Some examples of observatories that may benefit from standardized real-time QC testing include:

- Florida Atlantic University Harbor Branch Indian River Lagoon Observatory, <http://fau.loboviz.com/>
- Sanibel-Captiva Conservation Foundation River, Estuary and Coastal Observing Network (RECON), <http://recon.sccf.org/sites>

3.0 Quality Control

In order to conduct real-time QC on DN observations, the first pre-requisite is to understand the science and context within which the measurements are being conducted. DN 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. It is also important to note that advances in DN sensor technology have eliminated many of the problems encountered in older devices.

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, in the absence of reference data points such as water samples collected nearby, drift often cannot be detected or corrected. Drift correction for DN sensors during post-processing is difficult even with a post-calibration in hand because drift in DN 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 the set of flags and associated descriptions proposed by the International Oceanographic Data and Information Exchange (IODE) and adopted by the Intergovernmental Oceanographic Commission (IOC) in 2013. Operators may incorporate additional flags for inclusion in metadata records. For example, a DN 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. The exception to the rule occurs for test 6 spike check, where the most recent point must be flagged as “2 Not Evaluated” until the next point arrives, and the spike check can be performed.

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 Test Hierarchy

This section outlines the eleven real-time QC tests that are required or recommended for selected DN sensors. Tests are listed in order of increasing complexity, and generally, decreasing utility and are divided into three groups. The tests in group 1 are required for all DN 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. Table 3-2 shows the test hierarchy.

Table 3-2. QC Tests in order of implementation

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

Some effort will be needed to select the best thresholds, which are determined at the local level and may require multiple iterations of trial and error 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. Such flexibility is needed to support the U.S. IOOS effort, since the number of tests conducted and the justification for not applying some tests are useful for evaluating an operator's skill levels.

3.3 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 DN 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 DN_n , preceded by a value at DN_{n-1} , and so on backwards in time. They were developed from input by authors and reviewers of this manual, as well as from QARTOD workshops (QARTOD 2003-2009). The focus is primarily on the real-time QC of observation DN_n , DN_{n-1} , and DN_{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 clever and efficient coding, which are left to the programmers.

3.3.1 Applications of QC Tests to Stationary DN 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. For additional information regarding flags, see U.S. IOOS (2017) posted on the U.S. IOOS QARTOD website.

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	Codable Instructions
Fail=4	Data have not arrived as expected.	$NOW - TIM_STMP > TIM_INC$
Suspect=3	N/A	N/A
Pass=1	Applies for test pass condition.	N/A
Test Exception: None.		
Test specifications to be established locally by operator.		
Example: TIM_INC= 1 hour		

Test 2) Syntax Test (Required)

Check to ensure that the message is structured properly.

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.

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.	REC_CHAR ≠ NCHAR
Suspect =3	Data record can be parsed.	REC_CHAR ≠ NCHAR
Pass=1	Expected data record received; absence of parity errors.	N/A

Test Exception: None.

Test specifications to be established locally by operator.

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.

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 (DN_SENSOR_MIN, DN_SENSOR_MAX) are acceptable. Additionally, the operator can select a smaller span (DN_USER_MIN, DN_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.	$DN_n < DN_SENSOR_MIN$, or $DN_n > DN_SENSOR_MAX$
Suspect=3	Reported value is outside of user-selected span.	$DN_n < DN_USER_MIN$, or $DN_n > DN_USER_MAX$
Pass=1	Applies for test pass condition.	N/A

Test Exception: None.

Test specifications to be established locally by operator.

Examples: DN_SENSOR_MAX = (limited by the character output field, for example)
 DN_SENSOR_MIN =
 DN_USER_MAX =
 DN_USER_MIN =

Test 5) Climatology Test (Strongly Recommended)

Test that data point falls within seasonal expectations.

This test is a variation on the gross range check, where the gross range DN_Season_MAX and DN_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 DN, no fail flag is identified for this test.	N/A
Suspect=3	Reported value is outside of user-identified climatology window.	$DN_n < DN_Season_MIN$ or $DN_n > DN_Season_MAX$
Pass=1	Applies for test pass condition.	N/A

Test Exception: None.

Test specifications to be established locally by operator: A seasonal matrix of DN_{max} and DN_{min} values at all TIM_TST intervals.

