Manual for
Real-Time Quality Control of Ocean Optics Data

A Guide to Quality Control and Quality Assurance for Coastal and Ocean Optics Observations

Version 1.1
September 2017

Document Validation

U.S. IOOS Program Office Validation

September 5, 2017

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

QARTOD Project Manager Validation

September 5, 2017

Kathleen Bailey, U.S. IOOS Project Manager — Date

QARTOD Board of Advisors Validation

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September 5, 2017

Julianna O. Thomas, QARTOD Board of Advisors Chair — Date

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Revision History

Date	Revision Description	Notes
June 2015	Original Document Published	
September 2017	Revise cover to reflect correct version and publication date. Revise names and dates on *Document Validation* page (page ii). Update Table of Contents (pages iii-iv). Update *Revision History* (page v). Update email address in *Request to Manual Users* (page vi). Update *Acknowledgements* to include manual update version 1.1 team members (page vii). Update *Acronyms and Abbreviations* (pages viii). Add interoperable, sensor, variable to *Definitions of Selected Terms* and update definitions of CDOM and FDOM (page ix). Update section 1.0 to reflect QARTOD publications completed since original ocean optics manual; added digital object identifiers for each manual (page 1-2). Update sections 2.2.1, 2.2.3, and 2.3 to clarify and enhance existing content. Update section 3.3.1 to reflect more recent references and to make minor editing adjustments to Tests 4, 5, 6, 7, 8, 9, 10, 11, 12, and 13. Update QARTOD Board of Advisor and Regional Association Director listings in appendix B (B-1 through B-3). Perform general editing for consistency in style and terminology; update Web links.	Version 1.1

Endorsement Disclaimer

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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. We request that manual users notify us of their 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

We thank those who provided thoughtful comments and suggestions for the update of this manual, listed in appendix B on page B-1. We are grateful to our entire Ocean Optics team (appendix B, page B-4), especially to those who served on the Ocean Optics Manual Committee and provided content and suggestions for the initial draft, as well as all who reviewed each draft and provided valuable feedback for version 1.0 and 1.1.

Special thanks go to Dr. Steve Ackleson (U.S. Naval Research Laboratory), Dr. Emmanuel Boss (University of Maine), and the Ocean Optics Protocol Workshop Committee for the invitation and travel support to that workshop, which served as the kick-off meeting for this manual. The satellite ground-truth data collection experience and expertise provided by Emmanuel Boss was especially helpful, and we thank him for his enthusiastic support of this project. We also appreciate the support and encouragement provided by Dr. Ana Lara-Lopez (University of Tasmania/Integrated Marine Observing System).

Additional thanks go to outgoing QARTOD Technical Coordinator Ray Toll for his outstanding leadership in developing the U.S. IOOS QARTOD program and the initial six manuals.

Acronyms and Abbreviations

AOOS	Alaska Ocean Observing System
AOP	Apparent Optical Properties
CariCOOS	Caribbean Coastal Ocean Observing System
CDOM	Colored Dissolved Organic Matter
CeNCOOS	Central and Northern California Ocean Observing System
CO-OPS	Center for Operational Oceanographic Products and Services
FDOM	Fluorescent Dissolve Organic Matter
GCOOS	Gulf of Mexico Coastal Ocean Observing System
GLOS	Great Lakes Observing System
GOOS	Global Ocean Observing System
IOOS	Integrated Ocean Observing System
IOP	Inherent Optical Properties
ISO	International Organization for Standardization
LAGER	Local Automated Glider Editing Routine
MARACOOS	Mid-Atlantic Regional Association Coastal Ocean Observing System
NANOOS	Northwest Association of Networked Ocean Observing Systems
NDBC	National Data Buoy Center
NERACOOS	Northeastern Regional Association of Coastal Ocean Observing Systems
NERRS	National Estuarine Research Reserve System
NIST	National Institute of Standards and Technology
nm	Nanometers
NOAA	National Oceanic and Atmospheric Administration
NOS	National Ocean Service
OO	Optics Observation
PacIOOS	Pacific Islands Ocean Observing System
PAR	Photosynthetically Available Radiation
QARTOD	Quality-Assurance/Quality Control of Real-Time Oceanographic Data
QA	Quality Assurance
QC	Quality Control
SCCOOS	Southern California Coastal Ocean Observing System
SD	Standard Deviation
SECOORA	Southeast Coastal Ocean Observing Regional Association
UNESCO	United Nations Organization for Education, Science, and Culture

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.

Apparent Optical Properties (AOP)	AOPs are properties that (1) depend both on the medium (the IOPs) and on the geometric (directional) structure of the radiance distribution, and (2) display enough regular features and stability to be useful descriptors of a water body (Mobley 2010).
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.
Colored Dissolved Organic Matter (CDOM) and Fluorescent Dissolved Organic Matter (FDOM)	CDOM is the optically measurable component of the dissolved organic matter in water. DOM includes a broad range of organic molecules of various sizes and composition that are released by all living and dead plants and animals. Measuring the fraction of DOM that absorbs light at specific wavelengths and subsequently releases it at longer wavelengths (e.g., fluorescence) is diagnostic of DOM type and amount. Studies have often used the excitation and emission at 370 nanometers (nm) and 460 nm, respectively, to quantify the fluorescent fraction of colored DOM (referred to as CDOM fluorescence or FDOM) (Bergamaschi et al. 2009).
Data Record	A data record is one or more messages that form a coherent, logical, and complete observation.
Inherent Optical Properties (IOP)	IOP is any optical property of the water that does not depend on the illumination condition of the sun. An intrinsic property of the water.
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	A message is 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.
Photosynthetically available radiation (PAR)	PAR is the amount of light available for photosynthesis in the 400–700-nanometer wavelength range, e.g., mol Quanta m^-2 day^-1.
Quality Assurance (QA)	QA involves processes that are employed with hardware to support the generation of high quality data. (section 2.0 and appendix A)
Quality Control (QC)	QC involves follow-on steps that support the delivery of high quality data and requires both automation and human intervention. (section 3.0)
Real Time	Real time means data are delivered without delay for immediate use; time series extends only backwards in time, where the next data point is not available; and there may be delays ranging from a few seconds to a few hours or even days, depending upon the variable.
Thresholds	Thresholds are limits that are defined by the operator.
Turbidity	Turbidity is the reduction of transparency of a liquid caused by the presence of undissolved matter (ISO 1999). Turbidity instruments generally measure scattered light from a beam at a broad angle centered around 90°.
Sensor	A sensor is a device that detects or measures a physical property and provides the result without delay. A sensor is also an element of a measuring system that is directly affected by a phenomenon, body, or substance carrying a quantity to be measured. (JCGM 2012)
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 ocean optics data manual is the seventh in a series of guidance documents that address QC of real-time data of selected core variables and is also the seventh 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: 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, 2015. Manual for Real-Time Quality Control of Dissolved Nutrients Data: A Guide to Quality Control and Quality Assurance of Coastal and Dissolved Nutrients Observations. 56 pp. https://doi.org/10.7289/V52N50GF

