Second IODE Workshop on Quality Control of Chemical and Biological Oceanographic Data Collections

IOC Project Office for IODE
Oostende, Belgium, 22-24 October 2012
# TABLE OF CONTENTS

1. OPENING OF THE MEETING
   1.1 INTRODUCTIONS OF PARTICIPANTS
   1.2 ADOPTION OF THE AGENDA
   1.3 INTRODUCTION OF WORKING DOCUMENTS

2. AN OVERVIEW OF OCEANOGRAPHIC QUALITY CONTROL AND QUALITY ASSESSMENT SCHEMES AND THE BASIS FOR A STANDARD OF SCHEME
   2.1 PRESENTATIONS BY PARTICIPANTS
      2.1.1 DOKUZ EYLÜL UNIVERSITY, INSTITUTE OF MARINE SCIENCES AND TECHNOLOGY: NIHAYET BIZSEL
      2.1.2 EXAMPLES OF DATA QUALITY INDICATORS FOR DATA CONTRIBUTED TO BCO-DMO: MS CYNDY CHANDLER
      2.1.3 QUALITY CONTROL ON BIOLOGICAL DATA BEFORE AND AFTER DATA INTEGRATION: KLAAS DENEUDT, VLIZ, BELGIUM
      2.1.4 QUALITY CONTROL OF BOTTLE DATA AT INSTITUT MAURICE-LAMONTAGNE - FISHERIES AND OCEANS CANADA QUÉBEC REGION - LAURE DEVINE AND CAROLINE LAFLEUR
      2.1.5 THE QUALITY ASSURANCE/QUALITY CONTROL (QA/QC) PROCEDURE (GLODAP EXAMPLE) – ALEX KOZYR
      2.1.6 QUALITY CONTROL AND QUALITY FLAG OF PACIFICA – TORU SUZUKI, MARINE INFORMATION RESEARCH CENTER, JAPAN
      2.1.7 UKRAINIAN NODC (MARINE HYDROPHYSICAL INSTITUTE AND INSTITUTE OF BIOLOGY OF THE SOUTHERN SEAS, SEVASTOPOL) – SERGEY KONOVALOV, ALEXEY KHALIULIN (MHI), VOLODYMYR VLADYMYROV (IBSS)
      2.1.8 WORLD OCEAN DATABASE DATA QUALITY CONTROL – HERNAN GARCIA, NOAA NATIONAL OCEANOGRAPHIC DATA CENTER, SILVER SPRING, MD 20910, USA
      2.1.9 GLOBAL TEMPERATURE AND SALINITY PROFILE PROGRAMME (GTSPP) DATA QUALITY TESTS – CHARLES SUN, CHAIR SG-GTSPP
      2.1.10 QUALITY CONTROL OF CTD DATA USING PROPOSED IODE QF SCHEME – GREG REED, ANDREW WALSH, RAN HYDROGRAPHY AND METOC BRANCH
      2.1.11 SEADATANET QC, FLAGS AND EMODNET CHEMISTRY EXPERIENCE – MATTEO VINCI, ALESSANDRA GIORGETTI, OGS NODC, TRIESTE, ITALY

3. AN OVERVIEW OF THE PROPOSED STANDARD QF SCHEME
   3.1 JUSTIFICATION OF THE NEED FOR QF/QC STANDARD FOR DATA EXCHANGE
   3.2 THE STANDARD PROPOSAL
   3.3 COMMENTS BY THE AD HOC ODS GROUP
   3.4 CURRENT SITUATION AND FURTHER STEPS

4. QUALITY TESTS AND QUALITY FLAGS
   4.1 ASSIGNMENT AND RELATIONSHIP BETWEEN QUALITY FLAG (QF) AND MEASURED OR CALCULATED DATA (DATA FIT FOR PURPOSE)
   4.2 MINIMUM RECOMMENDED LIST OF SL FLAG CODES AND WORKING TOWARDS AND DOCUMENTED APPROACH
   4.3 RELATIONSHIP BETWEEN EXISTING QF AND RESULTS OF ADDITIONAL QUALITY TESTS (CLOSED VS OPEN SL FLAG LIST)

5. WRAP-UP SESSION

6. CLOSING OF THE MEETING
ANNEXES

ANNEX I: Agenda of the Meeting
ANNEX II: List of Participants
ANNEX III: Quality Flag Scheme for the exchange of oceanographic and marine meteorological data
The Intergovernmental Oceanographic Commission (IOC) of UNESCO celebrates its 50th anniversary in 2010. Since taking the lead in coordinating the International Indian Ocean Expedition in 1960, the IOC has worked to promote marine research, protection of the ocean, and international cooperation. Today the Commission is also developing marine services and capacity building, and is instrumental in monitoring the ocean through the Global Ocean Observing System (GOOS) and developing marine-hazards warning systems in vulnerable regions. Recognized as the UN focal point and mechanism for global cooperation in the study of the ocean, a key climate driver, IOC is a key player in the study of climate change. Through promoting international cooperation, the IOC assists Member States in their decisions towards improved management, sustainable development, and protection of the marine environment.
1. OPENING OF THE MEETING

Dr. Hernan Garcia (HG) and Dr. Sergey Konovalov (SK), Co-Chairs of the meeting, welcomed the participants to the meeting. Mr. Peter Pissierssens (PP) welcomed the participants to the IOC Project Office for IODE in Oostende, Belgium and provided information on local arrangements. He then introduced the agenda (attached in Annex I).

1.1 Introductions of participants

The participants were invited to introduce themselves. The list of participants is attached as Annex II.

1.2 Adoption of the agenda

The meeting adopted the agenda after a slight modification. The Agenda is attached as Annex I.