Examples: DN_SPRING_MIN =, DN_SPRING_MAX =

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 DN value at point $n-1$ (DN_{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 operator-selected thresholds, THRESHLD_LOW and THRESHLD_HIGH. Adjacent data points (DN_{n-2} and DN_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.	$ DN_{n-1} - SPK_REF > THRESHLD_HIGH$
Suspect=3	Low spike threshold exceeded.	$ DN_{n-1} - SPK_REF > THRESHLD_LOW$ $ DN_{n-1} - SPK_REF < THRESHLD_HIGH$
Pass=1	Applies for test pass condition.	N/A

Test Exception: None.

Test specifications to be established locally by operator.

Examples: THRESHLD_LOW =, THRESHLD_HIGH =

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. DN 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.

- **Example 1:** The rate of change between DN_{n-1} and DN_n must be less than three standard deviations ($3*SD$). The SD of the DN 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.
- **Example 2:** The rate of change between DN_{n-1} and DN_n must be less than $1\text{mg/L} + 2SD$.

Flags	Condition	Codable Instructions
Fail=4	Because of the dynamic nature of DN, no fail flag is identified for this test.	N/A
Suspect=3	The rate of change exceeds the selected threshold.	$ DN_n - DN_{n-1} > N_DEV * SD$
Pass=1	Applies for test pass condition.	N/A

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

Test specifications to be established locally by operator.

Example: $N_DEV = 3$, $TIM_DEV = 25$

Test 8) Flat Line Test (Strongly Recommended)

Invariate DN value.		
<p>When some sensors and/or data collection platforms fail, the result can be a continuously repeated observation of the same value. This test compares the present observation (DN_n) to a number (REP_CNT_FAIL or REP_CNT_SUSPECT) of previous observations. DN_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.</p>		
Flags	Condition	Codable Instructions
Fail=4	When the five most recent observations are equal, DN_n is flagged fail.	$DN_n \neq 0$ AND For $i=1, \text{REP_CNT_FAIL}$ $DN_n - DN_{n-i} < \text{EPS}$
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, DN_n is flagged suspect.	For $i=1, \text{REP_CNT_SUSPECT}$ $DN_n - DN_{n-i} < \text{EPS}$
Pass=1	Applies for test pass condition.	N/A
<p>Test Exception: Sensor failure introduces the possibility of repeated zero values. However, in oligotrophic waters, nutrient levels may be below the detection limit of DN sensors, and repeated zero values may be accurate. Operators must carefully choose how to flag data under these conditions.</p>		
<p>Test specifications to be established locally by operator. Examples: REP_CNT_FAIL = 5, REP_CNT_SUSPECT= 3</p>		

Test 9) Multi-Variate Test (Suggested)

Comparison to other variables.		
<p>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 DN manual.</p> <p>In this simple example, it is a pair of rate of change tests as described in test 7. The DN rate of change test is conducted with a more restrictive threshold (N_DN_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 DN and variable two is indeterminate. If the rate of change test on the second variable <i>fails</i> to exceed a threshold (e.g., an anomalous step is found in DN and is lacking in temperature), then the DN_n value is flagged.</p>		
Flags	Condition	Codable Instructions
Fail=4	Because of the dynamic nature of DN, no fail flag is identified for this test.	N/A
Suspect=3	DN _n fails the DN rate of change and the second variable does not exceed the rate of change.	$ DN_n - DN_{n-1} > N_DN_DEV * SD_DN$ AND $ TEMP_n - TEMP_{n-1} < N_TEMP_DEV * SD_T$
Pass=1	N/A	N/A
Test Exception: None.		
Test specifications to be established locally by operator.		
Examples: N_DN_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, dissolved oxygen, 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 pass a high rate of change DN 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.

The dissolved nutrients committee 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 DN 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.	N/A

Test Exception: None.

Test specifications to be established locally by operator.

Examples: TST_TIM = 12 hours
MIN_VAR_WARN=, MIN_VAR_FAIL=

Test 11) Neighbor Test (Suggested)**Comparison to nearby DN 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 DN 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 DN 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 test – comparison to other variables* where the second variable is the second DN 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 (DN1) are compared to a second site (DN2). The standard deviation for each site (SD1, SD2) is calculated over the period (TIM_DEV) and multiplied as appropriate (N_DN1_DEV for site DN1) 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 DN, no fail flag is identified for this test.	N/A
Suspect=3	DN _n fails the DN rate of change and the second DN sensor does not exceed the rate of change.	$ DN1_n - DN1_{n-1} > N_DN1_DEV * SD1$ AND $ DN2_n - DN2_{n-1} < N_DN2_DEV * SD2$
Pass=1	N/A	N/A

Test Exception: None.

