Joint European Research Infrastructure network for Coastal Observatory – Novel European eXpertise for coastal observaTories - **JERICO-NEXT**

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1. Introduction

One of the aims of JERICO NEXT is the improvement of synergies in methodologies and measuring systems of existing observing systems. One of the today's big challenges is the need to maximise the full potential of observing networks and use them into a vast range of services supporting the 'blue growth'. Furthermore, there is a need to harmonise the quality procedures of many different data collected during more than a century, in order to make all data of the same parameter compatible and comparable. Global historical databases, despite efforts by a number of research institutions, still contains a relatively large fraction of biased and substandard quality data and metadata that can confound applications.

A fundamental requirement in collaborative marine studies is the intercomparability of data obtained from participating laboratories irrespective of the country of origin. The production of comparable and compatible data requires that laboratories adopt good field and laboratory procedures as part and parcel of a Quality Assurance/Quality Control (QA/QC) regime. This includes the selection of internationally-validated methodologies for sampling and analysis, mandatory use of reference materials (certified reference materials, whenever possible) and participation in 'blind' international intercomparison exercises.

A number of quality control procedures and documents from NODCs and major international projects (e.g. SeaDataNet, WOCE, GTSPP, GOSUD, Argo, etc.) are existing. Most of them mainly deal with physical data (e.g. temperature and salinity and in some cases nutrients). Other documents exist for quality control for sea level (ESEAS and GLOSS) and met-ocean data – current meter data, waves, meteorological data (EU SIMORC project, WOCE Current Meter DAC). In addition, the ICES Working Group on Marine Data Management (WGMDM) guidelines are in use in a number of data centres. There is also the QARTOD effort in the USA, initially dealing with real time quality control.

Data quality control essentially and simply has the following objective: "To ensure the data consistency within a single data set and within a collection of data sets and to ensure that the quality and errors of the data are apparent to the user who has sufficient information to assess its suitability for a task." (IOC/CEC Manual, 1993).

If done well, quality control brings about a number of key advantages:

- Maintaining Common Standards - There is a minimum level to which all oceanographic data should be quality controlled. The data must be qualified by additional information concerning methods of measurement and subsequent data processing to be of use to potential users.
- Acquiring Consistency - Data within data centres should be as consistent to each other as possible. This makes the data more accessible to the external user.
- Ensuring Reliability - To serve the research community and others data must be reliable, and this can be better achieved if the data have been quality controlled to a internationally accepted standard.

Environmental and climatic issues are requiring well validated quality procedures based on reference methods and on inter-laboratory exercises. This is important also for the implementation of the European Water Framework Directive. It must be underlined that intercalibrations, availability of certified reference materials (CRMs), clean room techniques, etc., are not sufficient to assure good quality of data. It should be realized that sampling, sample pre-treatment, transport and storage, are an integral part of the analysis. These sample handling procedures have not received much attention in terms of quality assurance (QA) and good measuring practice (GMP).

From an historical point of view, although the problem was present from the pioneer analysis made by Redfield in 1934, the urgent need for nutrient standards was demonstrated during the World Ocean Circulation Experiment (WOCE) and the Joint Global Ocean Flux Study (JGOFS) when measurements were made by different laboratories. The internal consistency of nutrient data was evaluated by comparing measurements made in deep waters (depth over 3500 m) at nearby stations on different cruises. Offsets were found among the results of different laboratories indicating inconsistencies in the preparation of calibration standards.

In the 1970s the Japanese Sagami Chemical Research Center provided nutrient reference material for the Cooperative Study of Kuroshio Current (the so called CSK standard).

Today certified reference materials are provided by many institutions, such as:

- Canadian National Research Council
  - (http://www.nrc-cnrc.gc.ca/eng/solutions/advisory/crm_index.html),
- IAEA
  - (https://nucleus.iaea.org/rpst/referenceproducts/About/index.htm)
- Scripps Institution of Oceanography
  - (https://scripps.ucsd.edu/ships/shipboard-technical-support/odf/chemistry-services/seawater)
- Australian National Association of Testing Authorities
  - (https://www.nata.com.au/nata/54-nata-e-news/june2014/1010-nmi-releases-mx014-a-new-reference-material-certified-for-trace-elements-in-sea-water)

This document is reporting some important efforts for detailed examination of problems related to international ocean activities and studies of the marine environment, including improvements of scientific methods and quality methodologies. In particular it will provide an insight on activities carried out within some initiatives such as QUASIMEME, the Scientific Committee on Oceanic Research (SCOR), QARTOD. The document will present QA/QC procedures adopted or developed in international programmes (e.g. GO-SHIP, ARGO) and EU projects (e.g. MyOcean/ Marine Copernicus, JERICO).

In many cases, different projects are using the same or very similar QA/QC procedures, but they are elaborated in very specific context, or have added some additional procedures. For this reason there are apparent repetitions in reviewing the different initiatives, programmes and/or projects.

Finally a specific review on thermodynamic properties of sea waters and nutrients and chemical measurements will be presented. In many cases, different calculation algorithms are used for salinity and temperature and then there is a problem in the comparability of data. However, it must be underlined that the problem that is normally arising from data, is not the use of different algorithms, but the fact that there are no information in data related metadata on what has been used for calculations.

The document is also including a map of the quality flags used internationally.

2. Quasimeme

The "Quality Assurance of Information for Marine Environmental Monitoring in Europe" (QUASIMEME) project was supported by the European Commission between 1992 and 1996 with the aim to develop a holistic quality assurance programme for marine environmental monitoring information in Europe. As a result a marine network and laboratory performance studies have been established for most of the determinants measured in the marine environmental programmes for both monitoring and research purposes. After the end of the EU funding in 1995, the QUASIMEME scheme continued from 1996 on subscription basis.

The QUASIMEME project has been hosted from its inception in 1992 to April 1, 2005, by the Fisheries Research Institute in Aberdeen, United Kingdom. Wageningen University and Research (WUR) has taken over the responsibility for the QUASIMEME project on April 1, 2005. Since 1st January 2011, Quasimeme is part of WEPAL (Wageningen Evaluating Programmes for Analytical Laboratories. Today QUASIMEME is an interactive scheme. Participants can request specific determinands and matrices for inclusion in the programme, make suggestions for development exercises and workshop topics.

Exercises are conducted twice per annum. Data from the laboratories analysis are assessed electronically by QUASIMEME. The results are assessed against the assigned value for that determinand to obtain a z-score.

The routine performance studies provide the basis for the external quality assurance for institutes that make regular analytical measurements. The output from these studies is reviewed annually by the International Scientific Assessment Board, which comprises of experts in each of the main areas of the QUASIMEME programme.

Determinand Groups and environmental matrices for which laboratory performances are assessed:

Determinand Group	Water	Sediment	Biota
Nutrients	x		
Metals, Mercury, organics, chlorophyll	x		
DOC	x		
Trace Metals		x	x
PAH's	x	x	x
Organotins	x	x	x
Organics (eg PCBs &OCPs)	x	x	x
Brominated Flame Retardants		x	x
Passive Sampling	X		
Shellfish Toxins			x
Perfluorinated compounds			x
Chlorinated Organics		x	x

3. SCOR

The International Council for Science (ICSU) formed the Special Committee on Oceanic Research (SCOR) in 1957 to help address interdisciplinary science questions related to the ocean. SCOR's name was later changed to "Scientific Committee on Oceanic Research" to reflect its more permanent status.

SCOR activities focus on promoting international cooperation in planning and conducting oceanographic research, and solving methodological and conceptual problems that hinder research. SCOR covers all areas of ocean science and cooperates with other organizations with common interests to conduct many SCOR activities.

Within SCOR working groups are constituted to deliberate on a narrowly focused topic and develop a publication for the primary scientific literature. Their work is intended to be completed in 4 years or less. SCOR has sponsored—alone or with other organizations—147 working groups, some of them of interest for this report.