1.3 Introduction of working documents

The Co-Chair, Dr. Garcia introduced the working document “Proposal to adopt a quality flag scheme standard for data exchange in oceanography and marine meteorology, Version 1.2 March 2012”. Dr Garcia invited comments on the proposal not later than 12h00 on 23 October 2012.

2. AN OVERVIEW OF OCEANOGRAPHIC QUALITY CONTROL AND QUALITY ASSESSMENT SCHEMES AND THE BASIS FOR A STANDARD QF SCHEME

2.1 Presentations by participants

2.1.1 Dokuz Eylül University, Institute of Marine Sciences and Technology:
Nihayet Bizsel


Dr. Bizsel explained that the National Monitoring Programme of Turkey in the framework of MED POL Phase IV includes the monitoring of pollution trends at hot spots, the monitoring of river inputs, the compliance monitoring of effluents and the monitoring of contaminant levels in biota and sediments to follow long-term changes of the chemical pollution status of the coastal waters. This project is supported by The Ministry of Environment and Forestry and UNEP. A wide variety of parameters is sampled incl. total suspended material, Phosphate, Total phosphate, Nitrate, nitrite, ammonium, Silicate, Total Hg in water, Dissolved oxygen, BOD5, COD, PAH, Hg, Cd, Cr, Cu, Pb and Zn in sediment and biota, Organochlorine compounds in sediment and biota, Petroleum hydrocarbons in sediment and biota.

The National Monitoring Programme of Turkey included the monitoring of nutrient and chlorophyll-a levels in the water column in the Black Sea in 1992-1995. Dissolved oxygen and hydrogen sulphide concentrations were also measured in the monitoring programme. This study was supported by Turkish Scientific and Technological Research Council. Parameters sampled include Nutrients (phosphate, nitrate, nitrite, ammonium, silicate), Dissolved oxygen, Sulphide, Chlorophyll-a.
The programme has now ended. Instead the research institutions are stimulated to participate in international programmes such as SeaDataNet:

SeaDataNet Quality Flag Scale

- There are two types of flags in SeaDataNet:
  - Quality Flags
    - 0 – no qc
    - 1 – good value (looks good and no reported problems)
    - 2 – probably good value (associated with a known malfunction but looks OK)
    - 3 – probably bad value (associated with a known malfunction but looks wrong)
    - 4 – bad value (clearly wrong)
  - Information Flags
    - 5 – changed value (during quality control)
    - 6 – below detection (true value < quoted value)
    - 7 – value in excess (true value > quoted value)
    - 8 – interpolated value (special case of a changed value)
    - 9 – missing value
    - A – phenomenon uncertain (e.g. question over identification of biological specimen)

Countrywide in Turkey, the issues on royalty, usage rights, access rights in data management, are not backed by an elaborative legal background so that these issues are difficult to negotiate between or within an institution. Main practice is that the data are owned by the crew of the project in which they are collected. There are no any well defined terms or period for these ownership or privilege rights.

QC is an inherent and chronic problem for chemical and biological data and needs radical attempts regardless the excuse of high costs and time consumption.

Because, the essentiality of high quality time series data over an area is an inevitable fact that we challenge for

Suggestions:

**Chemical**

- Periodic control protocols for sampling and measurement devices
- At least 3 replicate measurements per samples and SD Variance
- Repetitive calibration with running standards at least for 5 times during measurements

**Biology**

- For identification and counts, there should be replicates per person for instance;
- Sub samples should be identified at least two different persons
- At least 3 counts per person
- Exploitation of expert knowledge on some species identification

Dr Konovalov noted there is another institute in Erdemli and Istanbul. So, are data sets collected and managed separately? Dr Bizsel said she could not obtain information from the other institutions. Even from the NODC no information was obtained. The issue of IPR is serious. Dr Bizsel expressed problems to obtain data from the NODC. Before 2000, there was a concrete structure. However, the national research council changed the policy and the institutions kept data themselves after 2000. There was no longer a data flow to the NODC.
Dr Konovalov said this is not unique to Turkey. Dr Bizsel added that there is no data management facility in her institution. There used to be a database in the institution before 2000 but this was ended in 2000. So Dr Bizsel has her own personal database.

Can GEBICH play a role to help your institute? There were 4-5 people from Turkey at the SDN training course. So there is data management capability in the different institutions but no data exchange between them.

Ms Bizsel’s presentation is available from the IODE web site on http://www.iode.org/index.php?option=com_oe&task=viewDocumentRecord&docID=9676

2.1.2 Examples of Data Quality Indicators for Data Contributed to BCO-DMO: Ms Cyndy Chandler

Presentation available through

Ms Cyndy Chandler (CC) of the Biological and Chemical Oceanography Data Management Office (BCO-DMO) contributed a presentation summarizing the quality indicators that BCO-DMO staff members have seen over the past couple of decades from the US GLOBEC (GLOBal ocean ECosystems dynamics ) and US JGOFS (Joint Global Ocean Flux Study) years to the present.

The BCO-DMO is funded by several programs within the US National Science Foundation Division of Ocean Sciences (OCE) to work with researchers to improve access to data resulting from NSF OCE funded ocean biogeochemistry and ecology research. BCO-DMO works with contributing investigators to gather documentation for the data they contribute. Investigators are encouraged to contribute descriptions of any quality assurance procedures and/or quality control done to improve the quality of the resultant data set. BCO-DMO adds the PI contributed data (including any quality indicators) to an online database, but no additional quality indicators are added by BCO-DMO. Data contributed to BCO-DMO are reviewed and any issues are referred to the contributing PI for resolution. If changes are required, this usually results in the data being modified and resubmitted to BCO-DMO.

