Status and Near-Term Plans for the U.S. IOOS Quality Assurance / Quality Control of Real-time Oceanographic Data (QARTOD) Project

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Abstract - The U.S. Integrated Ocean Observing System (IOOS) Quality Assurance / Quality Control of Oceanographic Data (QARTOD) project has produced a series of real-time quality control manuals for specific core variables and other variables of interest to the oceanographic community. Not all core variables warrant a QARTOD manual. We consider each remaining variable for which a QARTOD manual has not been produced and discuss the potential for development of a manual in the near term.

QARTOD QC tests are presently being implemented by IOOS Regional Associations. We review the challenges anticipated and encountered in this process and provide an example of a successful effort. Manuals are updated to ensure they remain accurate and relevant; feedback following implementation is a key component of the update process.

QARTOD manuals are used internationally, and we will continue to expand our global collaborative efforts. These include a review of the Global Ocean Observing System essential ocean variables to consider further candidates for a QC manual, and partnerships supportive of QC, QA, measurement uncertainty, and best practices. QARTOD manuals are also used by universities to train the individuals who will implement the next generation of advanced QC tests.

Keywords – QARTOD, quality control, quality assurance, real time data management, measurement uncertainty.

I. Introduction

The U.S. Integrated Ocean Observing System (IOOS®) Quality Assurance / Quality Control of Oceanographic Data (QARTOD) project has produced a series of real-time quality control manuals for specific core variables and other variables of interest to the oceanographic community [1]. The manuals are created with voluntary community support from hundreds of individuals, involving academic, governmental, and private sector engagement. The manuals provide specific tests to be applied to real-time data, including test and threshold examples and instructions, for those drafting program code for interoperable observational data streams.

Not all U.S. IOOS core variables warrant a QARTOD manual. Some variable observations are not interoperable, some observation systems are not sufficiently mature for

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automated quality control, and some simply do not require real-time QC. We consider each remaining core variable that does not yet have a manual and discuss the potential for development of a manual in the near term.

We have seen enthusiastic international participation in the creation and adoption of the existing QARTOD manuals. We will continue to expand our global collaborative efforts, including a review of the Global Ocean Observing System essential ocean variables to consider further candidates for a QC manual. QARTOD has already joined AtlantOS and others to begin the creation of a quality assurance (QA) manual and has strong interaction with the emerging Ocean Best Practices project. Future QARTOD tasks will shift slightly to include more quality assurance rather than exclusively focusing on quality control. One important component of this work includes the determination and documentation of measurement uncertainty.

Yet another rewarding finding is the use of QARTOD manuals by universities, training the next generation of operational oceanographers [2]. These are the skilled individuals who will eventually implement the most advanced QC tests described in the manuals, such as the multi-variate tests that compare different observations once useful relationships are established. They will become the subject matter experts that will create new manuals as technology emerges.

Finally, we review the efforts and challenges seen and anticipated when implementing QARTOD QC. Manuals will continue to be updated as appropriate in response to user community requirements and evolving measurement technology, to ensure they remain accurate and relevant.

II. Core Variable and QC Manual Feasibility

The initial intent was to develop a QARTOD manual for each IOOS core variable. While that is still an admirable goal, it has become apparent that real-time QC is not appropriate for all core variables at present, for a variety of reasons.

A. Completed Manuals

A QARTOD manual exists for the following variables: currents, salinity, sea level, surface waves, stream flow, temperature, wind speed and direction, dissolved nutrients, dissolved oxygen, ocean color, colored dissolved organic matter, optical properties, sound, phytoplankton species/abundance (see https://ioos.noaa.gov/project/qartod). Manuals for currents, salinity and temperature, sea level, surface waves, wind speed and direction, and dissolved nutrients have received incremental updates, and the dissolved oxygen manual has been updated twice. No substantial updates (which would have impact on operational use of the QC tests) have been necessary so far.

B. Future Manual

Manuals for these variables are currently being considered: acidity, partial pressure of CO2, and total suspended matter.