9) U.S. Integrated Ocean Observing System, 2016. Manual for Real-Time Quality Control of High Frequency Radar Surface Currents Data: 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: 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: 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, 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/10.25923/v9p8-ft24

This manual is a living document that reflects the state-of-the-art QC testing procedures for optics 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, and Technologies

The following sections describe the purpose of this manual, the constraints that operators may encounter when performing QC of ocean optics 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 optics community at large for the real-time QC of optics 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.

Optics observations covered by these test procedures are collected in oceans and lakes in real time or near-real time. These tests draw from existing expertise in programs such as the National Oceanic and Atmospheric Administration (NOAA) National Estuarine Research Reserve System (NERRS), and the NOAA-funded California Current Ecosystem research project.

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

Table 2-1. Platforms included and excluded in this manual.

Platforms Included	Platforms Excluded
Coastal and offshore buoys Gliders and profiling floats Oil platforms Coastal-Marine Automated Network (C-MAN) stations 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 an automated software program. Operators maintain a code repository (https://github.com/ioos/qartod) where others may find or post examples of code in use. Although certain tests are recommended, thresholds can vary among operators. The tests described here are designed to support a range of optics sensors and operator capabilities. Some well-established programs with the highest standards, such as the U.S. Naval Research Laboratory's Local Automated Glider Editing Routine: Optics, version 1 (LAGER Optics v1.0) system effort (Hou et al. 2010), 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 quality assurance (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. Although 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 Constraints

Measurements for several U.S. IOOS core variables of interest utilize optical techniques. 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, variables describing the optical properties of water measured below and immediately above the surface are identified; these variables include both IOP and AOP and are sufficiently common in nature to have similar QC checks. Table 2-2 shows the variables to be addressed in this ocean optics QC manual, as well as those that are excluded. Observations of the excluded variables may utilize optical techniques, but the application of that optical data is highly specialized and diverse, so excluded variables will be addressed in a future QC manual.

Table 2-2. Included and excluded variables addressed in this manual.

Variables Included	Variables Excluded
In-water radiance and irradiance Above-water radiance and irradiance Beam attenuation Turbidity PAR Chlorophyll CDOM FDOM Backscattering and volume scattering	Phytoplankton species Zooplankton abundance Total suspended matter Particulate matter concentration

2.2.1 Data Processing Methodology

The type of sensor system used to collect optics data and the system used to process and transmit the optics measurements determine which QC algorithms might be used. In-situ systems with sufficient on-board processing power within the sensor may substantially process the data to produce derived products, such as the particle size from fluctuations in the backscattering coefficient (Briggs et al. 2013). Many 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). It is critical for the operator to fully understand the effects of the on-board data processing employed by the manufacturer. If ample transmission capability is available, expanded data streams may be transmitted ashore, processed, 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.

2.2.2 Traceability to Accepted Standards

To ensure that optics 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.

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 accepted 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 radiance and irradiance (http://www.nist.gov/calibrations/spectroradiometric.cfm) may be required when conducting calibration checks on optics sensors. Where NIST standards are not available, an active research effort generally exists among operators, data users, and manufacturers regarding the use of primary and secondary standards for instrument calibration and calibration checks. Examples for fluorometry can be found in Earp et al. (2011), and for measurements such as absorption and attenuation, the current reference standard is the cleanest water available. Such ultrapure water can be created by a high-quality purification system that uses ultraviolet radiation, filters, and deionization to produce water with a high resistivity of 18.3 mega-Ohms.

2.2.3 Sensor Deployment Considerations and Hardware Limitations

Optics sensors can be deployed in several ways. Many sensors are fixed to platforms that observe the optical characteristics of the water below or above the surface. 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.

Instrumentation

Optics instruments can be constructed as a single-function device, such as a beam transmissometer, but are often housed with multiple optical sensors and commingled with additional sensors to form a multi-parameter package. Instrument capabilities range from highly accurate devices providing very specific optical characteristics in absolute units, to simple devices providing only relative changes in observations during the deployment time series. Optical observations are challenging because of the need to measure natural signals that can span over many orders of magnitude. Further, fundamental measurements of a specific target volume's characteristics often vary with wavelength, angle of incidence, particle shape, rotational dynamics, orientation, absorption and reflectance of suspended or dissolved constituents, wave focusing, and many other factors. Even extremely clear, particle-free water can exhibit optical turbulence caused by variations in temperature and salinity that affect the index of refraction (Hou et al. 2012).

To make meaningful observations, operators employ a wide 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 optical sensor.

- Beam transmissometer – a device used to measure the optical attenuation over a known path length using known spectral emitter and detector characteristics.
- Radiance meter – a device to measure energy incident upon a detector with known directional characteristics, often providing a spectral distribution.
- Irradiance meter – a device measuring incident radiance over a full hemisphere or sphere.
- Scattering particle size and distribution sensor – a sensor used to measure near-forward scattering from which the particle size distribution is derived.
- Turbidity sensor – any device used to observe "the reduction of transparency of a liquid caused by the presence of undissolved matter" (ISO 1999). A variety of optical techniques are employed to provide a measure of turbidity, including backscattering, scattering at right angles, and forward scattering.
- Backscattering sensor – a sensor used to measure the optical return signal in the backwards hemisphere at a specific centroid angle or angles using a known wavelength.