In preparing the presentation, Ms Chandler said she reviewed the 6000+ data sets that currently comprise the BCO-DMO data collection. The review showed that for the data now curated by BCO-DMO (predominantly ocean biogeochemistry and ecology data from US NSF-funded researchers since the late 1980s), only a small percentage included quality indicators (precise numbers are not available). Investigators, who did report quality indicators with their data, favored the use of three systems:

1.  Sampling device specific (an indicator of sampling quality, e.g. Niskin bottle)
2.  Measurement-specific (e.g. salinity)
3.  Standard deviation and standard error

Most of the code systems used to indicate overall sampling quality (#1 above) are integer-based: e.g. 1=good, -2=misfire, and -3=suspect; or 0 = good and -1 = suspect, but several investigators had adopted a system where “x” indicated a problem with sample quality, the details of which were reported in supplemental documentation. For the second type of system (measurement-specific), investigators used either integer codes, a color coded system (red = bad, yellow = questionable and no color indicated to quality-related concerns) or a single character (“a” or “c”) to represent the investigator’s “confidence” in a measurement.

Ms Chandler also included some general comments related to biology abundance data, in particular the importance of defining the meaning of zero (0) when reporting organism abundance. Knowing the difference is critical for species abundance data: an organism was looked for and not found (0) or there
are no data for this organism (blank). For experimental data (organism response to perturbation) it is important that are accompanied by descriptions of experimental design (e.g. controls, replicates, etc.).

Ms Chandler concluded with her observation that: “Data of known quality are more useful than data of unknown quality.”

URL:  [http://bco-dmo.org/](http://bco-dmo.org/)


**DISCUSSIONS**

Dr Konovalov stated that principal investigators (PIs) undertake some quality control of data but that they often only submit their high quality data. He based this statement on lab books where the original (raw) data were found. As such they do not provide quality flags.

Ms Chandler expressed the hope that in this process they would not remove the “poor quality” data as this would be a bad practice. She informed the meeting that in the US PIs will carry out quality control whereby the submitted data are the “best version” so the “noise” is not ignored.

### 2.1.3 Quality control on biological data before and after data integration: Klaas Deneudt, VLIZ, Belgium


Mr Klaas Deneudt (KD) addressed taxonomic quality control and additional quality control steps after data integration. Why perform taxonomic QC? (i) Taxonomic synonyms => accepted and alternative names  eg bottlenose dolphin: accepted name= Tursiops truncatus (Montagu, 1821) has 23 synonyms; (ii) Misspellings; (iii) Homonyms.

VLIZ developed taxon match tool. This tool uses the following components:
- TAXAMATCH fuzzy matching algorithm by Tony Rees
- PHP/MySql port of TAXAMATCH by Michael Giddens
- Scientific Names Parser by Dmitry Moztherin

![Figure 1: WoRMS Taxon match](image-url)
Quality control at integrated level:

EMODNet Biology portal: Marine biological data portal for Europe - Database system = EurOBIS

We have done a quality control analysis on the entire Eurobis database. Each record was evaluated for 22 QC-checks. Basically, each check is a question with a yes/no answer. The results of the qc’s are stored in a field in the database and enable users to filter data based on known quality criteria. The analysis is focused on completeness of records and detection of import errors. We checked the quality of taxonomic, geographical, temporal information and validate numerical values, limited list values and the completion of required fields. We distinguish essential en non-essential control checks.

Quality control steps:

- 22 Quality Control checks / record
QC: Questions with answer yes (1) or no (0)
 Stored in one field in database  filter
 Completeness of data and detection of import errors
 Quality control of
taxon names,
geographical information,
required fields,
numeric values,
limited values lists
information on date/time
 Essential & non-essential quality control checks

In addition there are non-essential QC checks. These are two qc’s we haven’t done yet. With these we want to detect spatial outliers. For example, spatial outliers in a dataset or outliers in the observations of a species. e.g. Geographic outliers:
Observation point in dataset = not an outlier in the dataset?
coordinate more than 4X standard deviation from the centroïd of the dataset?
Observation point of certain species = not an outlier in observations of species?
coordinate more than 4X the standard deviation from the centroid of the observations from that species?

Conclusion
 Taxonomic quality control is important,
tools are available
EurOBIS: 84% of the records  evaluated positively for essential QC
 Some of the qc steps only possible at the integrated level

DISCUSSIONS

Mr Deneudt further explained that they do not use 1 quality flag as this would not be able to contain all information. Instead the 22 QC steps are encoded in one field.

Dr Konovalov asked whether, after running taxonomy QC, only the corrected data are preserved. Mr Deneudt responded that they always try to preserve all data so the original taxonomic name will remain in the data set, but a new column is added with valid names so both are available. Mr Deneudt further informed the meeting that they do not use QC flags like “good, suspicious, etc” but rather they have quality checks.

Dr Konovalov agreed with keeping the original information but noted that we have different groups of users. Some may be able to choose which test to use for their purpose, while other users may just want the “best data”. For the latter we will need to provide quality flags. This will be the case for data that we make available through a portal.

2.1.4 Quality Control of Bottle Data at Institut Maurice-Lamontagne - Fisheries and Oceans Canada Québec Region - Laure Devine and Caroline Lafleur

Ms Laure Devine (LD) gave a short overview of the QC steps that were perform at her lab for data from discrete water samples. The main data types covered are dissolved oxygen, nutrients, and chlorophyll. The QC procedures discussed here are largely drawn from those used by NODC for
production of the World Ocean Database (WOD) as well as tests proposed in the GTSPP QC manual (global T-S pilot project / profile program).

Steps:

1. **Compilation of analyzed data:** Before the QC procedure can be run, we compile the analyzed data.