C. Not Needed

These variables either do not require real-time QC or alternative QC methods exist: ice distribution (manual evaluation is sufficient) and heat flux. Heat flux is derived from multiple met/ocean variables, therefore manuals for real-time QC of oceanic variables such as temperature, winds, and optical properties apply.

D. Not Feasible at Present

The following variables are not feasible for the reasons indicated in the parentheses: contaminants (lacks definition and is too vague for a specific real-time QC manual), pathogens (vague, without an interoperable data stream), bottom character (no interoperable data stream), biological vital rates (vague, without interoperable data stream), coral species and abundance, fish species/abundance, invertebrate species and abundance, marine mammal species/abundance, microbial species/abundance/activity, Nekton diet, sea birds species/abundance, sea turtles species/abundance, submerged aquatic vegetation species/abundance, and zooplankton species/abundance (data not disseminated in real-time, no interoperable data streams).

III. Near-term Plans

In fiscal year 2019, the IOOS QARTOD project plan is to update the waves manual (starting in October 2018), update the currents manual (starting in May 2019), and develop a real-time QC manual for pH (starting in February 2019). The pH manual will certainly be useful for data obtained from deployment of coastal sondes fitted with a pH sensor (Fig. 1) and may be useful to the ocean acidification community.

The IOOS/QARTOD project will continue to work with operators (data providers) striving to implement QARTOD tests, specifically supporting the development of standardized data set inputs and test results than can be used to evaluate test code developed by others. We will also encourage communities engaged in observations of specific variables to consider developing real-time QC manuals themselves, using the QARTOD process but without the U.S. IOOS QARTOD project necessarily leading the effort. We also intend to begin shifting toward broader QA considerations and support the further development of the emerging Ocean Best Practices System.

Fig. 1. Multiparameter sondes such as this YSI EXO water quality probe often include a pH sensor. Photo credit: YSI

IV. IMPLEMENTATION

There are several paths that may be taken by entities implementing QARTOD QC tests. In the best case, the operator has actively participated in the development of the QC manual(s). Operators may have provided tests already in use, or tests they believe would be appropriate and are willing to implement. These tests form the basis of the specific variable to be addressed by the QARTOD manual, and these operators find themselves readily aligned with QARTOD goals. Such was the case with the waves QC manual [3] and Scripps Institution of Oceanography Coastal Data Information Program (CDIP). CDIP is a well-established program, formed in 1975, with a long history of real-time QC of wave data. CDIP personnel were leaders in the initial grass-roots QARTOD effort, and they continue to provide strong support for this U.S. IOOS project. Consequently, many wave QC tests adopted by QARTOD have their genesis in CDIP: http://cdip.ucsd.edu/documents/index/product_docs/qc_summaries/waves/waves_table.php?&xtab=CDIP.

Detailed explanations of these tests and graphic examples are shown at: http://cdip.ucsd.edu/documents/index/product_docs/qc_summaries/waves/waves_table.php?&xtab=QARTOD

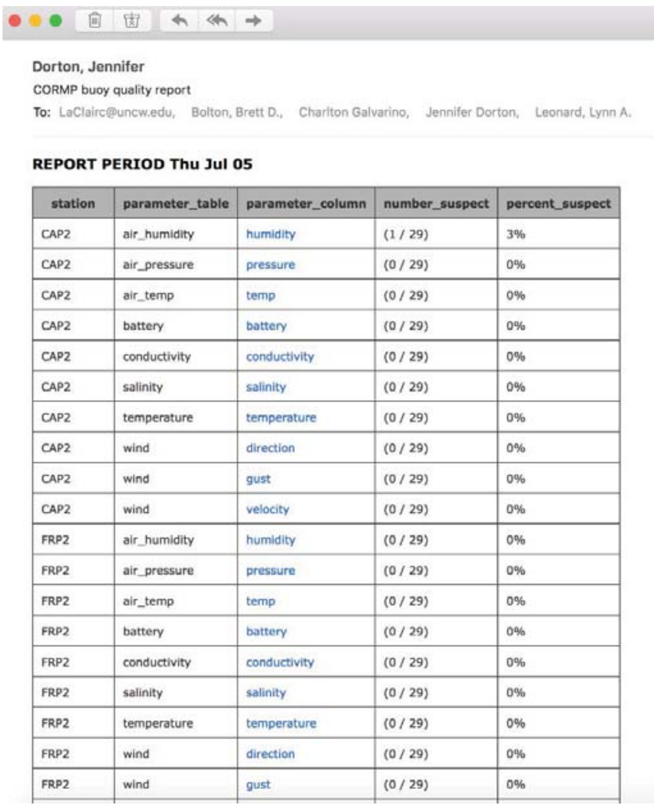
At the other extreme, operators may choose not to participate in the development of a QARTOD manual and, in the worst case, may view implementation the QC tests as onerous.