Table 2-3 provides examples of manufacturers and sensors that are typically used to observe optical variables in oceans and lakes. Figure 2-1 shows photographs of several sensors listed in table 2-3. Figures 2-2 through 2-6 show examples of sensors using different deployment scenarios.

Table 2-3. Frequently used sensors for optics observations in oceans and lakes.

Manufacturer/Sensor	Ocean Optic Variables Measured
ASD FieldSpec FR	Spectral radiance
AQUATEC 210TY	Turbidity (volume scattering) (15°-150°) FTU units
In-Situ Troll 9500	Turbidity (ISO 7027 method) (90°) NTU units
McVan Analite NEP395	Turbidity (infrared, 90° optics, ISO 7027)
WET Labs ECO-BB-SB	Backscattering at 124°
YSI 6136	Turbidity (backscattering)
WET Labs C-Star Transmissometer	Beam attenuation
Satlantic OCR-507	Spectral irradiance in air and water
WET Labs ECO FLNTUS	Chlorophyll and turbidity
WET Labs ECO FLBBrtd	Chlorophyll and backscattering
WET Labs ECO Triplet-w	Chlorophyll, CDOM, backscattering
WET Labs ECO Puck	Chlorophyll, CDOM, backscattering
WET Labs ac-S	Hyper-spectral absorption and beam attenuation
Biospherical Inst. QSP-2150	PAR
Biospherical Inst. QSP-2200	PAR
Sequoia Scientific LISST	Particle size distribution, volume concentration, and beam attenuation

Figure 2-1. Examples of widely used ocean optics sensors.

Figure 2-2. Shows the shipboard deployment of an ASD FieldSpec FR (right) and Spectralon plaque (left) used for observations of above-water radiance. The pistol grip and lens limit the field of view to one degree. (Photo courtesy of Dr. Ana Dogliotti/CONICET/UBA)

Figure 2-3. This WET Labs WQM (left) employs optical sensors to measure chlorophyll fluorescence, turbidity, and backscattering data (in addition to other variables). Bio-fouling measures include a wiper, bronze structural components, and PVC and copper tape. The WQM is deployed through a well in the Chesapeake Bay Interpretive Buoy System (CBIBS) buoy (right), allowing easy service from a small boat. (Photos courtesy of Mark Bushnell)

Figure 2-4. This Sequoia Scientific LISST 100X (left) was deployed during Deepwater Horizon water quality studies to observe particle size distribution and volume concentration. While on station, a short time series of surface data was collected using a boom mounted on the side of the RV Ocean Veritas (right). A second short time series was collected while underway to the next station. (Photos courtesy of Mark Bushnell)

Figure 2-5. Various optical instruments (including multi-spectral downwelling irradiance and upwelling radiance) are installed and deployed aboard this Satlantic Profiler II, which can free-fall through the water column or be lowered using a tether. (Photo courtesy of Todd Yeadon/Sea-Bird Scientific)

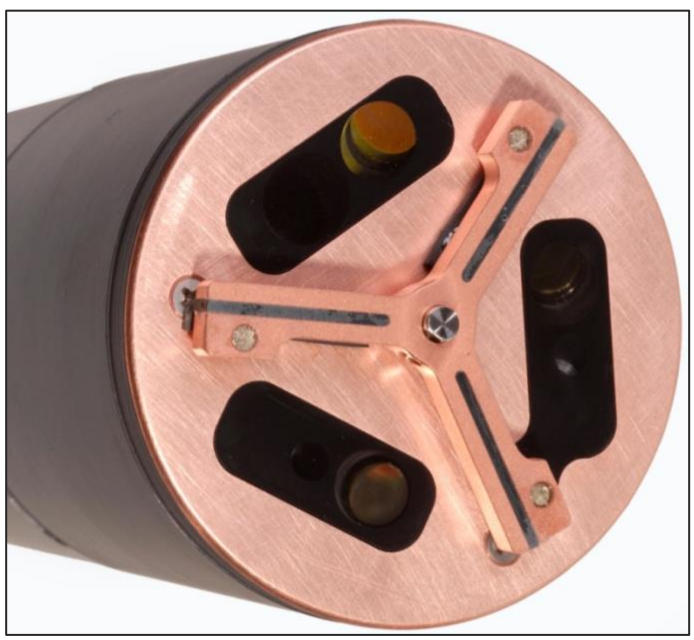

Figure 2-6. This WET Labs ECO Triplet-w is designed to measure chlorophyll, CDOM fluorescence, and red backscattering (turbidity). It uses both copper components and rotating wipers to reduce the effects of bio-fouling contamination. (Photo courtesy of Todd Yeadon/Sea-Bird Scientific)

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 field and factory calibration schedules and proper sensor maintenance.

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

Sensor redundancy is key to obtaining measurements and ensuring that uncertainties can be assigned to those measurements. Optical 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 parameter of interest. Variation in the estimated values can be useful in uncertainty calculations.

2.3 Applications of Optics Data

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

- Water quality
- Ocean biogeochemistry
- Ocean productivity
- Phytoplankton dynamics and physiology
- Sediment dynamics
- Department of Defense applications
- Satellite ground truth

Other applications utilizing post-processed data do not require real-time QC but benefit from it through early detection of optics sensors' issues.

3.0 Quality Control

The real-time QC of optics observations can be extremely challenging. Events such as upwelling or coastal runoff associated with storms can affect ocean optical characteristics and must be considered when determining acceptable data thresholds. Human involvement is therefore important to ensure that solid scientific principles are applied to data evaluation to ensure that good data are not discarded and bad data are not distributed (e.g., selection of appropriate thresholds and examination of data flagged as questionable).

To conduct real-time QC on optics observations, the first pre-requisite is to understand the science and context within which the measurements are being conducted. For example, and as was discussed in section 2.2.3, sensors can be deployed in a number of ways. Each deployment method imposes the need for specific QC methods, with different interpretations of 'real time.'

This manual focuses specifically on real-time data. For example, for real-time QC, gradual calibration changes or system responses (sensor drift) cannot be detected or corrected. Drift correction for optics measurements during post-processing is difficult even if a valid post-recovery calibration can be obtained. Drift is often caused by bio-fouling or changes in the transmission characteristics of lenses, emitter and detector performance, etc. and affects different systems in different ways (e.g., a sensor's response will be affected by the added mass of bio-fouling). Another example is the ability of some data providers to backfill data gaps. In both examples, the observations are not considered to be real time for purposes of QC checks. (However, in some sophisticated 24/7 QC operations, real-time dissemination may be switched from one sensor to another based on real-time QC flags.)