2. **Documentation—must include essential metadata:** Next we document the dataset. Essential elements include time and position information as well as the variables measured and their units. Nonessential but useful elements include mission and event info, collection gear, and methods used for collection, storage, and analysis.
   - Time and position information
   - Variables measured and units
   - Non-essential but useful: mission/event information; collection, storage, and analysis methods; etc.

3. **Preliminary examination of the dataset to detect gross, order-of-magnitude-type problems:** Finally, we look over the dataset to ID any order-of-magnitude-type errors, for example:
   - Were columns transposed?
   - Are units correct?
   - Were data handling problems noted? (at any point from collection through analysis)
   - How is “no data” indicated? (Don’t use « 0 »!!)
   - Do column headers align with the appropriate data values?
   - Are the units correct?
   - Were there data-handling errors noted in the field notebook?
   - Were there problems with sampling, sample storage, or analysis?
   - What value or symbol was used to indicate “no data”?

Quality control tests – overview

- Step 1 tests: Validating the important metadata such as time and position
- Step 2 tests: Comparing data values within a profile
- Step 3 tests: Comparing the profile to a climatology
- Step 5 tests: Visual inspections of the cruise track, station data, and data from the entire mission

Description of the quality flags (modified from GTSPP)

<table>
<thead>
<tr>
<th>Flag</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>No quality control</td>
</tr>
<tr>
<td>1</td>
<td>Value seems correct</td>
</tr>
<tr>
<td>2</td>
<td>Value appears inconsistent with other values</td>
</tr>
<tr>
<td>3</td>
<td>Value seems doubtful</td>
</tr>
<tr>
<td>4</td>
<td>Value seems erroneous</td>
</tr>
<tr>
<td>5</td>
<td>Value was modified as a result of QC</td>
</tr>
<tr>
<td>6</td>
<td>Reserved for future use</td>
</tr>
<tr>
<td>7</td>
<td>Possible problem with data point—further investigation required (IML temporary flag)</td>
</tr>
<tr>
<td>8</td>
<td>Reserved for future use</td>
</tr>
<tr>
<td>9</td>
<td>Value missing</td>
</tr>
</tbody>
</table>
QCFF: A QCFF (“quality control failed flag”) is assigned to each line of data (representing the analyses from a single depth). The QCFF is a number 2x associated with some tests (noted in blue). The QCFF values from the different failed tests are summed, allowing one to determine which QC test(s) failed.

She then described the 5 steps (for validating the important metadata) individually with special attention to the visual inspections.

Test 1.1: Platform identification: Verifies that all data were sampled from the same platform
Test 1.2: Impossible date/time: Verifies that date/times are not impossible and fall within mission dates
Test 1.3: Impossible location: Checks that latitudes and longitudes are globally possible
Test 1.4: Position on land: Plots cruise track overlaid on a land mask to make sure no positions are on land
Test 1.5: Impossible speed: Checks the ship speed between 2 consecutive station locations

Conclusions

When assigning flags: When faced with anomalous values, consider carefully before assigning quality flags:

– Could some real phenomenon have caused the unusual values (e.g., upwellings, currents, increased freshwater inputs)?
– Are there potential anthropomorphic sources that might explain the values?
– Are bad instrument calibrations or unstable standards responsible?

She closed with a quote from a colleague: “Flagging “bad” points in datasets is a tricky business. One should always worry about mislabeling as “doubtful” or “erroneous” data that are interesting or unusual but real. Good data should take precedence over expectations of what the numbers should be.” (P. Strain, Bedford Institute of Oceanography, DFO).

DISCUSSIONS

Dr Garcia informed the meeting that in the case of WOD the quality of the data is linked to the version of the database. This allows subsequent corrections that are then reflected in a new version of WOD.

Dr Sun noted that the method of “quality control failed flag” (QCFF) is similar to the GTSSP QC flag scheme with the difference that GTSSP applies the QCFF to all data quality tests.
2.1.5 The quality assurance/quality control (QA/QC) procedure (GLODAP example) – Alex Kozyr


Mr Alex Kozyer (CDIAC) introduced the quality assurance and quality control procedure developed by the GLobal Ocean Data Analysis Project (GLODAP).

- ANALYTICAL AND CALIBRATION TECHNIQUES
- RESULTS OF SHIPBOARD ANALYSIS OF CERTIFIED REFERENCE MATERIALS
- REPPLICATE SAMPLES
- CONSISTENCY OF DEEP CARBON DATA AT THE LOCATIONS WHERE CRUISES CROSS OR OVERLAP
- MULTIPLE LINEAR REGRESSION ANALYSIS
- ISOPYCNAL ANALYSES
- INTERNAL CONSISTENCY OF MULTIPLE CARBON MEASUREMENTS
- FINAL EVALUATION OF OFFSETS AND DETERMINATION OF CORRECTION TO BE APPLIED

**ANALYTICAL AND CALIBRATION TECHNIQUES**

**Total carbon dioxide (TCO2) analysis and calibration**

☐ All TCO2 samples that were retained in this synthesis work were analyzed by coulometric titration. The primary differences between the various groups were the sample volume use, the level of automation, and the primary calibration method. On many cruises the coulometer (UIC, Inc.) was coupled to a semi-automated sample analyzer (Johnson and Wallace 1992; Johnson et al. 1985, 1987, 1993, 1998). The most common system, a single-operator multiparameter metabolic analyzer (SOMMA), was typically outfitted with a 20- to 30-mL pipette and was calibrated by filling a gas loop with a known volume with pure CO2 gas, then introducing the gas into the carrier gas stream and performing subsequent coulometric titration (Johnson and Wallace 1992; Johnson et al. 1987,1993, 1998). Some systems were calibrated by analyzing sodium carbonate standards. In TCO2 systems that were not coupled with a semi-automated sample analyzer, the sample was typically introduced manually by a pipette or a syringe.