Contribution	Methodologies, studies
Joint Panel on Oceanographic Tables and Standards	• Algorithms for calculations of fundamental properties of seawater,*UNESCO Technical Papers in Marine Science* 44 (1983) • Progress on Oceanographic Table and Standards 1983-1986, *UNESCO Technical Papers in Marine Science* 50 (1986)
General Problems of Intercalibration and Standardization	• Report - pp. 34-36 of *SCOR Proceedings* Vol. 1(1) (1965)
Continuous Current Velocity Measurements	• An Intercomparison of Some Current Meters, *UNESCO Technical Papers in Marine Science* 11.
Estimation of Primary Production under Special Conditions	• Qasim, S.Z., P.M.A. Bhattathiri, and V.P. Devassy. 1972. Some problems related to the measurements using radiocarbon technique. Internationale Revue der gesamten Hydrobiologie und Hydrographie 57(4):535–549.
Tides of the Open Sea	• An intercomparison of open sea tidal pressure sensors, *UNESCO Technical Papers in Marine Science* 21.
Phytoplankton Methods	• *A Review of Methods Used for Quantitative Phytoplankton Studies. Final Report of SCOR Working Group 33*. 1974. UNESCO Technical Papers in Marine Science 18 • Sournia, A. 1978. Phytoplankton Manual. *UNESCO Monographs on Oceanographic Methodology* 6
River Inputs to Ocean Systems	• River Inputs to Ocean Systems: Status and Recommendations for Research, *UNESCO Technical Papers in Marine Science* 55
Evaluation of CTD Data	• The Acquisition, Calibration, and Analysis of CTD Data, *UNESCO Technical Papers in Marine Science* 54 (1988)
Coastal Off-Shore Ecosystems Relationships	• Coastal Offshore Ecosystems Relationships, *UNESCO Technical Papers in Marine Science* 48 (1986)

Methodology for Oceanic CO2 Measurements	• Methodology for Oceanic CO2 Measurements, *UNESCO Technical Papers in Marine Science* 65 (1992)
Determination of Photosynthetic Pigments in Seawater	• *Determination of Photosynthetic Pigments in Seawater*
Comparative Salinity and Density of the Atlantic and Pacific Ocean Basins	• Millero, F.J. 2000. Effect of changes in the composition of seawater on the density-salinity relationship. *Deep-Sea Research I* 47:1583-1590.
Sediment Trap and 234Th Methods for Carbon Export Flux Determination	• Buesseler et al. 2007. An assessment of the use of sediment traps for estimating upper ocean particle fluxes. *Journal of Marine Research, 65,* 345–416, 2007 - Used with permission from the Journal of Marine Research (http://peabody.yale.edu/scientific-publications/journal-marine-research/home)
Global Comparisons of Zooplankton Time Series	• Global Comparisons of Zooplankton Time Series. Special Issue of *Progress in Oceanography*, Volumes 97–100, Pages 1-186 (May–July 2012)
Thermodynamics and Equation of State of Seawater	• The international thermodynamic equation of seawater – 2010: Calculation and use of thermodynamic properties. IOC Manuals and Guides 56 • An Historical Perspective on the development of the Thermodynamic Equation of Seawater - 2010 Special issue of *Ocean Science*
Deep Ocean Exchanges with the Shelf	• Deep Ocean Exchanges with the Shelf - Special issue of *Ocean Science* and bibliography

4. QARTOD

QARTOD (Quality Assurance of Real Time Ocean Data) is a US IOOS Program Office initiated a community-based project for authoritative procedures for quality assurance (QA) and quality control (QC) of real-time ocean sensor data. The result of this effort is to develop standards that can become formal IOOS data standards for data from the Regional Associations.

For marine environmental variables, manuals are published describing the individual quality control procedures that are applied to the data stream prior to dissemination. The time lag between the data collection and dissemination dictates the number and types of tests applied to the data stream (i.e. the real time vs delayed mode issue). The description of each QC test is sufficient for a skilled software programmer to create software that implements the tests in different software environments.

These manuals are living documents that reflect the state-of-the-art QC testing procedures for real-time in-situ current observations.

- Real-Time Quality Control of HF Radar Observations
  - (https://ioos.noaa.gov/ioos-in-action/manual-real-time-quality-control-high-frequency-radar-surface-current-data/)
- Real-Time Quality Control of Dissolved Nutrients Observations
  - (https://ioos.noaa.gov/ioos-in-action/dissolved-nutrients/)
- Real-Time Quality Control of Wind Data
  - (https://ioos.noaa.gov/ioos-in-action/wind-data/)
- Real-Time Quality Control of Water Level Data
  - (https://ioos.noaa.gov/ioos-in-action/manual-real-time-quality-control-water-level-data/)
- Real-Time Quality Control of In-Situ Surface Wave Data
  - (https://ioos.noaa.gov/ioos-in-action/wave-data/)
- Real-Time Quality Control of Ocean Optics Data
  - (https://ioos.noaa.gov/ioos-in-action/oceanic-optics/
- Real-Time Quality Control of In-Situ Temperature and Salinity Data
  - (https://ioos.noaa.gov/ioos-in-action/temperature-salinity/)
- Real-Time Quality Control of Dissolved Oxygen Observations in Coastal Oceans
  - (https://ioos.noaa.gov/ioos-in-action/manual-real-time-quality-control-dissolved-oxygen-observations/
- Real-Time Quality Control of In-Situ Current Observations
  - (https://ioos.noaa.gov/ioos-in-action/currents/)
- Manual for Oceanographic Data Quality Control Flags
  - (https://www.ioos.noaa.gov/wp-content/uploads/2015/10/qartod_oceanographic_data_quality_manual.pdf)

5. GO-SHIP

The GO-SHIP program was developed to provide a sustained coordination mechanism for global repeat hydrography as outlined in the GO-SHIP strategy published in 2009 (available online at: http://www.go-ship.org/Docs/IOCTS89_GOSHIP.pdf). Central to this coordination is ensuring that measurements made by different groups are comparable, compatible, and of the highest quality possible. Under the guidance of the GO-SHIP committee and following the original work of Joyce (1991), the following measurement standards, or expectations, have been developed as goals for the data quality desired from GO-SHIP reference sections.

5.1. Standards for ctd sensors

Temperature	Accuracy = 0.002°C. Precision = 0.0005°C (ITS90).
Salinity	Accuracy = 0.002 g kg-1 (TEOS-10) depending on frequency and technique of calibration. Precision = 0.001 g kg-1 (TEOS-10), depending on processing techniques. 1
Pressure	Accuracy = 3 decibar (dbar) with careful laboratory calibration. Precision = 0.5 dbar, dependent on processing.2
O2	Accuracy † = 1%. Same for precision.
Notes:	† If no absolute standards are available for a measurement then accuracy should be taken to mean the reproducibility presently obtainable in the better laboratories. 1 Although conductivity is measured, data analyses require it to be expressed as salinity. Conversion and calibration techniques from conductivity to salinity should be stated. 2 Difficulties in CTD salinity data processing occasionally attributed to conductivity sensor problems or shortcomings in processing may actually be due to difficulties in accounting for pressure sensor limitations.

5.2. Standards for water samples

Salinity	Accuracy of 0.001 is possible with Autosal™ salinometers and concomitant attention to methodology, *e.g.*, monitoring Standard Sea Water. Accuracy with respect to one particular batch of Standard Sea Water can be achieved at better than 0.001 PSS-78. Autosal precision is better than 0.001 PSS-78. High precision of approximately 0.0002 PSS-78 is possible following the methods of Kawano (this manual) with great care and experience. Air temperature stability of ± 1°C is very important and should be recorded.1
O2	Target accuracy is that 2 sigma should be less than 0.5% of the highest concentration found in the ocean. Precision or reproducibility (2 sigma) is 0.08% of the highest concentration found in the ocean.
NO3	approximately 1% accuracy†, 2 and 0.2% precision, full scale.
PO4	approximately 1-2% accuracy†, 2 and 0.4% precision, full scale.
SiO2	approximately 1-3% accuracy†, 2 and 0.2% precision, full-scale.
DIC	Accuracy = 1-2 µmol kg-1
Alkalinity	Accuracy = 2-3 µmol kg-1
pCO2	Accuracy = 3 µatm; optimal 1 µatm
pH	Accuracy = 0.005 pH units.
3H	Accuracy 1%; precision 0.5% with a detection limit of 0.05 tritium unit (TU) in the upper ocean of the northern hemisphere and 0.005 TU elsewhere.