Most operators find themselves somewhere between these two cases. The following section details recent implementation of QARTOD QC by the University of North Carolina Wilmington's Coastal Ocean Research and Monitoring Program (CORMP). CORMP was established in 1999 and, as a partner in the Southeast Coastal Ocean Observing Regional Association (SECOORA), provides real-time oceanographic and meteorological data from nine stations off the coasts of North Carolina and South Carolina. Beginning in the early 2000s, CORMP implemented data quality checks for all real-time data. These checks, however, provided only basic tests (e.g., gross range, syntax error checks) and lacked consistency among parameters. In 2016, SECOORA required that all of its funded partners implement quality control measures as outlined in the IOOS QARTOD manuals, and this mandate turned into an opportunity for all CORMP personnel to participate in data QA/QC.

A. *Process Description*

The process began with CORMP and Second Creek Consulting, the CORMP data management contractor, reviewing the wind *Manual for Real-Time Quality Control of Wind Data* (https://ioos.noaa.gov/ioos-in-action/wind-data/) and identifying the required, strongly recommended, and suggested tests that needed to be implemented. Second Creek then developed the computer database algorithms to check real-time data based on QARTOD tests. These back-end processes worked well; however, it quickly became apparent that project principal investigators and technicians needed the ability to identify and review the specific tests that flagged data as suspect or failed. As the team further discussed QARTOD implementation, it was decided that a QARTOD dashboard and daily e-mail alert system were necessary.

Second Creek set up an automated, overnight e-mail alert to CORMP project personnel (Fig. 2). The e-mail alert allowed personnel to quickly identify a specific sensor on a mooring that is returning suspect data. From the e-mail, personnel can identify any data issues, click on the suspect data parameter, and then be taken to the CORMP Data Quality Dashboard (Fig. 3). The dashboard has built-in functionality that allows personnel to review the individual flags, graph data to identify trends, and ultimately accept the data flag or override the data flag in the roll-up column. The roll-up flag is the only quality flag shared with the SECOORA data management team, since this flag indicates the overall data quality. Once the CORMP team completed initial testing of the QARTOD system using the wind data, QARTOD tests were employed for the remaining data parameters provided by all of the CORMP moorings (http://cormp.org).



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CORMP buoy quality report
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REPORT PERIOD Thu Jul 05

station	parameter_table	parameter_column	number_suspect	percent_suspect
CAP2	air_humidity	humidity	(1 / 29)	3%
CAP2	air_pressure	pressure	(0 / 29)	0%
CAP2	air_temp	temp	(0 / 29)	0%
CAP2	battery	battery	(0 / 29)	0%
CAP2	conductivity	conductivity	(0 / 29)	0%
CAP2	salinity	salinity	(0 / 29)	0%
CAP2	temperature	temperature	(0 / 29)	0%
CAP2	wind	direction	(0 / 29)	0%
CAP2	wind	gust	(0 / 29)	0%
CAP2	wind	velocity	(0 / 29)	0%
FRP2	air_humidity	humidity	(0 / 29)	0%
FRP2	air_pressure	pressure	(0 / 29)	0%
FRP2	air_temp	temp	(0 / 29)	0%
FRP2	battery	battery	(0 / 29)	0%
FRP2	conductivity	conductivity	(0 / 29)	0%
FRP2	salinity	salinity	(0 / 29)	0%
FRP2	temperature	temperature	(0 / 29)	0%
FRP2	wind	direction	(0 / 29)	0%
FRP2	wind	gust	(0 / 29)	0%