**Total alkalinity (TALK) analysis and calibration.**

☐ All shipboard TALK measurements were made by potentiometric titration using a titrator and a potentiometer. TALK was determined either by characterizing a full titration curve (Brewer et al. 1986; Millero et al. 1993; DOE 1994; Ono et al. 1998) or by a single point titration (Perez and Fraga 1987). Analytical differences were in the volume of sample analyzed, the use of either an open or closed titration cell, and the calibration methods. Results were obtained from different curve-fitting techniques such as Gran plots, nonlinear fitting, or single-point analysis.

**Fugacity of CO2 (fCO2) analysis and calibration.**

Two different types of instruments were used to measure discrete fCO2 samples. With each, an aliquot of seawater was equilibrated at a constant temperature of either 4 or 20°C with a headspace of known initial CO2 content. Subsequently, the headspace CO2 concentration was determined by non-dispersive infrared analyzer (NDIR) or by quantitatively converting the CO2 to CH4 and then analyzing the concentration using a gas chromatograph (GC) with flame ionization detector. The initial fCO2 in the water was determined after correcting for loss (or gain) of CO2 during the equilibration process. This correction can be significant for large initial fCO2 differences between the
headspace and the water, and for systems with a large headspace-to-water volume ratio (Chen et al. 1995).

**pH analysis and calibration**

The pH measurements were determined by a spectrophotometric method (Clayton and Byrne 1993), with m-cresol purple as the indicator and either scanning or diode array spectrophotometers, or by using pH electrodes

**RESULTS OF SHIPBOARD ANALYSIS OF CERTIFIED REFERENCE MATERIALS**

Certified Reference Materials (CRMs) were used on many of the cruises as secondary standards for TCO2, with some exceptions during the Pacific Ocean and Atlantic survey. Routine analysis of shipboard CRMs helped verify the accuracy of sample measurements. Certification of the CRM for TCO2 is based on vacuum extraction/manometric analysis of samples in the laboratory of C. D. Keeling at Scripps Institution of Oceanography (SIO). A complete discussion of the technique developed for CRMs can be found at: http://www- mpl.ucsd.edu/people/adickson/CO2_QC/. Most groups which routinely ran CRM samples for TCO2 also analyzed the samples for TALK. The CRMs were certified for TALK in July 1996. However, archived CRMs produced prior to 1996 were calibrated as well so that post-cruise adjustments of TALK could be made (See Table 3 in Lamb et al, 2002) CRMs at the time of measurements were not available for the other carbon parameters

**REPLICATE SAMPLES**

Replicate samples were routinely collected and analyzed at sea, thus allowing the analyst to determine the overall precision of the measurement. The imprecision of replication includes the error associated with the collection and handling of the carbon sample, as well as the analytical precision. In addition, replicate samples for TCO2 were collected and stored for analysis ashore at SIO by laboratory of C.D. Keeling (see Guenther, P. R., C. D. Keeling, and G. Emanuele III. 1994b. Oceanic CO2 Measurements in the Pacific Ocean, 1990-1991: Shore Based Analyses. SIO Reference Series, Ref. No. 94-28. University of California, San Diego)

**CONSISTENCY OF DEEP CARBON DATA AT THE LOCATIONS WHERE CRUISES CROSS OR OVERLAP**

One approach for evaluating the consistency of the cruises was to compare data where cruises crossed or overlapped. A location was considered a crossover if stations from two cruises were within 1° (~100 km) of each other. If more than one station from a particular cruise fell within that limit, the data were combined for the comparison. For this analysis, only deep-water measurements (>2000 m for the Pacific Ocean, >2500 m for the Indian Ocean, and >3000 m for the Atlantic Ocean) were considered, because CO2 concentration in shallow water can be variable, and the penetration of anthropogenic CO2 can change relationships between the carbon parameters measured at different times. Once the stations were chosen, the data were plotted against potential density referenced to 3000 dB (or 4000 dB in the Atlantic) since water moves primarily along isopycnal surfaces. In order to quantitatively estimate the mean difference between legs, each of the two fitted curves for a restricted deep water density range was evaluated at evenly spaced intervals covering the range of space common to the selected stations from both legs. A mean was taken of the differences, and standard deviation was calculated

**MULTIPLE LINEAR REGRESSION ANALYSIS**

Another approach used to evaluate the data at the crossover locations was a multi-parameter linear regression analyses (MLR). Brewer, et al. (1995) and subsequently others (Wallace 1995; Slansky et al. 1997; Goyet and Davis 1997; Sabine et al. 1999), have shown that both TCO2 and TALK concentrations in deep and bottom waters can be fit well with MLR functions using commonly measured hydrographic quantities for the independent parameters. The geographic extent over which any such function is applicable depends on the number of water masses present, and the uniformity of
chemical and biological processes which have affected the carbon species concentration in each water mass.

**ISOPYCNAL ANALYSES**

At a few locations in the North Pacific the estimated offsets at the crossovers were not consistent with the offsets from the basinwide MLR analysis. In an attempt to determine whether the limited number of stations analyzed biased on the crossovers, we expanded the crossover analysis to include additional stations along each cruise and/or stations from neighboring cruises. The deep (> 2200 m) station data were averaged at specific potential density (sigma-theta) values and fitted with a 2nd-order polynomial function. The average differences and standard deviations were determined from evenly spaced differences along the curves. The range of values observed for a particular cruise at each isopycnal level indicated whether the stations initially used in the crossover analysis were offset from the surrounding stations. Although more assumptions about oceanographic consistency are necessary, the additional stations used in the isopycnal analysis can provide a better estimate of the difference between cruises because more data points are included in the analysis.