δ 3He	accuracy /precision = 1.5 ‰ in isotopic ratio; absolute total He of 0.5% with less stringent requirements for use as a tracer (e.g., He plume near East Pacific Rise).
CFCs	Approximately 1-2% accuracy and 1% precision, blanks at 0.005 pmol kg-1 with best technique.
SF6	Target precision for SF6 = 1.5% or 0.02 fmol kg-1 (1 fmol =10-15 mole), whichever is greater, with overall accuracies of about 3% or 0.04 fmol kg-1.
Carbon Isotopes	14C: Accuracy = 4-5 ‰; 13C : Accuracy = 0.03-0.04 ‰.
Notes:	† If no absolute standards are available for a measurement then *accuracy* should be taken to mean the *reproducibility* presently obtainable in the better laboratories. 1 Keeping constant temperature in the room where salinities are determined greatly increases their quality. Also, room temperature during the salinity measurement should be noted for later interpretation, if queries occur. Additionally, monitoring and recording the bath temperature is also recommended. The frequent use of IAPSO Standard Seawater is endorsed. To avoid the changes that occur in Standard Seawater, the use of the most recent batches is recommended. The bottles should also be used in an interleaving fashion as a consistency check within a batch and between batches. 2 Developments of reference materials for nutrients are underway that will enable improvements in the relative accuracy of measurements and clearer definition of the performance of laboratories when used appropriately and the results are reported with the appropriate meta data.

GO-SHIP is providing many documents on quality procedures

Contribution	Methodology application	Authors and link to the document
Data acquisition overview	Reference Quality Water Sample Data: Notes on Data Acquisition	J. H. Swift [pdf 2.2MB] https://www.go-ship.org/Manual/Swift_DataEval.pdf
Methods for water sampling and analysis	Method for Salinity (Conductivity Ratio) Measurement	T. Kawano [pdf 300KB] https://www.go-ship.org/Manual/Kawano_Salinity.pdf
	Recommendations for the Determination of Nutrients in Seawater to High Levels of Precision and Inter-Comparability using Continuous Flow Analysers	D.J. Hydes, M. Aoyama, A. Aminot, K. Bakker, S. Becker, S. Coverly, A. Daniel, A.G. Dickson, O. Grosso, R. Kerouel, J. van Ooijen, K. Sato, T. Tanhua, E.M.S. Woodward, and J. Z. Zhang [pdf 900 KB] https://www.go-ship.org/Manual/Hydes_et_al_Nutrients.pdf
	Determination of Dissolved Oxygen in Seawater by Winkler Titration Using the Amperometric Technique	C. Langdon [pdf 260KB] https://www.go-ship.org/Manual/Langdon_Amperometric_oxygen.pdf

	Guide to Best Practices for Ocean CO2 Measurement (2008)	A. G. Dickson, C.L. Sabine, and J. R. Christian [Web] http://cdiac.ornl.gov/oceans/Handbook_2007.html
	Sampling and Measurement of Chlorofluorocarbon and Sulfur Hexafluoride in Seawater	J.L. Bullister and T. Tanhua [pdf 140KB] https://www.go-ship.org/Manual/Bullister_Tanhua_CFCSF6.pdf
	Collection and Measurement of Carbon Isotopes in Seawater DIC	A.P. McNichol, P.D. Quay, A.R. Gagnon, and J.R. Burton [pdf 500KB] https://www.go-ship.org/Manual/McNichol_C1314.pdf
	Sampling and Measuring Helium Isotopes and Tritium in Seawater	W. J. Jenkins, D. E. Lott, K. Cahill, J. Curtice, P. Landry [pdf 290KB] https://www.go-ship.org/Manual/Jenkins_TritHe3.pdf
CTD Methods	Notes on CTD/O2 Data Acquisition and Processing Using Seabird Hardware and Software	K. E. McTaggart, G. C. Johnson, M. C. Johnson, F. M. Delahoyde, and J. H. Swift [pdf 280KB] https://www.go-ship.org/Manual/McTaggart_et_al_CTD.pdf
	CTD Oxygen Sensor Calibration Procedures	H. Uchida, G.C. Johnson, and K.E. McTaggart [pdf 590KB] https://www.go-ship.org/Manual/Uchida_CTDO2proc.pdf
	Calculation of the Thermophysical Properties of Seawater (2010)	T.J. McDougall, R. Feistel, D.G. Wright, R. Pawlowicz, F.J. Millero, D.R. Jackett, B.A. King, G.M. Marion, S. Seitz, P. Spitzer, and C-T.A. Chen [pdf 6MB] https://www.go-ship.org/Manual/TEOS-10_Manual_06Jul10.pdf
	A Manual for Acquiring Lowered Doppler Current Profiler Data	A.M. Thurnherr, M. Visbeck, E. Firing, B.A. King, J.M. Hummon, G. Krahmann, and B. Huber [pdf 2.14MB] https://www.go-ship.org/Manual/Thurnherr_LADCP.pdf
Underway Measurements	Ship-mounted Acoustic Doppler Current Profilers	E. Firing and J.M. Hummon [pdf 160KB] https://www.go-ship.org/Manual/Firing_SADCP.pdf
	A Guide to Making Climate Quality Meteorological and Flux Measurements at Sea (2006)	F. Bradley and C. Fairal [pdf 3.3MB] https://www.go-ship.org/Manual/fluxhandbook_NOAA-TECH%20PSD-311v3.pdf

6. JERICO - HFR data

The JERICO network is integrating new, promising observing technologies that can expand its spatial and temporal reach. High Frequency Radar (HFR) systems were identified as particularly attractive technology to complement the JERICO network. HFR technology offers the means to gather information on surface currents and sea state over wide areas with relative ease in terms of technical effort, manpower and costs.

The JERICO-NEXT deliverable 5.13 has provided some recommendations on the HFR data quality based on:

(1) the characteristics of HFR monitoring, considering that HFR surface current velocity data are somewhat unique in the oceanographic observation world since they are: i) two-dimensional ocean surface measurement; ii) derived from a fixed land-based remote sensor and iii) they are place on a fixed grid;
(2) the existing standards in non-EU networks (in particular in IOOS);
(3) the existing standards in Europe for Marine Data Management (EuroGOOS ROOSes, EuroGOOS HFR Task Team, CMEMS, SeaDataNet's NODC network, EMODnet Physics, JCOMMOPS in-situ Observing Platforms).

Integrated HFR networks providing real-time information with unified quality control have been operating in the United States (US-IOOS, http://www.ioos.noaa.gov/hfradar/) and in Australia (IMOS , http://imos.org.au/facilities/oceanradar/), providing key information for scientific and societal needs. In Europe, although some countries have started to implement operational HFR systems in the coastal area, a unified HF coastal radar network has not been implemented yet.

The QA/QC procedures in Europe have a high variability of approaches. The use of QA/QC advanced procedures is not frequent and highly diverse. Some of them include:

- At spectral level: use of SNR, 6dB peak width.
- System functioning diagnostic parameters at each radial station: radial vector count, average radial bearing, difference between the average radial bearing from measured and ideal patterns.
- For total data: velocity and GDOP Thresholds, spatial continuity, flags on spikes, gradients and out-of-range values.
- Spatial and temporal continuity, distributions of first and second order derivatives of radial and vector velocities, MAD filter, deviation from a reference signal.
- Validation exercises versus other in-situ or remote data as: current meters; different drifter designs (shapes and drogue); surface glider geostrophic velocities; SARAL/AltiKa altimetry velocity computation; Comparison with numerical operational models.

The one followed by SOCIB, http://www.socib.eu, include different levels of quality-controlled data sets both for real-time and delayed mode data (Lana et al., 2015):

[L0] Manufacturer QC procedures - Radial Components: Max Threshold - Total Vectors: Max Speed Threshold - 30º minimum required between radial vectors - First Order Limit settings – APM.
[L1] SOCIB battery of tests - For individual total vector (spikes, gradients and out-of-range values) are flagged - System functioning diagnostic parameters at each radial station: signal-to noise, radial vector count, average radial bearing, difference between the average radial bearing from measured and ideal patterns. QA/QC based on the international standards used in MARACOOS by Roarty et al. (2012).

6.1. Quality Control tests

The mandatory QC tests have been defined according to the EuroGOOS DATAMEQ working recommendations on real-time Quality Control (QC) and building on the QC tests defined for surface currents in the Quality Assurance/Quality Control of Real-Time Oceanographic Data (QARTOD) manual produced by the US Integrated Ocean Observing System (IOOS).

The mandatory QC tests are manufacturer-independent, i.e. they do not rely on particular variables or information provided only by a specific device.

These standard sets of tests have been defined both for radial and total velocity data and they are the required ones for labelling the data as Level 2B (for radial velocity) and Level 3B (for total velocity) data. Please refer to Appendix **Erreur ! Source du renvoi introuvable.** for the processing level definition.

Each QC test will result in a flag related to each data vector which will be inserted in the specific test variable. These variables can be matrices, in case the QC test evaluates each cell of the gridded data, or a scalar, in case the QC test assesses an overall property of the data.