3.1 QC Flags

Data are evaluated using QC tests, and the results of those tests are recorded by inserting 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. Additional flags may be incorporated to provide more detailed information to assist with troubleshooting. For example, an observation may fail the min/max test and be flagged as having failed. If the data failed the min/max by exceeding the upper limit, a "failed high" flag may indicate that the values were higher than the expected range. Such detailed flags primarily support maintenance efforts and are presently beyond U.S. IOOS requirements for QC of real-time data. However, all flags should be identified and defined in the metadata.

Further post-processing of the data may yield different conclusions from those reached during initial assessments. Flags set in real time should not be changed, ensuring that historical documentation is preserved. Results from post-processing should generate another set of flags corresponding to a revised version of the data.

Observations are time ordered, and the most recent observation is n_0, preceded by a value at n_{-1}, and so on backwards in time. The focus of the real-time QC is primarily on observations n_0, n_{-1}, and n_{-2}.

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

Flag	Description
Pass=1	Data have passed critical real-time QC 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 thirteen real-time QC tests that are required, recommended, or suggested for optics measurements. Operators should also consider that some of these tests can be carried out within the instrument, where thresholds can be defined in configuration files. Although more tests may imply a more robust QC effort, there are many reasons operators could use to justify not conducting some tests. In those cases, operators need only to document reasons these tests do not apply to their observations. 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. Tests are listed in table 3-2 and are divided into three groups: those that are required, strongly recommended, or suggested. However, for some critical, real-time applications with high risk operations, it may be advisable to invoke all groups.

Table 3-2. QC Tests in order of implementation and hierarchy.

Group 1 *Required*	Test 1	Timing/Gap Test
	Test 2	Syntax Test
	Test 3	Location Test
	Test 4	Gross Range Test
	Test 5	Decreasing Radiance, Irradiance, and PAR Test
Group 2 *Strongly Recommended*	Test 6	Photic Zone Limit for Radiance, Irradiance, and PAR Test
	Test 7	Climatology Test
	Test 8	Spike Test
	Test 9	Rate of Change Test
	Test 10	Flat Line Test
Group 3 *Suggested*	Test 11	Multi-Variate Test
	Test 12	Attenuated Signal Test
	Test 13	Neighbor Test

3.3 QC Test Descriptions

A variety of tests can be performed on the sensor measurements to evaluate data quality. Testing the timely arrival and integrity of the data transmission itself is a first step. If the data are corrupted during transmission, further testing may be irrelevant. The checks defined in these thirteen tests evaluate data through various comparisons to other data and to the expected conditions in the given environment. The tests listed in this section presume a time-ordered series of observations and denote the most recent observation as previously described. They were developed from input by authors and reviewers of this manual, as well as from QARTOD workshops (QARTOD 2003-2009).

Some effort will be needed to select the best thresholds, which are determined at the operator level and may require multiple iterations of trial and error before final selections are made. A successful QC effort is highly dependent upon selection of the proper thresholds, which should not be determined arbitrarily but can be based on historical knowledge or statistics derived from recently acquired data. Threshold selection can vary widely based on location, historical knowledge, and seasonal variations. Although this manual provides some guidance for selecting thresholds based on input from various operators, it is assumed that operators have the necessary expertise as well as a sincere interest in selecting the proper thresholds to maximize the value of their QC effort. Operators should openly provide thresholds as metadata for user support. This shared information will help U.S. IOOS to document standardized thresholds that will be included in future releases of this manual.

3.3.1 Applications of QC Tests to Optics Sensors

In the following test descriptions, a generic variable denoted by "OO" (optics observation) is used to represent any of the variables addressed by this manual. These thirteen tests require operators to select a variety of 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 latest data point. When this series of data points reveals that the entire group fails, the most recent data point is flagged, but the previous flags are not changed. This action supports the view that historical flags are generally not altered. The first example is in Test 10, the Flat Line Test, where this scenario will become clearer. The exception to this rule occurs in the Test 8, the Spike Test, where the most recent point must be flagged as "2 Not Evaluated" until the next point arrives and the spike check can be performed. For additional information regarding flags, see U.S. IOOS (2017) posted on the U.S. IOOS QARTOD website.

Some optics parameters with properties sensitive to particulate concentrations, such as chlorophyll fluorescence and backscattering, are more difficult to assess than other hydrographic properties such as temperature or salinity. This is a known limitation for QC of optics data. Operators will likely have to set the thresholds to generous values for some tests, such as the Spike Test and Rate of Change Test, to account for this limitation.

Test 1) Timing/Gap Test (Required)

Check for arrival of data.		
Test determines that the most recent data point has been measured and received within the expected time window (TIM_INC) and has the correct time stamp (TIM_STMP). Note: For those systems that do not update at regular intervals, a large value for TIM_INC can be assigned. The gap check is not a solution for all timing errors. Data could be measured or received 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.	If NOW – TIM_STMP > TIM_INC, flag = 4
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 the operator. **Example:** TIM_INC= 1 hour		

Test 2) Syntax Test (Required)