**INTERNAL CONSISTENCY OF MULTIPLE CARBON MEASUREMENTS**

An additional independent approach for evaluating the accuracy of data is the examination of the internal consistency of the CO2 system parameters. The CO2 system parameters in seawater can be characterized by temperature, salinity, phosphate and silicate, and two of the four measured inorganic carbon parameters: TCO2, TALK, fCO2, or pH. Thus, the carbon system is overdetermined on cruises where three or more carbon parameters were measured. By comparing estimates using different pairs of carbon measurements, one can evaluate potential offsets. In addition, examination of internal consistency over several cruises lends confidence to the reliability of the equilibrium constants. The constants of Mehrbach et al. (1973) as a refit by Dickson and Millero (1987) were used for this analysis, along with equilibrium constants for other components (e.g., boric acid dissociation, solubility of CO2, water hydrolysis, and phosphoric and silicic acid dissociation) necessary to characterize the carbonate system in seawater as recommended in Millero (1995). This choice was made based on the analysis of a large data set (15,300 samples) obtained from all the ocean basins (Lee et al. 2000; Millero et al. 2002). For this analysis, TALK was calculated using a combination of either TCO2 and fCO2, or TCO2 and pH [adjusted upward by 0.0047 (DelValls and Dickson 1998) for the Pacific and Indian Ocean but not for the Atlantic analysis].

**DISCUSSIONS**

Dr. Konovalov asked whether quality flags are applied for nutrients. Dr. Kozyr responded that no quality flags are applied because the data arrive at CDIAC with flags already. CDIAC may change the flags when outliers or inconsistencies are discovered. Some tests are applied. In this regard reference was made to the presentation of Dr. Suzuki under agenda item 2.1.6.
2.1.6 Quality Control and Quality Flag of PACIFICA – Toru Suzuki, Marine Information Research Center, Japan


Mr Toru Suzuki first explained the meaning of PACIFICA: Pacific Ocean Interior Carbon. Carbon and the related data synthesis project supported by S-CC (Section on Carbon and Climate) of PICES (North Pacific Marine Science Organization). Current version: 12.05 (2nd QC finalized in May 2012).

Contents of PACIFICA 12.05:

Source data: 306 hydrographic cruises, including 59 Line P and 34 GLODAP in the Pacific. 10,598 stations. Recommended adjustment values are estimated by secondary quality control. Additive for TCARBN, ALKALI, SALNTY. Multiplicative for OXYGEN, NO2+NO3, PHSPHT, SILCAT.

Primary Quality Control

- Assigned new EXPOCODE to identify cruise: 4 char. of ship code + 8 digits of cruise start date, e.g., 49NZ20070904 means 49 (country code of Japan) NZ (ship code of R/V MIRAI of JAMSTEC) on Sep.04, 2007
- Unified unit: µmol/L -> µmol/kg and Total scale for pH
- Check range and gradient/inversion
- Converted to WHP exchange format, i.e., WOCE Quality Code for water sample measurement is adopted

Secondary Quality Control

- Follow by CARINA (Carbon in Atlantic by CARBOOCEAN; Tanhua et al., 2010)
- Consist of two steps: Crossover analysis and Inversions
- Evaluation results of inversions and determination recommended adjustment values for 7 parameters

Find cruise/station pairs

- Cruise pairs: two cruise tracks are crossing, repeat or parallel each other within 250km
- Station pairs: within 250km or up to 60 closely stations

Interpolation of deeper profiles

Perform regression of parameters deeper than 2000m (or 1500m if max. depth is less than 2000m) as a piecewise cubic Hermite interpolating polynomial function of depth, potential temperature and sigma-4.
Calculation of offset/ratio

Figure 4: Calculation of offset

Determining “favourite” offset

<table>
<thead>
<tr>
<th></th>
<th>Offset</th>
<th>S.D.</th>
<th>Ratio</th>
<th>S.D.</th>
<th>Rating</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Sigma-4</td>
<td>2.334</td>
<td>2.474</td>
<td>1.001</td>
<td>0.001</td>
</tr>
<tr>
<td>2</td>
<td>Theta</td>
<td>2.783</td>
<td>1.104</td>
<td>1.001</td>
<td>0.000</td>
</tr>
<tr>
<td>3</td>
<td>Depth</td>
<td>2.167</td>
<td>1.459</td>
<td>1.001</td>
<td>0.001</td>
</tr>
<tr>
<td>4</td>
<td>Favorite</td>
<td>2.428</td>
<td>1.679</td>
<td>1.001</td>
<td>0.001</td>
</tr>
</tbody>
</table>

Figure 5: Determining favorite offset

2nd QC: step 2: Inversions

Calculation of adjustments of parameters using least square models (LSQ) with offset/ratio, standard deviation and information derived from the crossover analysis (Tanhua et al., 2010)

Methods (LSQ models)

1. No weighting
2. Weighting based on standard deviation (SD)
3. 2 + user rating (UR)
4. 3 + time difference (TD)… PACIFICA
5. 4 + latitude … CARINA
6. SD + UR + a-priori assumptions of quality
7. 6 + TD
8. 7 + latitude
PACIFICA DATA AND PRODUCTS

- 306 individual cruise data formatted WHP exchange
- Table of recommended adjustment values
- Unified data file
  - WHP exchange format (imported to ODP)
  - Adjusted 7 parameters
  - Including only good data (flag=2)
  - Measured pH, pH(TCARBN,ALKALI) (assigned flag=0), AOU, potential temperature/density, depth in meter
- Adjusted MAT file for MATLAB
- One-degree gridded statistics at standard depth

DISCUSSIONS

Dr Kozyr informed the meeting that a meeting will be held in November 2012 to discuss the possibilities for a GLODAP-2 and also to discuss how to handle new cruises beyond GLODAP-2. He stressed the need to continue data synthesis work. He also pointed out that Dr Robert Key (Princeton) will retire in two years and arrangements need to be made to take over his tasks.