Reference documentation on QC could be found in:

- IOOS-NOAA: HF-Radar Network Near-Real Time Ocean Surface Current Mapping
    - https://ioos.noaa.gov/wp-content/uploads/2016/06/HFRNet_QC-RTVproc.pdf
- SOCIB: Quality control of SOCIB HFR data.
    - http://www.socib.eu/files/documents/facilities/HFRADAR_QC_procedures.pdf

7. Glider

Mobile platforms are available in a variety of configurations and require different real-time QC considerations. Mobile platforms are, in order of increasing complexity: fixed vertical profilers, mobile surface vessels, and vessels freely operating in three dimensions (e.g., gliders, floats, powered AUVs).

Profiling gliders are self-propelled (buoyancy driven), autonomous underwater vehicles (AUVs) that are deployed for days-to- months and profile the water column collecting environmental data. There are many kind of gliders and quality control have agreed on the most commonly used. The QC procedures for temperature and salinity are derived from QARTOD and can be found in:

- IOOS: Manual for Quality Control of Temperature and Salinity Data Observations from Gliders.
    - https://ioos.noaa.gov/wp-content/uploads/2015/10/Manual-for-QC-of-Glider-Data_05_09_16.pdf

The FP7 GROOM project performed real time quality control (RTQC) tests on Chla, absolute diffuse irradiance and diffuse attenuation coefficient.

The project considered some aspects for Aanderaa optode oxygen sensor and real time salinity from un-pumped CTD.

GROOM defined procedures for automated Glider Data Quality Control to retrieve:
- Absolute Irradiances;
- Diffuse attenuation coefficient (K)

The focus was on the radiometric sensor OCR -504I for retrieving the upwelling irradiance (Ed) at four wavelengths (411.7 nm, 443.6 nm, 490.9 nm and 554.7 nm). The definition of DQC procedures has to take into account that OCR is a plane radiometer; therefore the best measurements are made when it is at 0 degrees angle with the horizontal

.

- http://www.groom-fp7.eu/lib/exe/fetch.php?media=public:deliverables:groom_d_3_02_ogs.pdf
- http://www.groom-fp7.eu/lib/exe/fetch.php?media=public:deliverables:groom_d_3_03_ifremer.pdf

In GROOM the following decisions were adopted:

- The NRT QC procedures for T&S derived from Argo QC procedure and EGO QC manual taking into account the changes agreed at meeting and updates already defined with MyOcean (now CMEMS).

- For Chlorophyll-A the NRT procedure developed jointly with BIO-Argo and are based on the development made within Pabim white book
    - (http://www.obs-vlfr.fr/OAO/file/PABIM_white_book_version1.3.pdf).

- For Oxygen parameter, there was an agreement to deliver Oxygen data using a common unit DOXY in micromole/kg whatever information is sent to shore by the float. The conversion method will be the one adopted by Argo and described in
    - http://www.argodatamgt.org/content/download/2928/21973/file/ARGO_oxygen_proposition_v1p2.pdf.

In a general way the QC procedures agreed for the gliders are adaptations of established Argo QC and the following implementations have been done:

- Valid range (e.g. TEMP, PRES, speed etc)
- Regional range
- Gradient
- Spike
- Stationary
- Position on land
- Density inversion

8. ARGO

Argo is an international program that calls for the deployment of 3,000 free drifting profiling floats, distributed over the global oceans, which will measure the temperature and salinity in the upper 2,000 m of the ocean providing 100,000 T/S profiles and reference velocity measurements per year. This allows continuous monitoring of the state of the ocean, with all data being made publicly available within hours after collection, for scientific use and assimilation into weather forecasting and climate prediction models.

The QC procedures for CTD and trajectory data are described with a two levels of control:

The first level is the real-time system that performs a set of agreed automatic checks.
The second level of quality control is the delayed-mode system.

These quality control procedures are applied to the parameters JULD, LATITUDE, LONGITUDE, PRES, TEMP, PSAL, and CNDC. The link to the 'Argo Quality Control Manual For CTD and Trajectory Data' is:

- http://archimer.ifremer.fr/doc/00228/33951/32470.pdf

The Argo quality control manual for biogeochemical data describes two levels of procedures:

The first level is the real-time system that performs a set of agreed automatic checks.

The second level is the delayed-mode quality control system.

The 'Argo quality control manual for biogeochemical data' is accessible through:

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- http://archimer.ifremer.fr/doc/00298/40879/42267.pdf

9. RTQC for Ferryboxes

Automated tests for ferrybox measurements are in a MyOcean Report ‘Real Time Quality Control of biogeochemical measurements’ (http://archimer.ifremer.fr/doc/00251/36232/34792.pdf). Recommended tests are based on RTQC for time series, but somehow modified due to the geospatial coverage of measurements.

The QC includes:

1. Impossible date test
2. Impossible location test
3. Frozen date/location/speed test

This tests checks whether the navigation system is updating. It should be performed on all measured parameters.

4. Speed range test

This test includes both a test for maximum speed and another one for minimum speed (some ferrybox systems are turned off at lower ship speed in order to avoid pumping of particles in harbours). Threshold values will depend on the ship capabilities and the area of navigation. This test replaces the impossible speed test.

5. Pump/ flow rate test

A test checking the state of the pump should be performed. If the Ferrybox is equipped with a flow rate meter (should be specified in metadata), threshold values should be applied for flagging of data

6. Pump history test

Pump should be working during a minimal period after it has been stopped in order to make sure water in the system has been renewed and stability has been achieved The correct threshold value will depend on the pump capacity and system design.

7. Global range test
8. Regional range test
9. Spike test
10. Gradient test

Horizontal spike and gradient tests must take into account the distance between adjacent measurements. This will depend on ship speed and data logging frequency. Moreover, only adjacent data measured at expected interval should be taken into account in the test. This test includes testing of spikes. Threshold values are likely to depend very much on regional specifications. However, as a first approach the same formulations and threshold values as for vertical profiles can be applied.

11. Stuck value test
12. Instrument comparison test
13. Parameter relationship test 19
14. Calibration status test
15. Subsequent trip test

The test is applied to Ferrybox Chl data only and aims to detect biofouling. Ferrybox systems are generally cleaned at regular intervals, but biofouling does still occur. The signal offset caused by the biofouling will increase with time as a result of increased amount of biofouling.

Most Ferrybox systems operate along fixed routes with a revisit frequency ranging from hours to several days. If the measured values of Chl-a fluorescence on one trip exceed the values from the previous trip along the entire (or most parts of the) transect, this indicates possible biofouling. This information can then be used to flag the data. The time step between two consecutive trips (or revisit time at specific locations) should also be taken into account. The test requires that the ferrybox is expected to pass different water masses (in order to reduce the risk of erroneous flagging of data during the start of a bloom event) and that it has a short revisiting time (max. 2-3 days).

Approach:

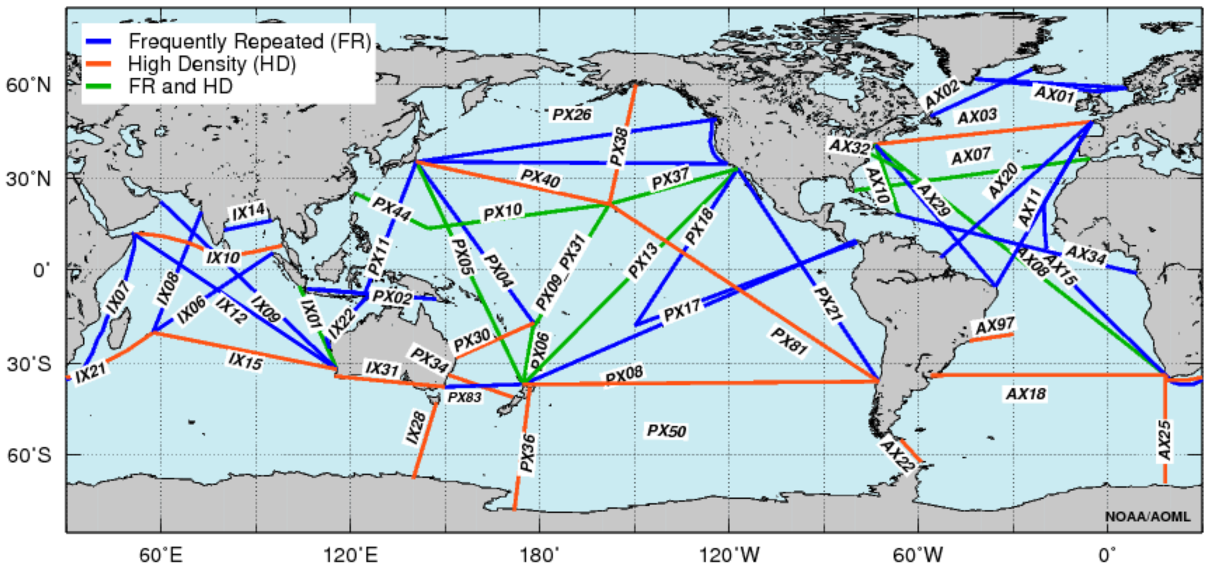
- The ferrybox transect is divided into 0.1x0.1 degree Lat/Lon boxes
  - For trip number N the mean of Chl values are calculated for each box and compared with values from the previous trip (N-1).
  - The test fails and data are flagged as bad data if CHLN > CHLN-1 for more than n % of the boxes. We propose to apply n = 75