Fig. 2. Daily e-mail with each mooring parameter identified and the number of suspect data points out of the total number of data points for a 24-hour period. Clicking on the blue text in the parameter column takes the user to the CORMP Data Quality Dashboard so that they can quickly identify the data quality issue.

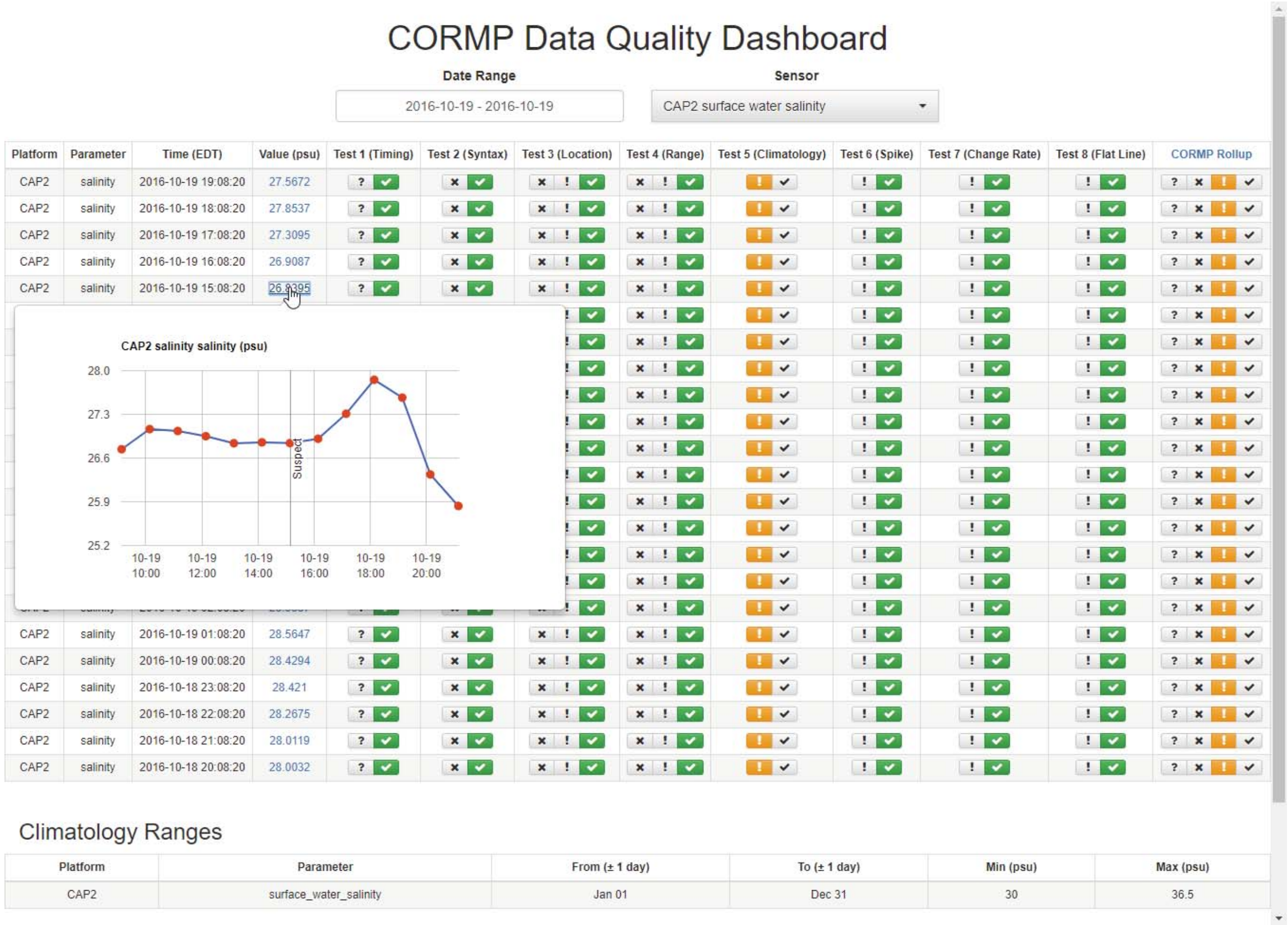
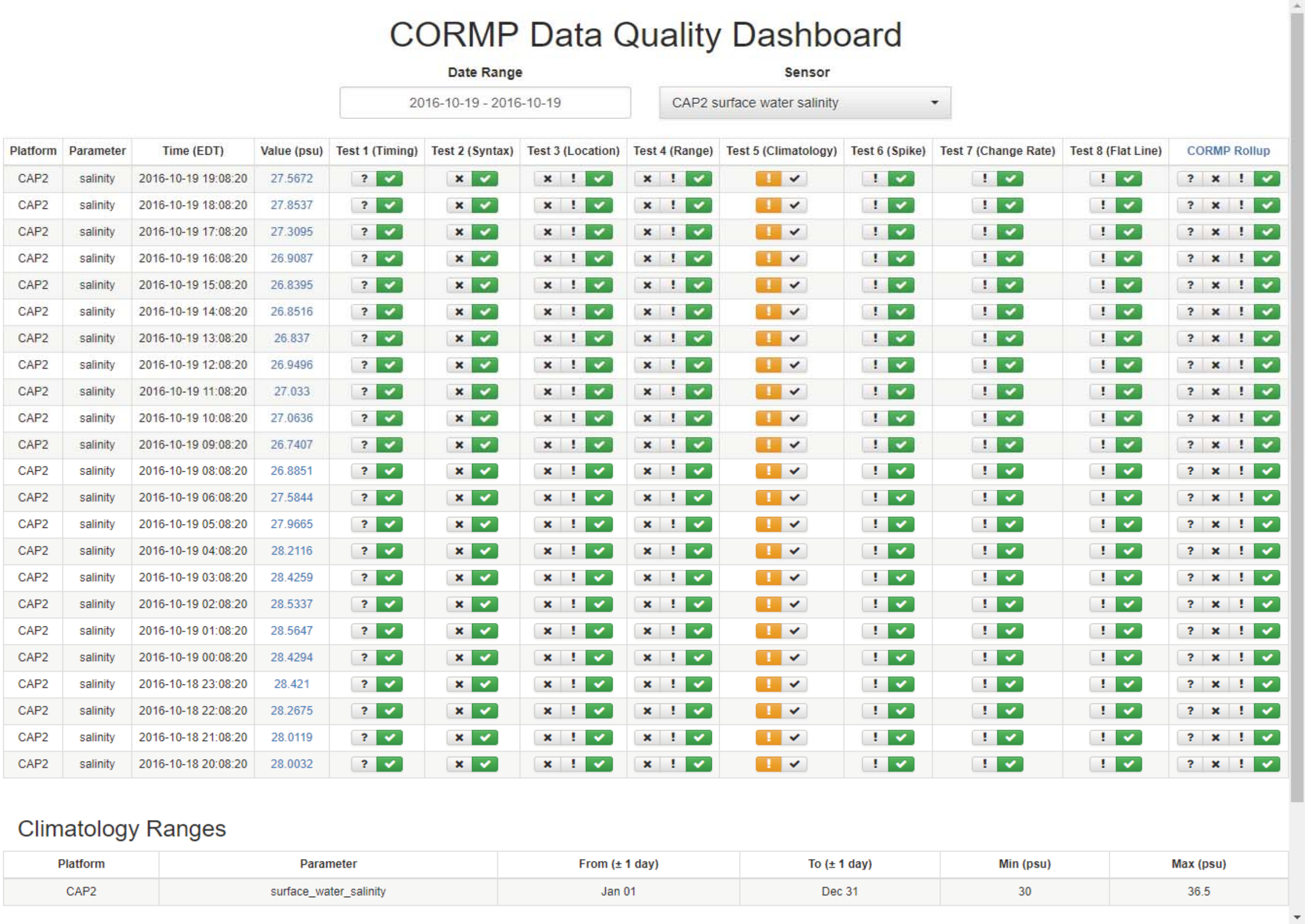