Dr Konovalov called for closer collaboration between the ocean carbon community and nutrients community. The nutrient community could e.g. recommend its methodology.
2.1.7 Ukrainian NODC (Marine Hydrophysical Institute and Institute of Biology of the Southern Seas, Sevastopol) – Sergey Konovalov, Alexey Khaliulin (MHI), Volodymyr Vladymyrov (IBSS)


Dr Konovalov shared some Ukrainian experience regarding quality flag schemes. He explained that their data go back to 1910. ONE approved Flag Scheme does not exist at MHI. The actual scheme has varied over time and from project-to-project. In some cases only 3 types of Flags (Good, Doubtful, Bad) are used. The SeaDataNet quality control flag scheme (vocabulary L201) has been used for the recent projects. He then showed the QC Flags used in NATO TU-Black Sea Project (see Table 1).

<table>
<thead>
<tr>
<th>No.</th>
<th>Flag Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>no quality control</td>
</tr>
<tr>
<td>1</td>
<td>good value</td>
</tr>
<tr>
<td>2</td>
<td>inconsistent but correct</td>
</tr>
<tr>
<td>3</td>
<td>doubtful</td>
</tr>
<tr>
<td>4</td>
<td>bad value</td>
</tr>
<tr>
<td>5</td>
<td>Corrected (changed) value</td>
</tr>
<tr>
<td>6</td>
<td>value is inconsistent with depth but all BGC data fit each other</td>
</tr>
</tbody>
</table>

Table 1: QC flags used in NATO-Black Sea Project

- **No quality control**: No quality control procedures have been applied to the data value. This is the initial status for all data values entering the working archive.
- **Good value**: Good quality data value that is not part of any identified malfunction and has been verified as consistent with real phenomena during the quality control process. Both automatic and expert control have been applied.
- **Inconsistent but correct**: Data value that is probably consistent with real phenomena (frontal zones, eddies, etc.) but inconsistent with the climate, for example.
- **Doubtful**: Data value recognized as unusual during quality control that forms part of a feature that is probably inconsistent with real phenomena. There are no recognized oceanographic and BGC reasons/data to prove or discard the unusual value.
- **Bad value**: An obviously erroneous data value. (It is possible in some cases to find the reason and correct the data. Misprint, for example.)
- **Corrected (changed) value**: Data value adjusted during quality control. Information on the way and reasons is added to the description file.
- **Value is inconsistent with depth but all BGC data fit each other**: For example, a sampler delivered water from a wrong depth, but all BGC data fit each other.
Figure 7: Results of quality assessment and flagging the data

<table>
<thead>
<tr>
<th>SeaDataNet quality control flags (vocabulary L201)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
</tr>
<tr>
<td>1</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>3</td>
</tr>
<tr>
<td>4</td>
</tr>
<tr>
<td>5</td>
</tr>
<tr>
<td>6</td>
</tr>
<tr>
<td>7</td>
</tr>
<tr>
<td>8</td>
</tr>
<tr>
<td>9</td>
</tr>
<tr>
<td>A</td>
</tr>
</tbody>
</table>
Range to climatology quality control

When trying to evaluate quality of chemical data we use 3 kinds of ranges depending on availability: Local (for sub-region of basin), Regional (for entire basin) or Global. The QC flag depends results of this test. If a tested value is within $+/-3\sigma$, the QC flag is "1" (good value). If a tested value exceeds $+/-3\sigma$ but within $+/-5\sigma$, the QC flag is "2" (probably good value). If a tested value exceeds $+/-5\sigma$, then the QC flag is “3” (probably bad value).

Check data vs. regional climatology

Checking data vs. regional climatology is the most powerful up-to-date tool for data quality assessment, if climatology is available. The better climatology is known, the more precise (spatially and seasonally resolved) data quality assessment is possible. Thus, the longer monitoring program is active, the more precise data and knowledge on a specific marine system become available. If climatology is available, the difference between new data and climatology may reveal either a lack of data quality or the presence of trends and/or abrupt shifts in climatology.

Example 1: oxygen at 100m in Black Sea (left 1955-1982; right 1983-2003)

Figure 8: climatology variations
Example 2: long-term variations in oxygen at 100m

![Figure 9: long-term variations in oxygen at 100m](image)

So we need software to assist us with the tests.

![Figure 10: software for expert quality control](image)

Often a question is whether spikes are artefacts or real features (see Figure 11).
When the problem was studied in more detail it turned out that local minimum in the vertical distribution of phosphate at ~16.0 sigma-t is the real feature.

**Sigma-t scale vs Depth scale**

The sigma-t scale allows to filter out the effect of spatial and intra-annual variations in the water stratification on the BGC structure, thus providing a basis for Quality Assessment of BGC properties, when climatology is not available or poorly resolved.

Dr Konovalov stated that Quality assessment of chemical data should include the next checks:

- Units and labels
- Range
- Climatology
- Gradients
- Spikes
- “Artificial” vertical and spatial irregularities
- Predictable relationships/stoichiometry (parameter ratios, sigma-t scale, solubility, etc.)
For biological data there are more problems and less “order” as compared to chemical and physical data. PIs kept their data for themselves and rarely contributed to one database or one data centre. It is now a big problem to get these data and make them available.

IBSS data centre data management experience: the level of biological data management activities in many former USSR institutes is very low (original data have been typically hold in personal or laboratory collections, thus formats, units, metadata, quality flags, etc. are not accounted). It takes less time to reformat original datasets in a datacentre, than to ask data holders to submit their data in some agreed formats and make additional errors. IBSS always ask data holders to provide data as is, archive them and then process.