10. XBT

An eXpendable BathyThermograph (XBT) is a probe that is dropped from a ship and measures the temperature as it falls through the water. A very thin wire transmits the temperature data to the ship where it is recorded for later analysis. The probe is designed to fall at a known rate, so that the depth of the probe can be inferred from the time since it was launched.

The transects are sampled in two modes: High Density (HD) and Frequently repeated (FR). All XBT transects are reviewed through an international consortium with oversight by the SOOP Implementation Panel (SOOPIP). Some transects include time series with more than 30 years of data.

Global XBT Network, OceanObs09 Recommendations



A number of papers with estimates of corrections have been published or submitted to scientific journals. The corrections proposed in some of these works are provided here to facilitate intercomparison by the scientific community.

Wijffels, Susan E., Josh Willis, Catia M. Domingues, Paul Barker, Neil J. White, Ann Gronell, Ken Ridgway, John A. Church, 2008: Changing Expendable Bathythermograph Fall Rates and Their Impact on Estimates of Thermosteric Sea Level Rise. J. Climate, 21, 56575672. doi: http://dx.doi.org/10.1175/2008JCLI2290.1 Wijffels et al. depth corrections: Table 1 (in situ comparison), Table 2 (in situ-altimeter comparison).

Ishii, M. and M. Kimoto, 2009: Reevaluation of Historical Ocean Heat Content Variations With An XBT depth bias Correction. J. Oceanogr. 65, 287299, doi:10.1007/s10872-009-0027-7. Ishii and Kimoto depth corrections. New corrections in conjunction with version 6.12* analysis of ocean temperature and salinity.

Gouretski, V. and F. Reseghetti, 2010, On depth and temperature biases in bathythermograph data: Development of a new correction scheme based on analysis of a global ocean database. Deep-Sea Research I, Vol. 57(6), pp. 812-834, doi:10.1016/j.dsr.2010.03.011, Gouretski, Reseghetti depth and temperature corrections, updated corrections.

Good, S.A, 2011,Depth biases in XBT data diagnosed using Bathymetry data ,Journal of Atmospheric and Oceanic Technology, 28, 287-300, doi: 10.1175/2010JTECHO773.1 Good depth corrections.

Hamon, M., G. Reverdin, P-Y Le Traon, 2012, Empirical correction of XBT data. Journal of Atmospheric and Oceanic Technology, doi:10.1175/JTECH-D-11-00129.1.

Gouretski, V., 2012, Using GEBCO digital bathymetry to infer depth biases in the XBT data, Deep Sea Research-I, 62,40-52. Gouretski depth and temperature corrections.

Cowley, R., S. Wijffels, L. Cheng, T. Boyer, S. Kizu: Biases in Expendable BathyThermograph data: a new view based on historical side-by-side comparisons, Journal of Atmospheric and Oceanic Technology, 30, 11951225, doi:10.1175/JTECH-D-12-00127.1. XBT pairs database used in study. Thermal gradient correction (TG), Cheng correction (CH).

Lijing Cheng, Jiang Zhu, Rebecca Cowley, Tim Boyer, and Susan Wijffels, 2014: Time, Probe Type, and Temperature Variable Bias Corrections to Historical Expendable Bathythermograph Observations. J. Atmos. Oceanic Technol., 31, 1793-1825, doi:10.1175/JTECH-D-13-00197.1. CH14 method to correct XBT Depth and Temperature bias. Note: Original Table 2 was replaced by an updated Table 2 on February 15, 2017. Updated table from personal communication - Lijing Cheng.

For the Mediterranean there are also many papers on XBT QA/QC procedures:

Manzella, G. M. R., Scoccimarro, E., Pinardi, N., and Tonani, M.: Improved near real-time data management procedures for the Mediterranean ocean Forecasting System-Voluntary Observing Ship program, Ann. Geophys., 21, 49-62, doi:10.5194/angeo-21-49-2003, 2003.

Manzella, G. M. R., Reseghetti, F., Coppini, G., Borghini, M., Cruzado, A., Galli, C., Gertman, I., Gervais, T., Hayes, D., Millot, C., Murashkovsky, A., Özsoy, E., Tziavos, C., Velasquez, Z., and Zodiatis, G.: The improvements of the ships of opportunity program in MFS-TEP, Ocean Sci., 3, 245-258, doi:10.5194/os-3-245-2007, 2007.

Reseghetti, F., Borghini, M., and Manzella, G. M. R.: Factors affecting the quality of XBT data – results of analyses on profiles from the Western Mediterranean Sea, Ocean Sci., 3, 59-75, doi:10.5194/os-3-59-2007, 2007.

11. Surface drifters

The modern drifter is a high-tech version of the "message in a bottle". It consists of a surface buoy and a subsurface drogue (sea anchor), attached by a long, thin tether. The buoy measures temperature and other properties, and has a transmitter to send the data to passing satellites. The drogue dominates the total area of the instrument and is centered at a depth of 15 meters beneath the sea surface.

11.1. Data transmission and drifter location

The drifter sensors measure data such as sea surface temperature, average the data over a window (typically 90 seconds), and transmit the sensor data at 401.65 MHz. Each drifter transmitter is assigned a Platform Terminal Transmitter (PTT) code, often referred to as the drifter ID.

Argos is a satellite-based system for collecting, processing and distributing data. It is operated by Collecte Localisation Satellites in Toulouse, France with a subsidiary (Service Argos, Inc.) in Largo, Maryland USA.

The position of a drifter is not usually given by the familiar Global Positioning System (GPS). Instead, it is inferred from the Doppler shift of its transmission as seen by the satellite and described in the Argos Users Manual. Argos specifies the accuracy of position fixes according to a location class: class one (350-1000 meters error), class two (150-350 meter error) and class three (less than 150 meter error).

11.2. Drifter data: quality control, interpolation and coverage

Drifter locations are estimated from 16-20 satellite fixes per day, per drifter. AOML's Drifter Data Assembly Center (DAC) assembles these raw data, applies quality control procedures, and interpolates them to regular 1/4-day intervals. The raw observations and processed data are archived at the DAC and at Canada's Marine Environmental Data Service.

11.3. Quality control

The DAC first visually examines drifter data for evidence that the data were transmitted while on the deck of a ship, the drifter was aground, or the drifter has been picked up by a boater. These drifters are usually apparent from their trajectories, and can be supported by submergence values and the diurnal variations in temperature. These observations are removed from the data set.

Next, the DAC identifies drifters which have lost their drogues. This is done using the submergence or tether strain observations. The drogue lost dates are compiled in a directory file that includes each drifter's deployment time and location, ending time and location, and the type of death (picked up, ran aground, stopped transmitting, ...). These dates are stored using a modified Julian day convention in which "day 1" is January 1, 1979. For a drifter that never lost its drogue, the directory file holds the placeholder value 0 for drogue off time while it is still alive (still transmitting good data), or the date of its final reliable transmission if it has died.

To eliminate the more egregious errors in raw Argos fixes, the DAC applies a two-step quality control scheme (Hansen and Poulain, 1996). In this scheme the velocity is calculated by finite differencing the raw fixes both forward and backward in time. A fix is flagged as "bad" if it produces a velocity greater than four standard deviations from the mean for both forward and backward passes. Two-way differencing is used because a forward-only calculation may fail to identify a bad fix if it comes immediately after a gap in data acquisition.

11.4. Interpolation

The raw fixes are interpolated to uniform six hour intervals using an optimal interpolation procedure known as kriging. For more information, see Hansen and Poulain (1996). Latitude, longitude and temperature are interpolated independently.