Fig. 3. Precipitation from Hurricane Matthew caused coastal and inland flooding throughout SC. Large amounts of run-off over a two-week period resulted in lower salinity throughout Long Bay and Winyah Bay. The QARTOD climatology test provided a "suspect" flag for all of the CAP2 surface water salinity data for almost two weeks after the storm. The CORMP Data Quality Dashboard provides analysts the ability to visually inspect data quality records. In this example, the salinity data were graphed to review the salinity trend over a 10-hour period. The CORMP Rollup flag (far right column) provides an overall quality flag (pass, suspect, or fail) for the data. Consistently low salinity caused personnel to investigate conditions at the mooring to determine if the sensor was bad.

B. Hurricane Matthew Tests the System

Within weeks of the full CORMP QARTOD implementation, the system was tested by Hurricane Matthew. The hurricane delivered large amounts of rain along the U.S. southeast Atlantic coastline. Extensive freshwater run-off affected coastal waters along the South Carolina coast and caused water temperature, salinity, and conductivity data from the CAP2 mooring to be flagged every hour for almost two weeks (Fig. 3). Initially, project personnel were uncertain as to the cause of the data flags since the CTD (conductivity, temperature, and density) sensor could have been damaged by the storm, so they reached out to South Carolina Department of Natural Resources (SC DNR) staff and asked if they would conduct CTD casts near the buoy at 1-meter water depth, the depth of the sensor under the mooring. SC DNR personnel made several casts over the two-week period and found that the CTD data from the CAP2 mooring were accurate. Large volumes of fresh water had reduced salinity, causing the climatology test to be suspect. Once it was confirmed that the data from the mooring were correct, project personnel marked the data as "pass" in the roll-up flag. The "suspect" flag for climatology, however, remains in place because the data were below the climatological range for that location (Fig. 4).

QARTOD implementation has improved efficiency by allowing CORMP technicians to identify sensor problems sooner and to take the most appropriate action. For example, in situations where redundant sensors are located on a mooring, the data manager immediately can shift the data feed to the back-up sensor, thereby minimizing data loss. In cases when sensor redundancy is lacking, such as with CTDs or acoustic Doppler current profilers, technicians can schedule at-sea maintenance activities, thereby reducing the number of days where bad or suspect data are being returned. Finally, QARTOD implementation also allows technicians to avoid unnecessary costs such as ship time to swap a sensor that is actually providing good data (such as the example with CAP2) or sending sensors back for unneeded calibration.