Check to ensure that the message is structured properly.		
Test checks that received data message (full message) contains the proper structure without any indicators of flawed transmission such as parity errors. Possible tests are: a) the expected number of characters (NCHAR) for fixed-length messages equals the number of characters received (REC_CHAR), or b) passes a standard parity bit check, cyclic redundancy check, etc. Many such syntax tests exist, and the operator should select the best criteria for one or more syntax tests. 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. A syntax check is performed only at the message level and not within the message content. In cases where a data record requires multiple messages, this check can be performed at the message level but is not used to check message content.		
Flags	**Condition**	**Codable Instructions**
Fail=4	Data sentence cannot be parsed to provide a valid observation.	If REC_CHAR ≠ NCHAR, flag = 4
Suspect =3	N/A	N/A
Pass=1	Expected data sentence received; absence of parity errors.	N/A
Test Exception: None.		
Test specifications to be established locally by the 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 (SENSOR_MIN, SENSOR_MAX) are acceptable. Additionally, the operator can select a smaller span (OP_MIN, OP_MAX) based upon local knowledge or a desire to draw attention to extreme values. A good example of an OP_MIN value is the true dark current; often the one provided by the manufacturer is not exact. Ideally, the dark current is determined with the sensor on the platform upon which it will be deployed, powered, etc. **NOTE:** Operators may choose to flag as suspect values that exceed the calibration span but not the hardware limits (e.g., a value that sensor is not capable of producing).		
Flags	**Condition**	**Codable Instructions**
Fail=4	Reported value is outside of sensor span.	If OO_n < SENSOR_MIN, or OO_n > SENSOR_MAX, flag = 4
Suspect=3	Reported value is outside of operator-selected span.	If OO_n < OP_MIN, or OO_n > OP_MAX, flag = 3
Pass=1	Applies for test pass condition.	N/A
Test Exception: None.		
Test specifications to be established locally by the operator. **Examples:** SENSOR_MAX = 5 mg/m^3 OP_MAX = 1 mg/m^3 SENSOR_MIN = 0 mg/m^3 OP_MIN = 0 mg/m^3		

Test 5) Decreasing Radiance, Irradiance, and PAR Test (Required)

Test that subsurface radiance, irradiance, and PAR decrease with increasing depth.

This test can be used to check for decreasing radiance, irradiance, and PAR as the sensor is lowered and raised in the water column. Generally, these variables are expected to decrease with depth. Sources of noise, such as wave-focusing near the surface, instrument tilt toward/away from the sun, or changes in cloud cover can cause increases (variations in cloud cover can be corrected with a reference unit).

In the codable instructions below, a profile of downwelling irradiance, Ed(z), is inspected to ensure there is no increase with depth. A time series of depth and irradiance is presumed during a downcast, but there is no guarantee of a monotonically increasing depth series with each step z_{n-1} to z_n. There are no operator-selected thresholds for this test.

Flags	Condition	Codable Instructions
Fail=4	Reported value shows an increase in irradiance with increasing depth.	If $z_n > z_{n-1}$ and $Ed_n > Ed_{n-1}$, flag = 4
Suspect=3	No suspect flag is identified for this test.	N/A
Pass=1	Applies for test pass condition.	N/A

Test Exception: The test can be applied only to profiles of radiance, irradiance, and PAR.

Test specifications to be established locally by operator: None.

Test 6) Photic Zone Limit for Radiance, Irradiance, and PAR Test (Strongly Recommended)

Test that radiance, irradiance, and PAR are nearly zero below the photic zone.

This test can be used to check for near-zero observations of upwelling/downwelling radiance, irradiance, and PAR as the sensor is lowered and raised below the photic zone. While fluorescence and Raman scattering may increase these observations, these effects are generally quite small (except in the red, where it might be the only source of light).

In the codable instructions below, upwelling irradiance Eu(z) is inspected to ensure it is less than the operator-selected minimum value (Eu_{min}) at depths below the operator-selected photic zone depth (z_{photic}). When selecting Eu_{min}, operators should consider sensor dark current and system noise. A common definition of z_{photic} is the depth at which irradiance (350–700 nm) is reduced to 1% of the surface irradiance (Jerlov 1968).

Flags	Condition	Codable Instructions
Fail=4	Reported value below z_{photic} is greater than the operator-selected minimum value Eu_{min}.	If $z_n > z_{photic-1}$ and $Eu_n > Eu_{min}$, flag = 4
Suspect=3	No suspect flag is identified for this test.	N/A
Pass=1	Applies for test pass condition.	N/A

Test Exception: This test may not apply where high chlorophyll fluorescence increases energy at approximately 683 nm.
(see http://www.opticsinfobase.org/ao/abstract.cfm?uri=ao-18-8-1161)

Test specifications to be established locally by operator.
Example: z_{photic} = 80 m, Eu_{min}= $5x^{10-3}$ µW cm^{-2} nm^{-1}

Test 7) 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 (SEASON_MIN_FAIL, SEASON_MAX_FAIL, SEASON_MIN_SUSPECT, and SEASON_MAX_SUSPECT) is adjusted monthly, seasonally, or at some other operator-selected time period (TIM_TST). Expertise of the local operator is required to determine reasonable seasonal averages. Locations with existing multi-year time series permit more refined identification of appropriate thresholds. Examples: • An above-surface downwelling radiance SEASON_MAX that can be determined by latitude and time of day assuming the clearest possible atmosphere. • A larger SEASON_MAX may be used for a coastal turbidity measurement where increased melt water stream runoff is expected in the spring. • Guidance for the selection of seasonal chlorophyll ranges can be obtained at https://oceancolor.gsfc.nasa.gov/cgi/l3.		
Flags	**Condition**	**Codable Instructions**
Fail=4	Reported value is outside the seasonal span defined by the failure thresholds.	If OO_n < SEASON_MIN_FAIL, or OO_n > SEASON_MAX_FAIL, flag = 4
Suspect=3	Reported value is outside the seasonal span defined by the suspect thresholds.	If OO_n < SEASON_MIN_SUSPECT or OO_n > SEASON_MAX_SUSPECT, flag = 3
Pass=1	Applies for test pass condition.	N/A
Test Exception: The test may not be feasible where observations lack a seasonal signal, or where insufficient data exists to establish a signal.		
Test specifications to be established locally by operator: A seasonal matrix of OO_{max} and OO_{min} values at all TIM_TST intervals. **Examples:** SPRING_MIN = 1.0 mg/m^3, SPRING_MAX = 7.0 mg/m^3		

Test 8) Spike Test (Strongly Recommended)

Data point *n*-1 exceeds a selected threshold relative to adjacent data points.

Optical data can spike due to the presence of aggregates in the water (e.g., Briggs et al. 2011, Deep Sea Research), so the high-spike threshold must be carefully set. However, frequent data spikes may indicate a faulty sensor. While spikes are expected with particulate sensors, they are not expected for dissolved sensors, such as a CDOM fluorometer.

This check is for single-value spikes, specifically the value at point n_{-1}. Spikes consisting of more than one data point are difficult to capture, but their onset may be flagged by the rate of change test.

Note that instruments with internal averaging that carries over more than one data output report will need a different spike identification methodology than presented here.

