Quality Assurance/Quality Control of Real-Time Oceanographic Data

Status and Implementation Efforts

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***Abstract*— The Quality Assurance/Quality Control of Real-Time Oceanographic Data (QARTOD) project was formally adopted in 2012 as a part of the U.S. Integrated Ocean Observing System (IOOS) Data Management and Communication (DMAC) system. A well-established process has resulted in eight manuals that provide specific quality control tests for a variety of U.S. IOOS core variables of interest. Specifically, the manuals address quality control (QC) for observations of dissolved oxygen, currents, waves, water levels, winds, temperature and salinity, ocean optics, and dissolved nutrients. Regional Associations within the U.S. are now working toward implementing these test procedures, which are also being incorporated by international ocean-observing organizations, the private sector, and manufacturers developing sensor improvements.**

The manuals are initially drafted and reviewed by a committee of subject matter experts. The resulting draft is distributed to the U.S. Regional Associations for a second round of reviews, followed by a third review from the wider international community. As such, the manuals represent the best processes desired by those who will implement the tests. An important aspect of the tests is the selection of thresholds and other test criteria by local operators, who are in the best position to understand and determine such limits. The tests are neither overly prescriptive nor overly generic and are designed to support a wide range of sensors and operator capabilities. Tests are identified as required, strongly recommended, or suggested, with test results falling into one of three categories: pass, suspect/of high interest, or fail. Test examples are provided in the manuals, and the instructions are sufficiently explicit for a programmer to use them to write software code for automated QC processes.

The manuals are living documents. They are updated as the QARTOD project evolves and as input is received from operators, data users, and manufacturers. The dissolved oxygen, waves, and currents manuals received updates in 2015.

***Keywords*— QARTOD, data quality control, real-time data**

I. Introduction

Access to oceanographic data in real time is increasingly the norm for several reasons: ingestion into operational meteorological or ocean models, support for safe and secure commerce, enhanced defense, or confirmation of proper operations of a research system. Most data users expect real-time data to receive some form of quality control (QC) before being widely shared.

The first in a series of workshops addressing real-time QC was held in December 2003, hosted by the National Oceanic and Atmospheric Administration's (NOAA's) National Data Buoy Center (NDBC) at the Stennis Space Center in Bay St. Louis, Mississippi. Although the workshop results were comprehensive (and, in retrospect, quite prescient), attendees determined that additional workshops were required to advance the development of real-time QC. The acronym *QARTOD* was coined and the workshop became known as QARTOD I.

NOAA's National Ocean Service/Center for Operational Oceanographic Products and Services (CO-OPS) hosted QARTOD II in Norfolk, Virginia in February 2005 with a focus on the QC of wave and current measurements. QARTOD III was held in November 2005 at the Scripps Institution of Oceanography, La Jolla, California. QARTOD IV was held at the Woods Hole Oceanographic Institution in June 2006, and QARTOD V was co-hosted by NDBC and CO-OPS and held in Atlanta, Georgia in November 2009. These early grassroots QARTOD efforts and their outcomes are well documented by [1] and in the workshop proceedings, which can be found at http://nautilus.baruch.sc.edu/twiki/bin/view.

In April 2012 a project plan was completed and accepted by U.S. IOOS, making QARTOD a formal activity of their Data Management and Communications (DMAC) system. The plan described a management structure as shown in Fig. 1, called for the formation of a Board of Advisors (BOA), and identified the process for the generation of variable-specific QC manuals. This project plan and all subsequent QARTOD documents are posted at http://www.ioos.noaa.gov/qartod.

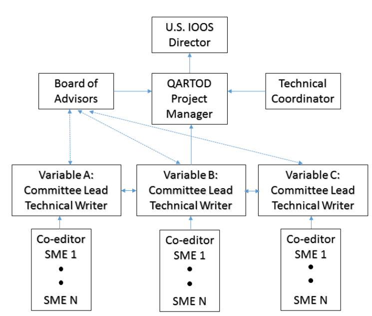

Fig. 1. The adopted management structure for the QARTOD project.

The process for generating QARTOD manuals consists of the following steps:

- A Board of Advisors proposes the next variable to be addressed, and the variable is accepted by US IOOS.
- The Technical Coordinator (TC) establishes a committee of subject matter experts (SMEs).
- SMEs provide input to the TC and technical writer, who produce a draft manual.
- The committee provides the first manual review.
- The document is distributed to the Regional Associations for a second review.
- The document is broadly distributed nationally and internationally for a third review.
- The document is accepted by the IOOS Director and BOA, receives signatures, and is posted to the U.S. IOOS website.
- The posting is publicized via periodicals, newsletters, and social media.

This process has been successfully used to generate manuals for: dissolved oxygen [2], waves [3], currents [4], water levels [5] wind speed and direction [6], temperature and salinity [7], ocean optics [8], and dissolved nutrients. Another manual that identifies a scheme for assigning data quality flags has also been created [9].

For the ocean optics and dissolved nutrients manuals, one or two committee members have been recruited to serve as co-editors to assist the TC and technical writer in drafting the manual.

A key element of the entire review process is the establishment of an adjudication matrix. Every comment or suggested revision received is logged into an Excel spreadsheet, which includes the identification of the source and a response about why the suggested input was or was not incorporated. Most comments and suggested revisions are readily addressed by the TC, but in cases where the response is less obvious, the TC consults with co-editors, SME committee members, and/or the BOA.

A requirement of the resulting manuals is that they are sufficiently detailed to provide instructions to programmers who are writing the software code for implementation of the QC tests. Each manual contains a pseudo-code description of each test, along with examples of the test thresholds. Final selection of the specific test thresholds is made by the operators, who are best situated to understand their unique requirements and regional conditions.