Along with the interpolated positions, the DAC provides formal error bars on the positions. These error bars identify large gaps (as long as two weeks) across which the data have been interpolated.

Following interpolation, the zonal and meridional components of velocity are calculated via centered finite differencing over 1/2 day displacements. Many investigators interested in subinertial motion (e.g., Ralph and Niiler, 1999; Fratantoni, 2001; Lumpkin and Garzoli, 2005) apply a lowpass filter to these velocities before proceeding with their analyses.

11.5. Velocity observations

SVP drifters do not perfectly follow the water column averaged over the drogue depth. For example, water can downwell (sink to great depths from the surface), while the drifter is forced to stay at the sea surface. Also, the drifter can "slip" through the water. The resulting speed of the drifter is thus a combination of the large-scale currents at 15 meters depth, plus the upper-ocean wind-driven flow, plus the slip.

11.6. Slip

Slip is the horizontal motion of a drifter that differs from the lateral motion of currents averaged over the drogue depth. Slip is caused by wind on the surface float, drag on the float and tether, and rectification of surface waves (Niiler et al., 1987; Geyer, 1989). In order to reduce rectification, the surface float is spherical (Niiler et al., 1987, 1995). The original SVP design included a 20 cm diameter subsurface float between the surface float and drogue, intended to decouple their motion and to provide additional buoyancy offsetting the weighted drogue. The subsurface float has been omitted in the recent mini drifter redesign.

The most important design characteristics that minimize slip are low tension between the surface buoy and drogue, which avoids aliasing wave motion, and a large drag area ratio (Niiler et al., 1987). As long as the drogue remains attached to the drifter, the downwind slip is estimated at 0.7 cm/s per 10 m/s of wind speed (Niiler and Paduan, 1995). If an SVP drifter loses its drogue, it will slip downwind at a speed of 8.6 cm/s per 10 m/s of wind (Pazan and Niiler, 2001).

11.7. Ekman drift

Currents at the ocean surface are caused by many different forces. At very large scales, many currents are associated with a dynamical balance between a pressure force and the Coriolis force. These currents are called "geostrophic". Currents described by a balance of different forces are "ageostrophic". The most common ageostrophic current seen in the upper ocean is the directly wind-driven Ekman drift (Ekmank 1905; see here for a detailed description of Ekman drift).

Several recent studies have examined how the combination of geostrophic and Ekman drift determines how a drifter moves through the water. For more details, see Niiler and Paduan (1995), Ralph and Niiler (1999), Niiler (2001) and Rio and Hernandez (2003).

11.8. Other observations

- Sea surface temperature (SST): All standard SVP drifters measure temperature 20-30 cm beneath the sea surface. These data are disseminated on the Global Telecommunication System (GTS) by Argos within two hours of reception for use in numerical weather forecasting and operational SST analysis, and for calibrating satellite-derived SST fields such as the NOAA Optimum Interpolation and TMI/AMSRE products.
- Barometric pressure: Many drifters, known as SVP-Bs, have been outfitted with a barometer to measure air pressure. Large-scale experimental deployments began in 1994; operational barometric observations have been collected since 1997. These data are particularly valuable in numerical weather prediction at high latitudes, where few in-situ observations are available if a storm develops outside the major shipping lanes. The barometer port extends 20 cm above the top of the surface float to minimize spuriously high spikes in the pressure record associated with submergence.
- Wind: Some drifters include a hydrophone for noise level, which can be converted to wind speed and precipitation estimates, and a 25 cm by 20 cm wind vane mounted to the barometer port of the surface float (with accompanying two-axis tilt sensor in the float, and swivel connection for the tether) to measure wind direction. SVP drifters of this type are known as Minimets (Milliff et al., 2003). The WOTAN hydrophone is typically mounted either on the tether, at a depth of 11 m, or between the tether and drogue top. Recent air deployments of these drifters in the paths of hurricanes Fabian and Isabel (2003), Frances and Jeanne (2004) and Rita (2005) have demonstrated the ability to measure the wind direction to within 10 degrees, mapping the circulation of the hurricane more clearly than in QuikSCAT satellite data.
- Ocean color: Some drifters have included an upwelling radiance sensor mounted on the surface float just beneath the sea surface, along with a downwelling irradiance sensor (Letelier et al., 1996).
- Salinity: The first salinity-measuring drifters were developed at Scripps Institution of Oceanography (SIO) by attaching a SeaBird SeaCat (thermistor and conductivity) to the top of the drogue (11 m depth). In 1992-3, 72 of these drifters were deployed in the tropical Pacific and provided observations which compared favourably to the TAO mooring data (Kennan et al., 1998). Four of these drifters were recovered after 310 days at sea, with post-calibration revealing a maximum offset of 0.02 psu. More recently, drifters have been developed which can measure surface salinity. Biofouling presents the major challenge to obtaining extended observations of surface salinity. Ongoing experiments are varying the antifouling paint and the pumping systems for the SeaBird Microcats. A current Global Drifter Program project involves SVP-Microcat pairs deployed in the Bay of Biscay west of France, each pair consisting of one drifter with pumping and one without, with sequential recoveries to evaluate the success and necessity of pumping. In the future, drifter salinity observations will provide calibration and validation for satellite-derived sea surface salinity products.
- Subsurface temperature: Several drifter manufacturers are developing drifters with thermistor chains to measure temperature profiles of the ocean s upper O(100 m). These observations would be invaluable for measuring mixed layer heat content variability, which can be poorly correlated with SST changes (Kelly, 2004). An array of drifters including eight with thermistor chains were air-deployed ahead of Hurricane Rita in September 2005, successfully providing upper ocean heat measurments in the Gulf of Mexico prior to the storm's landfall near the Texas/Louisiana border.

12. Thermodynamic properties of sea waters

There is still a certain variety of algorithms used for the calculation of the temperature (IPTS-68, ITS-90) and salinity (PSS-78, EOS-80, TEOS-10).

In recent years some considerations on the thermodynamics aspects of seawater, ice and moist air suggested to redefine the thermodynamic properties of these substances. The following reasons leaded to new formulations of the sea water properties:

1. Polynomial expressions of the International Equation of State of Seawater (EOS-80) were not totally consistent each other as they were not exactly obeying the thermodynamic Maxwell cross-differentiation relations.
2. More accurate and more broadly applicable thermodynamic description of pure water was developed since the late 1970s as well as more accurate measurements of heat capacity and temperature maximum density.
3. A new standard model of sea water composition was conceived as a result of an improved understanding of the impact on sea water density of the variation of its composition.

TEOS-10 is based on a Gibbs function formulation from which all thermodynamic properties of seawater (density, enthalpy, entropy sound speed, etc.) can be derived in a thermodynamically consistent manner. TEOS-10 was adopted by the Intergovernmental Oceanographic Commission at its 25th Assembly in June 2009 to replace EOS-80 as the official description of seawater and ice properties in marine science.

A notable difference of TEOS-10 compared with EOS-80 is the adoption of Absolute Salinity (mass fraction of salt in seawater) instead of the Practical Salinity (which is essentially a measure of the conductivity of seawater). Absolute Salinity (g/kg) is an SI unit of concentration. The thermodynamic properties of seawater, such as density and enthalpy, are now correctly expressed as functions of Absolute Salinity rather than being functions of the conductivity of seawater. Spatial variations of the composition of seawater mean that Absolute Salinity is not simply proportional to Practical Salinity; TEOS-10 contains procedures to correct for these effects.

To avoid some drastic and probably not safe changes with respect to the previous practices, it was decided that the salinity that is reported to national databases must remain Practical Salinity as determined on the Practical Salinity Scale of 1978. The practice of storing one type of salinity in national databases (Practical Salinity), but using a different type of salinity in publications (Absolute Salinity), was thought to be analogous to existing practice with temperature; in situ temperature should be stored in databases (since it is the measured quantity), but the temperature variable that is used in publications is a calculated quantity, being potential temperature to date under EOS-80, and from 2010, Conservative Temperature under TEOS-10. To avoid confusion while the use of Practical Salinity in scientific publications is phased out, authors and editors are requested to ensure that salinity is specifically identified as being either Practical Salinity (SP) or Absolute Salinity (SA). In addition, the method used to compute the location-dependent relationship between SP and SA should be explicitly stated.