CORMP Data Quality Dashboard

Date Range: 2016-10-19 - 2016-10-19

Sensor: CAP2 surface water salinity

Platform	Parameter	Time (EDT)	Value (psu)	Test 1 (Timing)	Test 2 (Syntax)	Test 3 (Location)	Test 4 (Range)	Test 5 (Climatology)	Test 6 (Spike)	Test 7 (Change Rate)	Test 8 (Flat Line)	CORMP Rollup
CAP2	salinity	2016-10-19 19:08:20	27.5672	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓
CAP2	salinity	2016-10-19 18:08:20	27.8537	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓
CAP2	salinity	2016-10-19 17:08:20	27.3095	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓
CAP2	salinity	2016-10-19 16:08:20	26.9087	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓
CAP2	salinity	2016-10-19 15:08:20	26.8395	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓
CAP2	salinity	2016-10-19 14:08:20	26.8516	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓
CAP2	salinity	2016-10-19 13:08:20	26.837	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓
CAP2	salinity	2016-10-19 12:08:20	26.9496	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓
CAP2	salinity	2016-10-19 11:08:20	27.033	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓
CAP2	salinity	2016-10-19 10:08:20	27.0636	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓
CAP2	salinity	2016-10-19 09:08:20	26.7407	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓
CAP2	salinity	2016-10-19 08:08:20	26.8851	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓
CAP2	salinity	2016-10-19 06:08:20	27.5844	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓
CAP2	salinity	2016-10-19 05:08:20	27.9665	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓
CAP2	salinity	2016-10-19 04:08:20	28.2116	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓
CAP2	salinity	2016-10-19 03:08:20	28.4259	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓
CAP2	salinity	2016-10-19 02:08:20	28.5337	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓
CAP2	salinity	2016-10-19 01:08:20	28.5647	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓
CAP2	salinity	2016-10-19 00:08:20	28.4294	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓
CAP2	salinity	2016-10-18 23:08:20	28.421	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓
CAP2	salinity	2016-10-18 22:08:20	28.2675	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓
CAP2	salinity	2016-10-18 21:08:20	28.0119	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓
CAP2	salinity	2016-10-18 20:08:20	28.0032	? ✓	× ✓	× ! ✓	× ! ✓	! ✓	! ✓	! ✓	! ✓	? × ! ✓

Climatology Ranges

Platform	Parameter	From (± 1 day)	To (± 1 day)	Min (psu)	Max (psu)
CAP2	surface_water_salinity	Jan 01	Dec 31	30	36.5

Fig. 4. After further analysis and on-site salinity measurements taken by SC Department of Natural Resources personnel, it was determined that the salinity data from the CAP2 mooring were correct. CORMP personnel manually changed the rollup flag from "suspect" to "pass". The climatology "suspect" flag remains in place, since the data were truly below the climatological range for the mooring location. Note that the climatology range specific to the CAP2 mooring location is 30-36.5 psu. The range is listed on the Dashboard for ease of reference.

C. *QARTOD Implementation Take Away Messages*

- This is not just a data manager effort—it is a team effort. The subject matter expert of the data in question also needs to be involved in QARTOD implementation and execution.
- When implemented correctly, all team members have an "ownership" in the real-time data and work together to ensure that data are flagged appropriately.
- Data flags provide an early alert system for sensor failures. Field work can quickly be scheduled to swap sensors or provide further maintenance as needed.
- Data roll-up flags can be passed to the QC team so that every data point has a pass, suspect, or fail flag attached to it.

V. QARTOD MANUAL USE IN THE CLASSROOM

To make the purpose of the tests clear to readers, each manual includes fundamental information—the reasons for making the measurements, the sensors used and how they work (and fail), and how the data are used. Interesting examples of data and test results are included to demonstrate the utility of the tests. These components make the manuals ideal for educational purposes. Rutgers University has initiated a new master's program with studies that include QA/QC of data using QARTOD manuals.

However, the manuals state that a knowledgeable operator is presumed. The local operator is responsible for selecting the proper test thresholds for each particular sensor they deploy, so knowledge of the variable being measured is critical. What are the best thresholds for good, questionable, and bad data? What is the lowest dissolved oxygen expected before it becomes questionable or of high interest and requires human evaluation? When does a dissolved oxygen pass beyond questionable and become unreasonable? Such questions will interest students, and the answers are based upon an understanding of fundamentals, previous observations, time series analysis, statistics, and similar skills.

VI. Summary

Real-time quality control of operational oceanographic data observations is now the norm, expected by most data users and required by many funding agencies. With this development comes the critical need for standardization and automation of optimized real-time QA/QC algorithms. QC tests such as those provided by QARTOD simplify implementation by providing community accepted standards, without being overly prescriptive or challenging.

Acknowledgment

We greatly appreciate the efforts from the hundreds of volunteers who have assisted in the develop of the series of QARTOD QC manuals and supporting documents. They are individually identified in each document. We are rewarded by the work of those implementing these QC tests.

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