The spike test consists of two operator-selected thresholds, THRSHLD_LOW and THRSHLD_HIGH. Adjacent data points (n_{-2} and n_0) are averaged to form a spike reference (SPK_REF). The absolute value of the spike is tested to capture positive and negative spikes. Large spikes are easier to identify as outliers and flag as failures. Smaller spikes may be real and are only flagged suspect. The thresholds may be fixed values or dynamically established (for example, a multiple of the standard deviation over an operator-selected period).

An alternative is a third difference test defined as $Diff_n = OO_{n-3} - 3*OO_{n-2} + 3*OO_{n-1} - OO_n$.

Flags	Condition	Codable Instructions
Fail=4	High spike threshold exceeded.	If $\lvert OO_{n-1}$ - SPK_REF$\rvert$ > THRSHLD_HIGH, flag = 4
Suspect=3	Low spike threshold exceeded.	If $\lvert OO_{n-1}$ - SPK_REF$\rvert$ > THRSHLD_LOW and $\lvert OO_{n-1}$ - SPK_REF$\rvert$ $\leq$ THRSHLD_HIGH, flag=3
Pass=1	Applies for test pass condition.	N/A

Test Exception: None.

Test specifications to be established locally by the operator.
Examples: THRSHLD_LOW = 3 mg/m^3, THRSHLD_HIGH = 6 mg/m^3

Test 9) 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. OO values can change substantially over short periods in some locations, 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. Test implementation can be challenging. Upon failure, it is unknown which point is bad. Further, upon failing a data point, it remains to be determined how the next iteration can be handled. The following suggest two ways to select the thresholds:

- The rate of change between OO_{n-1} and OO_n must be less than three standard deviations (3*SD). The SD of the OO time series is computed over an operator-selected period representing fluctuations of interest. The local operator determines both the number of SDs (N_DEV) and the period over which the SDs are calculated (TIM_DEV).
- The rate of change between OO_{n-1} and OO_n must be less than a fixed value +2SD.

Flags	Condition	Codable Instructions
Fail=4	No fail flag is identified for this test.	N/A
Suspect=3	The rate of change exceeds the selected threshold.	If $\lvert OO_n - OO_{n-1} \rvert$ > N_DEV*SD, flag = 3
Pass=1	Applies for test pass condition.	N/A

Test Exception: The test may not be feasible where insufficient data exists to establish a rate of change threshold.

Test specifications to be established locally by operator.
Examples: TIM_DEV = 24 hours, N_DEV = 3

Test 10) Flat Line Test (Strongly Recommended)

Invariant value.

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 *n* to a number (REP_CNT_FAIL or REP_CNT_SUSPECT) of previous observations. Observation *n* is flagged if it has the same value as previous observations within a tolerance value, EPS, to allow for numerical round-off error. Note that historical flags are not changed.

Flags	Condition	Codable Instructions
Fail=4	When the five most recent observations are equal, OO_n is flagged fail.	For i = 1,REP_CNT_FAIL, If OO_n - OO_{n-i} < EPS, flag = 4
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, OO_n is flagged suspect.	For i = 1,REP_CNT_SUSPECT, If OO_n - OO_{n-i} < EPS, flag = 3
Pass=1	Applies for test pass condition.	N/A

Test Exception: Some deployments may experience prolonged invariant optics observations.

Test specifications to be established locally by the operator.
Examples: REP_CNT_FAIL = 5, REP_CNT_SUSPECT= 3, EPS = 0.2 mg/m^3

Test 11) Multi-Variate Test (Suggested)

Comparison to other variables.

This is an advanced family of tests, starting with the simpler test described here and anticipating growth toward full co-variance testing in the future. It is doubtful that anyone is conducting tests such as these in real time. As these tests are developed and implemented, they should be documented and standardized in later versions of this manual.

The multi-variate QC test may be especially useful for ocean optics observations, since optical sensors frequently co-vary among themselves (e.g., backscattering and beam attenuation), and often co-vary with other sensors (e.g., temperature and salinity).

This example pairs rate of change tests as described in Test 9. The OO rate of change test is conducted with a more restrictive threshold (N_OOMV_DEV). If this test fails, a second rate of change test operating on a second variable (perhaps another OO variable or temperature) is conducted. The absolute value rate of change should be tested, since the relationship between OO and the second variable may be indeterminate. If the rate of change test on the second variable fails to exceed a threshold (e.g., an anomalous step is found in OO and is lacking in temperature), then the OO_n value is flagged.

Flags	Condition	Codable Instructions
Fail=4	No fail flag is identified for this test.	N/A
Suspect=3	OO_n fails the rate of change and the second variable (T [temperature], for example) does not exceed the rate of change.	If $\lvert OO_n - OO_{n-1} \rvert$ > N_OOMV_DEV*SD_OO AND $\lvert T_n - T_{n-1} \rvert$ < N_T_DEV*SD_T, flag = 3
Pass=1	Applies for test pass condition.	N/A

Test Exception: None.

Test specifications to be established locally by the operator.
Examples: N_OOMV_DEV = 2, N_T_DEV=2, TIM_DEV = 25 hours

NOTE: In a more complex case, more than one secondary rate of change test can be conducted. Salinity, wind speed, or current speed are possible secondary candidates and could be checked for anomalous rate of change values. In this case, a knowledgeable operator may elect to assign a pass flag to a high rate of change 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 QARTOD ocean optics committee recognized the high value in full co-variance testing but also noted the challenges. Such testing remains in the realm of research, but is not yet ready for operational implementation.

Test 12) Attenuated Signal Test (Suggested)

A test for inadequate variation of the time series.

A common sensor failure mode can provide a data series that is nearly but not exactly a flat line (e.g., if an optical emitter or receiver becomes bio-fouled). This test inspects for an 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.	If During TST_TIM, SD < MIN_VAR_FAIL, or During TST_TIM, MAX-MIN < MIN_VAR_FAIL, flag = 4
Suspect=3	Variation fails to meet the minimum threshold MIN_VAR_WARN.	If During TST_TIM, SD < MIN_VAR_WARN, or During TST_TIM, MAX-MIN < MIN_VAR_WARN, flag = 3
Pass=1	Applies for test pass condition.	N/A

Test Exception: None.

Test specifications to be established locally by the operator.