The more prominent advantages of TEOS-10 compared with EOS-80 are:

- For the first time the influence of the spatially varying composition of sea water is systematically taken into account through the use of Absolute Salinity. In the open ocean, this has a non-trivial effect on the horizontal density gradient, and thereby on the ocean velocities and transports calculated via the ‘‘thermal wind’’ relation.
- The new salinity variable, Absolute Salinity, is measured in SI units (e.g. g kg^{-1}).
- The Gibbs function approach of TEOS-10 allows the calculation of internal energy, entropy, enthalpy, potential enthalpy and the chemical potentials of sea water as well as the freezing temperature, and the latent heats of freezing and of evaporation. These quantities were not available from EOS-80 but are essential for the accurate accounting of ‘‘heat’’ in the ocean and for the consistent and accurate treatment of air-sea and ice-sea heat fluxes in coupled climate models.

- In particular, Conservative Temperature Θ accurately represents the "heat content" per unit mass of sea water, and is to be used in place of potential temperature θ in oceanography.
- The thermodynamic quantities available from TEOS-10 are totally consistent with each other; this was not the case with EOS-80.

12.1. Comments on sea water properties management

During the approval process of TEOS-10 it was clearly underlined that the algorithms for the computation of temperature and salinity will evolve in the future (especially salinity).

It was also considered that most of the databases have stored salinity in PS units, and transformation in AS units would be not easy and could create some inconsistencies. For this reason was suggested to maintain salinity in PS units and in situ temperature in databases, as a practice for long term archival.

However comparability and compatibility problems could remain due to legacy of old databases, where could be found salinity values in PPT or in PSS. It is necessary that the databases contain also information on units, instruments and methodologies used to derive salinity and temperature values. This information allows the use for studies on long term changes, climatology, trends, etc.

The way the instruments are affecting studies is shown in table 1, where temperature accuracy is reported for different technologies.

Instrument	Temp precision (°C)	Depth precision	Year (from)
Nansen bottles	0.01	1.5%–6% FS	1897
STD	0.1	?	1965
CTD	0.001	0.015% FS	1967
MBT	0.2	1% Z	1940
XBT	0.1	2% Z	1966

Table 1. Temperature and depth accuracy for different instruments (from Manzella and Gambetta, 2013).

The estimated accuracy during the decades of temperature, salinity, density and depth is given in table 2.

Parameter	1908 - 1970	1970 – 1980	1980 – 2009
Temp (°C)	0.01	0.05	0.005
Salinity (PSU)	0.02	0.1	0.02
Density	0.02	0.1	0.002
Depth	5 m	1 dbar	0.5 dbar

Table 2. Estimated accuracy during decades (from Manzella and Gambetta, 2013)

A recommendation for data managers could be the storage of 'primitive' parameters, such as conductivity instead of salinity and in situ temperature, providing at the same time the necessary information that would allow the conversion with new algorithms.

Manzella and Gambetta (http://journals.ametsoc.org/doi/pdf/10.1175/JTECH-D-11-00218.1) have proposed a series of QC tests that can provide information on how data are comparable in the context of climate changes.

It must be underlined that there are currently established certified standardizations for temperature measurements (ITS90, traceable to SI using Standard Platinum Resistance Thermometer, SPRT) and salinity measurements (comparability ensured using IAPSO salinity standard seawater provided by OSI, UK).

GSW Oceanographic Toolbox has been developed within SCOR-IAPSO initiatives to calculate the thermodynamic properties of sea water (reference is: McDougall, T.J. and P.M. Barker, 2011: Getting started with TEOS-10 and

the Gibbs Seawater (GSW) Oceanographic Toolbox, 28pp., SCOR/IAPSO WG127, ISBN 978-0-646-55621-5. – link to software: http://www.teos-10.org/software.htm).

13. Nutrients and chemical measurements

There have been important initiatives in Europe and at global level to assess the validity of chemical data. In Europe a project named 'Quality Assurance of Information for Marine Environmental Monitoring in Europe' (QUASIMEME) was founded in 1992 for four years. A routine laboratory performance studies has provided the basis of an external quality assurance for institute collecting chemical data in the marine environment. Actually QUASIMEME is part of an accreditation system based on ISO 17043 carried out within the Dutch initiative WEPAL (Wageningen Evaluating Programmes for Analytical Laboratories).

The 2007 IPCC Report highlighted the problem inherent to chemical data sets stating that: "Uncertainties in deep ocean nutrient observations may be responsible for the lack of coherence in the nutrient changes. Sources of inaccuracy include the limited number of observations and the lack of compatibility between measurements from different laboratories at different times" (Bindoff et al., 2007 – https://www.ipcc.ch/publications_and_data/ar4/wg1/en/ch5.html).

13.1. Nutrients

Nutrients have been measured since the very earliest day of scientific ocean observations, back in the 19th century. However, studies on ocean climate changes based on nutrient data have hardly been made, because to poor comparability of historical nutrient data sets.

Discrepancies up to 10% was resulting from analysis of nutrient concentrations from global crossover station (Aoyama et al., 2015)[1].

An inter-laboratory comparison exercise similar to QUASIMEME since 2003 showed a similar magnitude of discrepancy among some participant laboratories ([1]). The errors were attributed to analytical problems and to the need to have Certified Reference Materials (CRM) to be established by the authority of a SCOR Working Group.

Established certified standardisations are existing for temperature and salinity, as well as carbonate system parameter measurements (comparability and traceability ensured using CRMs). Similarly, changes to oceanic oxygen can now also be accurately observed (Standardo and Gruber, 2012 – http://onlinelibrary.wiley.com/doi/10.1029/2012JC007909/abstract). CRMs for oceanographic use have been developed during the last decade. These include a Danish RM from Water Quality Institute (VKI), National Research Council - Canada CRM (MOOS-3), and one developed by KANSO-Japan. In 2015 the National Metrology Institute of Japan (NMIJ) started to provide CRMs (NMIJ CRM 7601-a, NMIJ CRM 7602-a, and NMIJ CRM 7603-a) with nutrient concentrations appropriate for the nutrient concentration ranges of Nitrate, Nitrite, Silicate and Phosphate found in the Pacific and Atlantic Oceans. MOOS-3 covers nutrient concentrations specifically for the Atlantic Ocean.

By putting together all the experiences the SCOR WG #147 established the mechanisms required to provide comparability of oceanic nutrient data, using globally accepted CRMs. A major challenge with this SCOR WG is to develop a system by which the comparability of data within and between laboratories is better than 1% at full scale of nitrate, phosphate and silicate concentrations.

Water samples have been collected in different oceans by different institutions at different levels, as shown in the table below (updated to January 2017):

No.	Level of seawater	Resource of seawater	Bottling	Certification

[1] For all Ayoama et al. Publications refer to https://researchportal.port.ac.uk/portal/en/publications/ioccpjamstec-2015-interlaboratory-calibration-exercise-of-a-certified-reference-material-for-nutrients-in-seawater(5cfcc734-fd96-4a32-8bc8-a796e935228e).html

1	Low in Atlantic	NIOZ	Oct. 2015	Sep 2016
2	Middle in Atlantic			
3	Middle in Pacific	JAMSTEC	Apr. 2016	Jan 2017
4	High in Pacific	JAMSTEC	Dec 2015	Sep 2016
5	High in Atlantic			

13.2. Greenhouse gases

Understanding and quantifying ocean-atmosphere exchanges of the climate-relevant trace gases nitrous oxide (N_2O) and methane (CH4) is important for understanding the global biogeochemical cycles of carbon and nitrogen in the context of ongoing global climate change.

The SCOR WG #143 started actions to improve and consolidate measurements of the greenhouse gases nitrous oxide (N_2O) and methane (CH4) dissolved in seawater. The work is based on inter-calibration exercises targeting discrete N_2O and CH4 measurements and on recommendations and protocols for calibration, quantification, and data reporting. A second base of the activity is an overall assessment on the status of dissolved N_2O and CH4 measurements in the global oceans and the identification of key regions and recommendations on the necessary temporal and spatial scale for sampling.

Production of the gas standards became a top priority. A contractual agreement was established between NOAA PMEL and the University of Hawaii for the production of the standards. The gas standards have been shipped in June 2016 to the Working Group members.

13.3. Comments on nutrients and chemicals management

The primary goal for the SCOR Working Group #147 is for nutrient data collected at any one place by an individual laboratory and data collected over long time periods by one or more laboratories to be consistent with certified comparability. The initiative is based on previously developed collaboration with the IOC-ICES SGONS that ended in 2012.

The SCOR Working Group #143 is working on climate-relevant trace gases nitrous oxide (N_2O) and methane (CH4).