Test specifications to be established locally by operator.

Examples: N_DN1_DEV = 2, N_DN2_DEV=2, TIM_DEV = 25 hours

3.3.2 Applications of QC Tests to DN 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 earlier in section 3.3 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) 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	No change
		Fixed Vertical	
		Mobile	
		3-D	
2) Syntax Test (Required) 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	No change
		Fixed Vertical	
		Mobile	
		3-D	
3) Location Test (Required) 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	No change
		Fixed Vertical	
		Mobile	
		3-D	
4) 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 (DN_SENSOR_MIN, DN_SENSOR_MAX) are acceptable. Additionally, the operator can select a smaller span (DN_USER_MIN, DN_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	No change
		Fixed Vertical	
		Mobile	
		3-D	

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

Test	Condition	Platform	Codable Instructions
5) Climatology Test (Strongly Recommended) This test is a variation on the gross range check, where the gross range DN_Season_MAX and DN_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
6) Spike Test (Strongly Recommended) This check is for single value spikes, specifically the DN value at point n-1 (DN_{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 operator-selected thresholds above or below adjacent data points, THRESHLD_LOW and THRESHLD_HIGH. Adjacent data points (DN_{n-2} and DN_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

Test	Condition	Platform	Codable Instructions
7) Rate of Change Test (Strongly Recommended) This test inspects the time series for a time rate of change that exceeds a threshold value identified by the operator. DN 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. <ul style="list-style-type: none"> • Example 1: The rate of change between DN_{n-1} and DN_n must be less than three standard deviations ($3*SD$). The SD of the DN 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. • Example 2: The rate of change between DN_{n-1} and DN_n must be less than $1\text{mg/L} + 2SD$. 	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) When some sensors and/or data collection platforms fail, the result can be a continuously repeated observation of exactly the same value. This test compares the present observation (DN_n) to a number (REP_CNT_FAIL or $REP_CNT_SUSPECT$) of previous observations. DN_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.	Invariant DN 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) 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. In the simplest case, it is a pair of rate of change tests as described in test 7. The DN rate of change test is conducted with a more restrictive threshold (N_DN_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 DN and variable two is indeterminate. If the rate of change test on the second variable <i>fails</i> to exceed a threshold (e.g., an anomalous step is found in DN and is lacking in temperature), then the DN 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) A DN 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) The check has the potential to be the most useful test when a nearby second sensor is determined to have a similar response. This test is the same as test 9) <i>multi-variate check – comparison to other variables</i> where the second variable is the second DN 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 DN sensors.	Stationary	No change
		Fixed Vertical	Test is conducted along z axis
		Mobile	No change
		3-D	No change

4.0 Summary

The QC tests in this DN manual have been compiled using the guidance provided by QARTOD workshops (QARTOD 2003-2009) and from operators with extensive experience. Wherever possible, redundant tests have been merged. These tests are designed to support a range of DN sensors and operator capabilities. Some well-established programs with the highest standards have implemented very rigorous QC processes. Others, with different requirements, may utilize sensors with data streams that cannot support as many QC checks—all have value when used prudently. It is the responsibility of the users to understand and appropriately utilize data of varying quality, and operators must provide support by documenting and publishing their QC processes. A balance must be struck between the time-sensitive needs of real-time observing systems and the degree of rigor that has been applied to non-real-time systems by operators with decades of QC experience.

The eleven data QC tests identified in this manual apply to DN observations from a variety of sensor types and platforms that may be used in U.S. IOOS. Several existing programs, such as the USGS National Real-Time Water Quality program, have already developed QC tests that are similar to the U.S. IOOS QARTOD tests in this manual. The QARTOD dissolved nutrients committee's objective is for the QC tests of these programs to comply with U.S. IOOS QARTOD requirements and recommendations without being overly prescriptive, by providing meaningful guidance and thresholds that everyone can accomplish within a National framework. The individual tests are described and include codable instructions, output conditions, example thresholds, and exceptions (if any).