Examples: TST_TIM = 24 hours
MIN_VAR_WARN = 0.4 mg/m^3, MIN_VAR_FAIL = 0.1 mg/m^3

Test 13) Neighbor Test (Suggested)

Comparison to nearby sensors.

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

Ideally, redundant 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.

However, there are few instances where a second sensor is sufficiently proximate to provide a useful QC check. Although optics observations can have large spatial disparity, this test should not be overlooked where it may have application.

This test is the same as Test 11, *Multi-Variate Test – comparison to other variables* where the second variable is the second 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 (OO1) are compared to a second site (OO2). The standard deviation for each site (SD1, SD2) is calculated over the period (TIM_DEV) and multiplied as appropriate (N_OO1_DEV for site OO1) to calculate the rate of change threshold. Note that an operator could also choose to use the same threshold for each site, since the sites are presumed to be similar. A unique and highly valuable version of the neighbor check is the surrogate use of OO forecasts. These 'virtual neighbor' constructs offer a QC check that is also presumed to be similar—again, within operator-selected thresholds.

Flags	Condition	Codable Instructions
Fail=4	No fail flag is identified for this test.	N/A
Suspect=3	$OO1_n$ fails the rate of change and the second sensor $OO2_n$ does not exceed the rate of change.	If $\lvert OO1_n - OO1_{n-1} \rvert$ > N_OO1_DEV*SD1 AND $\lvert OO2_n - OO2_{n-1} \rvert$ < N_OO2_DEV*SD2, flag = 3
Pass=1	Applies for test pass condition.	N/A

Test Exception: There is no adequate neighbor.

Test specifications to be established locally by the operator.
Examples: N_OO1_DEV = 2, N_OO2_DEV = 2, TIM_DEV = 25 hours

4.0 Summary

The QC tests in this ocean optics manual have been compiled using the guidance provided by QARTOD workshops (QARTOD 2003-2009). Test suggestions came from operators with extensive experience. Wherever possible, redundant tests have been merged. The tests described here are designed to support a range of optics 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 thirteen data QC tests identified in this manual apply to optics observations from a variety of sensor types and platforms that may be used in U.S. IOOS. Since several existing programs (such as the LAGER Optics v1.0 system operated by the Oceanography Division of the Naval Research Laboratory) have already developed QC tests that are similar to the tests in this manual, the QARTOD ocean optics committee's objective is for the QC tests of these programs to comply with QARTOD requirements and recommendations. 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 optical 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.

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.

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

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U.S. IOOS QARTOD Project Plan, February 18, 2012. Updated February 2017. https://doi.org/10.7289/V5JQ0Z71

Supporting Ocean Optics Documents:

(https://ioos.noaa.gov/ioos-in-action/oceanic-optics/)

These documents were particularly useful to the committee and reviewers when developing this manual. They do not contain copyright restrictions and are posted on the U.S. IOOS QARTOD website for easy reference.

Report from the COL-NASA Data QA/QC Workshop

Development and testing of Local Automated Glider Editing Routines for Optical Data Quality Control

Ambient Water Quality Criteria for Dissolved Oxygen, Water Clarity and Chlorophyll a for the Chesapeake Bay and Its Tributaries

Data Systems Relevant to JCOMM Activities

Optical Tools for Ocean Monitoring and Research

Supporting Web Links:

http://www.act-us.info/evaluations.php (Various evaluation reports listed under Turbidity and Fluorometer)

http://www.oceanopticsbook.info/view/references/brief_definitions

http://www.sequoiasci.com/library/

http://www.sequoiasci.com/product_category/marine

http://water.usgs.gov/osw/techniques/TSS/ZieglerT.pdf

Appendix A. Quality Assurance

A major pre-requisite for establishing quality control standards for optics measurements is a strong quality assurance program. Remember the mantra that good QC requires good QA, and good QA requires good scientists, engineers, and technicians.

The lists in the following sections suggest ways to ensure QA by using specific procedures and techniques. Operators should also follow instructions provided by the sensor manufacturer.

A.1 Sensor Calibration Considerations

Observations must be traceable to one or more accepted standards through a calibration performed by the manufacturer and/or the operator. If the calibration is conducted by the manufacturer, the operator must also conduct some form of an acceptable calibration check.

NIST provides a wealth of information on standards and calibrations for many variables, including time, temperature, and pressure. Virtually all manufacturers provide calibrations traceable to NIST standards as part of their standard product services.

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 towards corporate conglomeration, those wishing to employ a consensus standard should ensure that the different manufacturers are truly independent.

A known deficiency of some optical sensors is that their dark value (i.e., value provided by instrument when no signal arrives to the detector) depends on the system upon which it is deployed. This deficiency requires operators to measure the dark value prior to deployment—when the instrument is on the frame it will be deployed and powered from. This issue is most important in clear water and/or at the depth where the offset in dark values can be a significant part of the total signal measured. The calibrations for each sensor should be plotted as a function of time, thus developing a history of the sensor. This is an easy way to highlight sensor changes or bad calibrations. Calibration coefficients between sensors/manufactures can then also be compared.

A.2 Sensor Comparison

An effective QA effort continuously strives to ensure that end data products are of high value and to prove they are free of error. Operators should seek out partnering opportunities to inter-compare systems by co-locating differing sensors. Agreement of multiple systems would provide a robust observation, while disagreement may offer a measure of data uncertainty. If possible, operators should retain an alternate sensor or technology from a second vendor 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, and they must be understood in order to properly report results. For those who succeed, the additional sensors provide a highly robust demonstration of capability. Such efforts form the basis of a strong QA/QC effort. Further, it provides the operator with an expanded supply source, permitting less reliance upon a single manufacturer and providing competition that is often required by procurement offices.

A.3 Bio-fouling and Corrosion Prevention Strategies

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

- Use anti-fouling paint with the highest copper content available (up to 75%) when possible (not on aluminum).
- Wrap the body of the sensor with clear packing tape for a small probe or plastic wrap for a large instrument. This keeps the PVC tape from leaving residue on the sensor. Heavy PVC underground cable tape is the best for bad bio-fouling.
- Wrap with copper tape (again, beware of aluminum).
- Coat with zinc oxide (Desitin ointment).
- Remember that growth is sensor, depth, location, and season dependent.
- 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.
- Avoid or isolate dissimilar metals.
- Maintain sacrificial anodes and ensure they are properly installed (good electrical contact).
- Maximize use of non-metallic components.
- Use UV-stabilized components that are not subject to sunlight degradation.
- If bio-fouling has occurred, document this (e.g., photos) and include the information in the metadata such that users are aware of the problem.