The manuals make a clear distinction between QC and quality assurance (QA). QC is defined as efforts taken to ensure that data provided by the sensor are sufficiently accurate, while QA is a larger task, which includes proper selection of instruments, calibration, deployment, and other activities that cannot be undertaken in real time. QA is equally important and is often discussed in the manual and appendix as a utility to operators; however, detailed QA is beyond the scope of these manuals.

Also important, but beyond the scope of the manuals, are 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 data 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 are key components in establishing the observational error bounds. Operators are strongly encouraged to consider the impact of the QC tests on data uncertainty, as these two components greatly enhance the utility of their data.

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. The tests described are designed to support a range of 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. Data users must understand and appropriately utilize data of varying quality; 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.

Table I shows, as an example, the thirteen tests described in [8]. Operators may not adopt all of these tests, but they should document the tests they implement and explain the reasons for not implementing the others. Such justification can be as simple as “no adequate neighbors” or “multi-variate test capabilities have not yet been developed”. The intent is to identify a few advanced test opportunities without demanding adherence for operators with constrained resources.

TABLE I. THESE ARE THE THIRTEEN TESTS IDENTIFIED FOR OCEAN OPTICS OBSERVATIONS, AND THEIR DESIGNATION AS REQUIRED, STRONGLY RECOMMENDED, OR SUGGESTED.

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

II. DATA QC FLAGS

The results of the tests must accompany the data during dissemination so that data users can see that data quality checks have occurred, as well as the outcome of those checks. Many standard data flagging schemes exist. Reference [10] describes the quality flag code definitions of sixteen widely used oceanographic flagging schemes, as well as the mappings between them. In late 2013, U.S. IOOS QARTOD formally adopted the recent International Oceanographic Data and Information Exchange flagging scheme [11] to replace the earlier flagging structure drafted during the QARTOD grass roots days. The QARTOD flags document referenced in the introduction of this paper [9] is posted at http://www.ioos.noaa.gov/qartod/temperature_salinity/qartod_oceanographic_data_quality_manual.pdf.

III. QARTOD STATUS

The eight existing QC manuals address roughly half of the 26 ocean observing core variables "required to detect and/or predict changes in a maximum number of phenomena of interest to user groups" (http://www.iooc.us/ocean-observations/variables). Table II identifies the variables that now have supporting documents, as well as those that remain.

The QARTOD BOA now recognizes the possibility that all 26 core variables may not presently be candidates for real-time QC processes, and the identification of those remaining is becoming increasingly challenging.

To assist the implementation effort, in June 2015 at the annual DMAC system meeting, the creation of an IOOS DMAC QARTOD Working Group was proposed and subsequently established. The preliminary purpose is:

"This working group will be keeping the pulse of QARTOD implementation efforts for the purpose of coordinated implementation. This working group will provide a forum for feedback/communication between the Regional Associations and program office implementation developers. Representatives from this working group will report to the QARTOD BOA quarterly with status updates, which provide the working group the opportunity to make requests for clarification from the BOA and to raise BOA awareness of implementation challenges."

TABLE II. STATUS OF QARTOD

QARTOD CORE VARIABLE MATRIX				
Manuals Completed	**Date Completed**	**Update Completed**	**Core Variable (s) Covered**	**Other Variables Covered**
Dissolved Oxygen	Dec_2012	Apr_2015	Dissolved Oxygen	
In-Situ Currents	Jun 2013	Sep 2015	Surface Currents	
In-Situ Waves	Jun_2013	Jul_2015	Surface Waves	
Temperature and Salinity	Dec_2013		Temperature Salinity	
Water Level	May 2014		Sea Level	
Wind Speed and	Oct 2014		Wind Speed and Direction	
Ocean Optics	Jun_2015		CDOM Ocean Color Optical Properties	In-water radiance/irradiance Above-water radiance/irradiance Beam attenuation Turbidity PAR Cholorophyll FDOM
Dissolved Nutrients	Sep_2015		Dissolved Nutrients	Nitrogen (NO3, NO2, and NH4) Phosphate Silicate
Remaining Manuals	**Projected Completion**		**Remaining Core Variables To Be Covered**	
Zooplankton			Zooplankton Abundance	
			Zooplankton Species	
			Phytoplankton Species	
CO2/Acidity			Partial Pressure of CO2	
			Acidity	
Sea Floor			Bathymetry	
			Bottom Character	
Contaminants			Contaminants	
Fish			Fish Abundance	
			Fish Species	
Heat and Ice			Heat Flux	
			Ice Distribution	
Pathogens			Pathogens	
Stream Flow			Stream Flow	
Total Suspended Matter			Total Suspended Matter	
HFSCM				

IV. QARTOD PLANS

One major goal of the QARTOD project includes providing assistance to operators as they implement QARTOD QC practices. Implementation of existing tests will yield more detailed information about the challenges that operators are encountering. Each manual contains an email link to IOOS to enable operators to provide specific feedback about each test so that the TC can correct or adjust tests as needed. Starting in FY16, the QARTOD project will work with the IDQWG and others to evaluate the practicality of the tests and the adequacy of the test descriptions.

Other plans for FY16 include a QC manual for high frequency radar surface current mapping (HFRSCM), and another variable yet to be determined. Both the water level manual, and the temperature and salinity manual, will be updated. While updating the temperature and salinity manual, a focus on the mobile profiling section will specifically: 1) support the US IOOS Glider Data Assembly Center's effort to establish real-time QC within that DAC, and 2) serve to assist those operators striving towards real-time QC implementation, and 3) provide the highly valued feedback mentioned above.

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