Selection of the proper thresholds is critical to a successful QC effort. Thresholds can be based on historical knowledge or statistics derived from more recently acquired data and should not be determined arbitrarily. This manual provides some guidance for selecting thresholds based on input from various operators, but also notes that operators need the subject-matter expertise in selecting the proper thresholds to maximize the value of their QC effort. Because long-term data for DN variables are relatively scarce, it is expected that refinement of thresholds and exceptions will occur over time globally as well as becoming more specific to regional databases.

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

Future QARTOD manuals will address standard QC test 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 test procedures may even take place within the sensor package. Significant components of metadata will

reside in the sensor and be transmitted either on demand or automatically along with the data stream. Users may also reference metadata through Uniform Resource Locators to simplify the identification of which QC steps have been applied to data. However, QARTOD QC test procedures in this manual address only real-time, in-situ observations made by sensors on fixed or mobile platforms. The tests do not include post-processing, which is not conducted in real time but may be useful for ecosystem-based management, or delayed-mode, which is required for climate studies.

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 carefully following them 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.

Each QC manual is a dynamic document and is posted on the QARTOD website (<https://ioos.noaa.gov/project/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 existing 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 DN 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.

5.0 References

- Bushnell, M., Presentation at QARTOD III: November 2005. Scripps Institution of Oceanography, La Jolla, California.
- Joint Committee for Guides in Metrology (JCGM), 2012. International Vocabulary of Metrology: Basic and General Concepts and Associated Terms. 3rd Edition.
- Martini, K.I., Walsh, I.D., Branham, C.W., 2017. Measuring Nitrate in Puget Sound Using Optical Sensors. Sea Technology, October 2017, pp. 10-13.
- Neumann, Gerhard and Pierson, W. J., 1966. Principles of Physical Oceanography, Prentice Hall, p. 154.
- Paris. Intergovernmental Oceanographic Commission of UNESCO, 2013. Ocean Data Standards, Vol.3: Recommendation for a Quality Flag Scheme for the Exchange of Oceanographic and Marine Meteorological Data. (IOC Manuals and Guides, 54, Vol. 3.) 12 pp. (English) (IOC/2013/MG/54-3) http://www.nodc.noaa.gov/oceanacidification/support/MG54_3.pdf
- Pellerin, B.A., Bergamaschi, B.A., Downing, B.D., Saraceno, J.F., Garrett, J.A., and Olsen, L.D., 2013, Optical techniques for the determination of nitrate in environmental waters: Guidelines for instrument selection, operation, deployment, maintenance, quality assurance, and data reporting: U.S. Geological Survey Techniques and Methods 1–D5, p. 37. <http://pubs.usgs.gov/tm/01/d5/pdf/tm1d5.pdf>
- QARTOD I-V Reports 2003-2009: <https://ioos.noaa.gov/project/qartod/>
- U.S. IOOS Office, November 2010. A Blueprint for Full Capability, Version 1.0, 254 pp. https://www.ioos.noaa.gov/wp-content/uploads/2015/09/us_ioos_blueprint_ver1.pdf
- U.S. Integrated Ocean Observing System, 2017. Manual for the Use of Real-Time Oceanographic Data Quality Control Flags Version 1.1. 41 pp. <https://doi.org/10.7289/V5B56GZJ>
-

Additional References to Related Documents:

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/resourcepool-mainmenu-7>.

<http://www.oceandatastandards.org> is the higher-level page (see menu to the right for subpages). Argo Quality Control Manual can be found at:
<http://www.argodatamgt.org/content/download/341/2650/file/argo-quality-control-manual-V2.7.pdf>

National Data Buoy Center (NDBC) Technical Document 09-02, Handbook of Automated Data Quality Control Checks and Procedures, August 2009. National Data Buoy Center, Stennis Space Center, Mississippi 39529-6000.

National Oceanographic Partnership Program (NOPP) January 2006. The First U.S. Integrated Ocean Observing System (IOOS) Development Plan – A report of the national Ocean Research Leadership Council and the Interagency Committee on Ocean Science and Resource Management Integration. The National Office for Integrated and Sustained Ocean Observations. Ocean US Publication No. 9.