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.
- Perform periodic calibration of ready-to-use spares.
- Monitor with redundant sensors whenever possible.
- Take photos of sensor fouling for records.
- Record all actions related to sensors – calibration, cleaning, deployment, etc.
- Monitor battery voltage and watch for unexpected fluctuations.
- Perform serial standard dilutions during calibration to improve sensor characterization for appropriate sensors (e.g., chlorophyll solutions for fluorometric sensors).
- Perform regular (seasonal or greater) co-located, in-situ sampling for cross comparison and characterization. Sensor factory settings are often related to a particular algae standard that may not be representative of the community that is being observed.

When evaluating which instrument to use, consider these factors:

- Selection of a reliable and supportive manufacturer and appropriate model
- Operating range (i.e., some instruments won't operate at a certain temperature, depth or pressure range)
- Resolution/precision required
- Sampling frequency – how fast sensor can take measurements
- Reporting frequency – how often the sensor reports the data
- Response time of the sensor – sensor lag – time response
- Instrument check – visual inspection for defects, bio-fouling, etc.
- Power check – master clock, battery, etc. – variability in these among sensors
- Standardize sensor clock to a reference such as GPS timing
- Capability to reveal a problem with data

When evaluating which specifications must be met:

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

General comments regarding QA procedures:

- A diagram (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.
- Do not make the checklist so detailed that it will not be used.
- 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., temperature).
- Use NIST-traceable instrumentation when conducting calibrations or calibration checks.
- A sensor that maintains an internal file of past calibration constants is very useful since it can be downloaded instead of transcribed manually, introducing human error.
- The calibration constants or deviations from a standard should be plotted over time to determine if the sensor has a drift in one direction or another. A sudden change can indicate a problem with the sensor or the last calibration.

A.5 QA Levels for Best Practices

A wide variety of techniques are used by operators to assure that sensors are properly calibrated and operating within specifications. While all operators must conduct some form of validation, there is no need to force operators to adhere to one single method. A balance exists between available resources, level of proficiency of the operator, and target data reproducibility requirements. 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	Sensors are swapped and/or serviced at sufficient regular intervals. Calibrations checks are conducted before and after deployment.
Better Process	The good process, plus an overlapping operational period during sensor swap-out to demonstrate continuity of observations.
Best Process	The better process, plus follow a well-documented protocol, use an alternative sensor to validate in-situ deployments, and/or employ manufacturer conducted pre- and post-calibrations.

A.6 Additional Sources of QA Information

Optics sensor operators 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 test bed 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. The NOAA Center for Operational Oceanographic Products and Services (CO-OPS) 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://www.ioos.noaa.gov/qartod/
- ACT - http://www.act-us.info/
- CO-OPS - http://tidesandcurrents.noaa.gov/pub.html under the heading Manuals and Standards
- World Ocean Circulation Experiment - https://www.nodc.noaa.gov/woce/
- National Data Buoy Center (NDBC) - http://www.ndbc.noaa.gov/
- Australian Integrated Marine Observing System Bio-Optical Working Group - http://imos.org.au/bwgdocs.html
- Consortium for Ocean Leadership (COL) and the National Aeronautical and Space Administration (NASA) Report - https://www.ioos.noaa.gov/wp-content/uploads/2016/04/data_qc_workshop_final_report2012_08_7.pdf

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

Pre-deployment QA Checklist

- ❐ Read the manual.
- ❐ Establish, use, and submit (with a reference and version #) a documented sensor preparation procedure (protocol); include cleaning sensor according to the manufacturer's procedures.
- ❐ Calibrate sensor against an accepted standard and document (with a reference and version #).
- ❐ Compare the sensor with an identical, calibrated sensor measuring the same thing in the same area (in a calibration lab).
- ❐ View calibration specifications with a critical eye (don't presume the calibration is infallible). Execute detailed review of calibrated data.
- ❐ Check the sensor history for past calibrations, including a plot over time of deviations from the standard for <u>each</u> (this will help identify trends such a progressively poorer performance). Control chart calibrations.
- ❐ Check the sensor history for past repairs, maintenance, and calibration.
- ❐ Consider storing and shipping information before deploying.
- ❐ Heat, cold, vibration, etc.
- ❐ Provide detailed documentation.
- ❐ Record operator/user experiences with this sensor after reading the manual.
- ❐ Search the literature for information on your particular sensor(s) to see what experiences other researchers may have had with the sensor(s).
- ❐ Establish and use a formal pre-deployment checklist.
- ❐ Ensure that technicians are well-trained. Use a visual tracking system for training to identify those technicians who are highly trained and then pair them with inexperienced technicians. Have data quality review chain.

Deployment Checklist

- ❐ Scrape bio-fouling off platform.
- ❐ Verify sensor serial numbers.
- ❐ Deploy and co-locate multiple sensors (attention to interference if too close).
- ❐ Perform visual inspection; take photos if possible (verify position of sensors, connectors, fouling, and cable problems).
- ❐ Verify instrument function at deployment site prior to site departure. Allot sufficient time for temperature equilibration.
- ❐ Monitor sensors for issues (freezing, fouling).
- ❐ Automate processing so you can monitor the initial deployment and confirm the sensor is working while still on-site.
- ❐ Specify date/time for all recorded events. Use GMT or UTC.
- ❐ Check software to ensure that the sensor configuration and calibration coefficients are correct. Also check sampling rates and other timed events, like wiping and time averaging.
- ❐ Visually inspect data stream to ensure reasonable values.
- ❐ Compare up and down casts and/or dual sensors (if available).
- ❐ Note weather conditions and members of field crew.
- ❐ Avoid leaving optical sensors on the deck of the ship without covering them. Most sensors are painted black, and the heat from the sun will degrade the optical components. Cover with a tarp when not being deployed.

Post-deployment Checklist

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

Appendix B. QARTOD Ocean Optics Manual Team

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