Both groups have put their attention on intercalibration and on the establishment of Certified Reference Materials. But the most important output of the SCOR WG is that the influence of the spatially varying composition of sea water must be systematically taken into account. Also in this case, it is important to complement the data with information on instruments used for the analysis with other information on CRM and methodology used.

14. IOC Quality flag scheme and existing second level applications

IOC in the Manuals and guides No. 54, Ocean Data Standards, Vol.3: Recommendation for a Quality Flag Scheme for the Exchange of Oceanographic and Marine Meteorological Data is proposing a two level quality flag scheme:

14.1. Primary Level

The first or primary level is composed of five quality values and their definitions (Table 1).

Table 1: Primary level

Value	Primary-level flag short name	Definition
1	Good	Passed documented required QC tests
2	Not evaluated, not available or unknown	Used for data when no QC test performed or the information on quality is not available
3	Questionable/suspect	Failed non-critical documented metric or subjective test(s)
4	Bad	Failed critical documented QC test(s) or as assigned by the data provider
9	Missing data	Used as place holder when data are missing

The flagging scheme can be applied to any type of data. The Primary Level is intended for data users that need only basic data quality flags.

14.2. Secondary level

The secondary level complements the primary level flags by reporting the results of specific QC tests performed and data processing history. The secondary level content varies in number and description and is chosen by those who implement the scheme, representing information on the applied quality tests (e.g., excessive spike check, regional data range check) and data processing history (e.g., interpolated values, corrected values).

Table 2: An example of quality control tests and data processing history

Example quality control tests / data processing history (description)
Globally impossible value
Monthly climatology standard deviation test
Excessive spike check
Excessive offset/bias when compared to a reference data set
Excessive data uncertainty
Unexpected X/Y ratio (e.g., chemical stoichiometry or property-property X to T, S, density, among others)
Excessive spatial gradient or pattern check (“bullseyes”)
Below detection limit of method
Interpolated value (not measured)
Data offset corrected value relative to a reference data
Expert review

The secondary level tests and their results can be specified as needed. While providing the secondary level information is not mandatory, it is highly recommended that the secondary level be used to explain fully the primary level flags. As shown in the example below, the results of many quality tests can be represented by values.

14.3. ODV generic quality flags

Code	Description
0	Good

1	Unknown
4	Questionable
8	Bad

14.4. QARTOD quality flags – proposed, not yet definitive

Code	Description
0	Quality not evaluated
1	Bad
2	Questionable/suspect
3	Good
9	Missing data

14.5. OceanSITES quality flags – proposed, not yet definitive

Code	Description
0	No QC was performed
1	Good data
2	Probably good data
3	Bad data that are potentially correctable
4	Bad data
5	Value changed
7	Nominal value
8	Interpolated value
9	Missing value

14.6. GTSPP quality flags

Code	Description
0	No quality control has been assigned
1	QC was performed; appears to be correct
2	QC was performed; probably good
3	QC was performed; appears doubtful
4	QC was performed; appears erroneous
5	The value was changed as a result of QC
9	The value is missing

14.7. SeaDataNet quality flags

Code	Description
0	No quality control
1	Good value
2	Probably good value
3	Probably bad value
4	Bad value
5	Changed value
6	Value below detection

7	Value in excess
8	Interpolated value
9	Missing value
A	Value phenomenon uncertain

14.8. BODC

Code	Description
<	Below detection limit
>	In excess of quoted value
A	Taxonomic flag for affinis (aff.)
B	Beginning of CTD down/up cast
C	Taxonomic flag for confer (cf.)
D	Thermometric depth
E	End of CTD down/up cast
H	Extrapolated value
I	Taxonomic flag for single species (sp.)
K	Improbable value, unknown QC source
L	Improbable value, originators QC
M	Improbable source, BODC QC
N	Null value
O	Improbable value, user QC
P	Trace/calm
Q	Indeterminate
R	Replacement value
S	Estimated value
T	Interpolated value
U	Uncalibrated
W	Control value
X	Excessive difference

14.9. NODC WOD (observed levels)

Code	Description
0	Accepted value
1	Range outlier
2	Failed inversion check
3	Failed gradient check
4	Observed level “bullseye” flag and zero gradient check
5	Combined gradient and inversion checks
6	Failed range and inversion checks
7	Failed range and gradient checks
8	Failed range and questionable data checks
9	Failed range and combined gradient and inversion checks

15. Mapping the IODE quality flag scheme to existing quality flag schemes.

15.1. Mapping the ODV scheme

ODV scheme		Proposed quality flag scheme			Comments
Flag code	Flag description	Primary-level flag code	Primary-level flag description	Secondary-level flag description (held in a code table)	
0	Good	1	Good	Expert review	Unless the exact list of quality checks is provided
1	Unknown	2	Not evaluated, not available or unknown	Expert review	Unless the exact list of quality checks is provided
4	Questionable	3	Questionable	Expert review	Unless the exact list of quality checks is provided
8	Bad	4	Bad	Expert review	Unless the exact list of quality checks is provided

15.2. Mapping the WOCE water sample scheme

WOCE water sample		Proposed quality flag scheme			Comments
Flag code	Flag description	Primary-level flag code	Primary-level flag description	Secondary-level flag description (held in a code table)	
1	Sample for this measurement was drawn from water bottle, but analysis not received	9	Missing data	Sample was collected, but analysis not received due to unknown reason	
2	Acceptable measurement	1	Good	Expert review	Unless the exact list of quality checks is provided
3	Questionable measurement	3	Questionable	Expert review	Unless the exact list of quality checks is provided
4	Bad measurement	4	Bad	Expert review	Unless the exact list of quality checks is provided
5	Data were expected to be measured, but the observation is missing due to sample loss, contamination, etc.	9	Missing data	Sample was collected, but the observation is missing due to sample loss, contamination, etc.	

6	Mean of replicate measurements	2	Not evaluated, not available or unknown	Mean of replicate measurements	Because no information was provided on the quality of the replicate measurements, this can only be mapped to 2 in the new scheme. However, once checks are applied and the data are considered good then the primary flag can be changed to 1 and secondary flags are added.
7	Manual chromatographic peak measurement	2	Not evaluated, not available or unknown	Manual chromatographic peak measurement	
8	Irregular digital chromatographic peak integration	2	Not evaluated, not available or unknown	Irregular digital chromatographic peak integration	
9	Sample not drawn for this measurement from this bottle	9	Missing data	Sample not collected for this measurement	

15.3. Mapping the GTSPP scheme

GTSPP scheme		Proposed quality flag scheme			
Flag code	**Flag description**	**Primary-level flag code**	**Primary-level flag description**	**Secondary-level flag description (held in a code table)**	**Comments**
0	No quality control has been assigned	2	Not evaluated, not available or unknown	Sample collected but QC tests were not applied	
1	QC was performed; appears to be correct	1	Good	Expert review	Unless the exact list of quality checks is provided
2	QC was performed; probably good	1	Good	Expert review	Unless the exact list of quality checks is provided
3	QC performed; appears doubtful	3	Questionable	Expert review	Unless the exact list of quality checks is provided
4	QC performed; appears erroneous	4	Bad	Expert review	Unless the exact list of quality checks is provided

5	The value was changed as a result of QC	1	Good	Changed value; Expert review	Once checks are applied, secondary flags are added.
9	The value is missing	9	Missing data	Not reported	

15.4. Mapping the SDN scheme

SDN scheme		Proposed quality flag scheme			Comments
Flag code	**Flag description**	**Primary-level flag code**	**Primary-level flag description**	**Secondary-level flag description (held in a code table)**	
0	No quality control	2	Not evaluated, not available or unknown	Sample collected but QC tests were not applied	
1	Good value	1	Good	Expert review	Unless the exact list of quality checks is provided
2	Probably good value	1	Good	Expert review	Unless the exact list of quality checks is provided
3	Probably bad value	3	Questionable	Expert review	Unless the exact list of quality checks is provided
4	Bad value	4	Bad	Expert review	Unless the exact list of quality checks is provided
5	Changed value	1	Good	Changed value; Expert review	Once checks are applied, secondary flags are added.
6	Value below detection	4	Bad	Detection limit	
7	Value in excess	4	Bad	Excess limit	
8	Interpolated value	1	Good	Interpolated value	
9	The value is missing	9	Missing data	Not reported	
A	Value phenomenon uncertain	3	Questionable	Expert review	Unless the exact list of quality checks is provided