Wagner, R.J., Boulger, R.W., Jr., Oblinger, C.J., and Smith, B.A., 2006, Guidelines and standard procedures for continuous water-quality monitors—Station operation, record computation, and data reporting: U.S. Geological Survey Techniques and Methods 1–D3, 51 p. <http://pubs.water.usgs.gov/tm1d3>

Villagarcía, M. 2005. Calibration of Biogeochemical Data from Nitrate Sensors. Instituto Canario de Ciencias Marinas (ICCU) Las Palmas, Spain.

Supporting Documents Found on the QARTOD Website:

<https://ioos.noaa.gov/ioos-in-action/dissolved-nutrients/>

NDBC Handbook of Automated Data Quality Control

Argo Quality Control Manual, V 2.7 3 January 2012

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)

UHM Stormwater Monitoring System Servicing Checklist

Optical Techniques for the Determination of Nitrate in Environmental Waters: Guidelines for Instrument Selection, Operation, Deployment, Maintenance, Quality Assurance, and Data Reporting

Appendix A Quality Assurance

A major pre-requisite for establishing data quality for dissolved nutrient 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 such as NIST through a calibration performed by the manufacturer and/or the operator. If the calibration is conducted by the manufacturer, the operator must also conduct some form of an acceptable calibration 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.

Wet chemical sensors also have defined reagent stability and storage considerations that should be accounted for. For example, if reagents are beyond a "best-by date" the data are likely suspect. If reagents drift (NH₄ or NO₃ reagent degradation), that drift must be known or monitored.

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.

Gas-segmented continuous flow auto-analyzers are the standard instrument/method for routine nutrient measurement onboard the ship and in the shore-based laboratory. The most important check for the DN

sensor's performance is taking samples from DN sensor deployment sites, analyzing them using a nutrient auto-analyzer in the lab, and comparing the results with those from the DN sensors.

For nitrate sensors using the cadmium reduction method, the reduction efficiency of the cadmium coil/column should be tested before and after the sensor deployment. Preparation of the cadmium column should follow the method established in the literature. A threshold (e.g., 95%) should be defined for an acceptable cadmium reduction efficiency before deployments.

Users often take samples during deployment, recovery, or service. These times are risky for ensuring quality sensor data—often due to initial stabilization, sensor/environment disturbance, or high fouling near the end of the deployment. At least one sample should be obtained mid-deployment without disturbing the sensor.

A.3 Bio-fouling and Corrosion Prevention Strategies

Bio-fouling is a frequent cause of DN 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 DN 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 lens on optical DN 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 (using care in the vicinity of optics and other sensitive components).
- Carefully maintain and clean filters.
- Obtain mid-deployment validation field samples.

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., conductivity and 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 DN 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	DN sensors are swapped and/or serviced at sufficiently regular intervals so as to avoid data steps (unexpected offsets) upon swap/service. Pre- and post-deployment calibration checks are conducted on each sensor.
Better Process	The good processes are employed, plus pre- and post-deployment calibration checks are conducted using alternative sensors to confirm performance.
Best Process	The better processes are employed, 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 DN 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 - <https://ioos.noaa.gov/project/qartod/>
- ACT - <http://www.act-us.info/>
- 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 - <https://www.nodc.noaa.gov/woce/>
- 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 each (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.)

Appendix B Dissolved Nutrients Manual Committee and Reviewers

Dissolved Nutrients Manual Committee and Reviewers, Version 1.1	
Name	Organization
Mark Bushnell	U.S. IOOS
Brett Johnston	USGS
Vince Kelly	Green Eyes LLC
Matthias Lankhorst	University of California San Diego
Ana Lara-Lopez	University of Tasmania
Robert Maxfield	Environmental Protection Agency
Margaret McManus	University of Hawaii
Jim Potemra	University of Hawaii
Brian Pellerin	USGS
Cassie Schwanger	CSIRO Oceans and Atmosphere

QARTOD Board of Advisors, Version 1.1	
Name	Organization
Kathleen Bailey, Project Manager	U.S. IOOS
Julie Bosch	NOAA/National Centers for Environmental Information
Eugene Burger	NOAA/Pacific Marine Environmental Laboratory
Matt Howard	GCOOS/Texas A&M University
Bob Jensen	U.S. Army Corps of Engineers
Shannon McArthur	NOAA/National Data Buoy Center
Chris Paternostro	NOS/Center for Operational Oceanographic Products and Services
Mario Tamburri	University of Maryland Center for Environmental Science / Chesapeake Biological Laboratory
Julie Thomas, BOA Chair	SCCOOS/Scripps Institution of Oceanography/Coastal Data Information Program

U.S. IOOS Regional Associations, Version 1.1	
Name	Organization
Josie Quintrell	IOOS Association
Clarissa Anderson	SCCOOS
Debra Hernandez	SECOORA
Melissa Iwamoto	PacIOOS
Barbara Kirkpatrick	GCOOS
Gerhard Kuska	MARACOOS
Molly McCammon	AOOS
Julio Morell	CariCOOS
Ru Morrison	NERACOOS
Jan Newton	NANOOS
Kelli Paige	GLOS
Henry Ruhl	CeNCOOS

Dissolved Nutrients Manual Team, Version 1.0

Manual Committee and Reviewers

Name	Organization
Mark Bushnell, Lead Editor	CoastalObsTechServices LLC - NOS/CO-OPS
Emilio Mayorga, Editor	NANOOS/University of Washington
Daniel Schar, Editor	Alliance for Coastal Technology/University of Hawaii
Helen Worthington, Editor	REMSA - NOS/CO-OPS
Eric Breuer	NOAA/CO-OPS
Bryan Downing	USGS
Karen Grissom	NOAA/National Data Buoy Center
Nichole Halsey	Sea-Bird Scientific
Dennis Hanisak	Florida Atlantic University
Nathan Holcomb	NOAA/CO-OPS
Carol Janzen	Sea-Bird Electronics
Corey Koch	WET Labs
Brian Lapointe	Florida Atlantic University
Brian Melzian	Environmental Protection Agency
Eric Milbrandt	Sanibel/Captiva Conservation Foundation
Brian Pellerin	USGS
Jeff Scudder	University of South Florida
Denice Shaw	Environmental Protection Agency
Rik Wanninkhof	NOAA
Jia-Zhong Zhang	NOAA/Atlantic Oceanographic and Meteorological Laboratory

DMAC Committee, Version 1.0

Name	Organization
Rob Bochenek	AOOS/CeNCOOS Axiom Consulting & Design
Eric Bridger	NERACOOS/Gulf of Marine Research Institute
Jorge Capella	CariCOOS/University of Puerto Rico
Jeremy Cothran	SECOORA/University of South Carolina
Matt Howard	GCOOS/Texas A&M University
Eoin Howlett	MARACOOS/Applied Science Associates, Inc.
Kelly Knee	MARACOOS/Applied Science Associates, Inc.
Emilio Mayorga	NANOOS/University of Washington
Jennifer Patterson	CeNCOOS/Monterey Bay Aquarium Research Institute
Jim Potemra	PacIOOS/University of Hawaii
Rob Ragsdale	U.S. IOOS
Tad Slawecki	GLOS/LimnoTech
Derrick Snowden	U.S. IOOS
Shane StClair	AOOS/Axiom Consulting & Design
Vembu Subramanian	SECOORA/University of South Florida
Darren Wright	SCCOOS/Scripps Institution of Oceanography/CDIP

QARTOD Board of Advisors, Version 1.0	
Name	Organization
Joe Swaykos, Chair	NOAA/National Data Buoy Center
Kathy Bailey	U.S. IOOS
Julie Bosch	NOAA/National Centers for Environmental Information
Eugene Burger	NOAA/Pacific Marine Environmental Laboratory
Janet Fredericks	Woods Hole Oceanographic Institution
Matt Howard	GCOOS
Bob Jensen	USACE
Chris Paternostro	NOS/CO-OPS
Julie Thomas	University of California San Diego/Scripps Institution of Oceanography

U.S. IOOS Regional Associations, Version 1.0	
Name	Organization
Josie Quintrell	U.S. IOOS Association
David Anderson	CeNCOOS
Debra Hernandez	SECOORA
Barbara Kirkpatrick	GCOOS
Gerhard Kuska	MARACOOS
Molly McCammon	AOOS
Julio Morell	CariCOOS
Ru Morrison	NERACOOS
Jan Newton	NANOOS
Chris Ostrander	PacIOOS
Kelli Paige	GLOS
Julie Thomas	SCCOOS