**Quality control of biological data**

There are no standard quality control procedures applied for the biological data at IBSS and most former USSR institutes. QC procedures are data type dependent (benthos, zooplankton, etc.). Expert control in corresponding taxonomic group is required. Abundance (phytoplankton) can be 0, 1, 10, 1000, 10000, 100000 cells/L. No range limits often exist and in most cases correctness of the parameter value can be estimated only by expert (taking into account region, season, depth, sampling gear etc.). QC automatic procedures can only notify data manager on local dataset outliers.

For historical datasets, for which person processed sample can not be contacted, QC procedures are often impossible. As metadata have never been attached to data many datasets became useless (loss of date, coordinates, volumes etc.).

**Problems**

There are no regional databases on marine biological data that can be used for statistical checks. Within Ocean-Ukraine and EMODNET Bio pilot projects large amount of historical data for the Black Sea submitted to OBIS/EMODNET. But still huge gaps in geographical, taxonomic and temporal coverage.

![Figure 13: Black Sea zooplankton data provided by the OBIS/Emodnet and problems with their spatial and temporal resolution](image)
Individual parameters are extremely variable. Typical ranges, distribution patterns, predictable ratios can be derived from only large databases.

Data management software for data processing is essential. The software is data type dependent and it should allow the storage/management of the full set of information (including metadata, summaries of analytical methods etc.). A proper reporting format, use of vocabularies, on-the-fly checks will reduce the possible errors in data entry procedures and ensures further interoperability.

- Use species lists and notify user if non-standard name is used
- Ensure that values of parameters will be proper type and within limits (if exist)
- Can notify user if value exceed some predefined limits (ex. cell size is larger that described in identification books)

One of the key element of the data quality control of biological data on species level can be regional and global checklists with information on:

- Reference to literature (database) where species mentioned for the region
- Morphometry
- Info on blooming, introduced species
- Images, photos
- Min, max, average cell volume, weight etc.
- Check spelling
- Possible wrong identification
- Inter-calibration - species reported only for one subregion – one species can be identified as different in different laboratories

IBSS use Black Sea phytoplankton check-list for QC of regional phytoplankton data

So, **Quality assessment of biological data should include the next checks:**

- Units and labels/species
- Range (including data on blooms, introduced species, etc.)
- Climatology

**Questions:**

- Can we expect chemical and biological data to inherit one of the existing flag scheme and quality checks developed for basically physical properties (temperature, salinity)?
- What type of quality flag system do we need to generate and maintain multidisciplinary databases?

**DISCUSSIONS**

The meeting noted that most users are interested in “good data” and therefore prefer a short list of quality flags. Nevertheless it is important to maintain information on the various tests that were done on the data as these are required by experienced data users.
2.1.8 World Ocean Database Data Quality Control - Hernan Garcia, NOAA National Oceanographic Data Center, Silver Spring, MD 20910, USA


Dr Garcia recalled that the World Ocean Database (WOD) is a global, scientifically quality-controlled oceanographic database in one well documented digital format + unrestricted access to original data (1772-yesterday). As an example, the number of profiles in the WOD 2009 release for each parameter are shown in Table 2.

<table>
<thead>
<tr>
<th>Parameter (*)</th>
<th>Number of profiles (preliminary count)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>8,896,052 (1772-2009)</td>
</tr>
<tr>
<td>Salinity</td>
<td>3,533,325 (1874-2009)</td>
</tr>
<tr>
<td>Dissolved oxygen</td>
<td>848,519 (1898-2008)</td>
</tr>
<tr>
<td>Phosphate</td>
<td>454,933 (1922-2008)</td>
</tr>
<tr>
<td>Silicic Acid</td>
<td>335,140 (1921-2008)</td>
</tr>
<tr>
<td>Nitrate</td>
<td>268,388 (1925-2008)</td>
</tr>
<tr>
<td>pH</td>
<td>196,844 (1910-2007)</td>
</tr>
<tr>
<td>Chlorophyll</td>
<td>212,825 (1933-2008)</td>
</tr>
<tr>
<td>Alkalinity</td>
<td>52,313 (1921-2008)</td>
</tr>
<tr>
<td>pCO$_2$</td>
<td>3,382 (1967-2008)</td>
</tr>
<tr>
<td>Dissolved inorganic carbon</td>
<td>13,146 (1958-2008)</td>
</tr>
<tr>
<td>Tritium</td>
<td>1,618 (1984-2003)</td>
</tr>
<tr>
<td>Delta Helium-3</td>
<td>2,086 (1985-2003)</td>
</tr>
<tr>
<td>Argon</td>
<td>75 (1993-1993)</td>
</tr>
<tr>
<td>Neon</td>
<td>1,308 (1987-2002)</td>
</tr>
<tr>
<td>CFC-11</td>
<td>11,272 (1985-2008)</td>
</tr>
<tr>
<td>CFC-12</td>
<td>11,279 (1985-2008)</td>
</tr>
<tr>
<td>CFC-113</td>
<td>2,799 (1990-2006)</td>
</tr>
<tr>
<td>PLankton</td>
<td>218,695 (1905-2008)</td>
</tr>
<tr>
<td>Transmissivity (BAC)</td>
<td>13,190 (1963-2007)</td>
</tr>
</tbody>
</table>
Figure 14: WOD 2009 release spatial and temporal coverage

The World Ocean Atlas provides climatologies:

Figure 15: WOA climatologies

Dr Garcia recalled some definitions:

**Quality Assurance**: Integrated procedures (Quality Control and Quality Assessment) to produce data output of known quality (Dux, 1990; Taylor, 1987):

**Quality Control (QC)** — *Activities to control* the quality of a measurement so that it meets the needs of users (Fit for Purpose).
Quality assessment (QA) — Activities to monitor over time that quality control continues to meet the needs of the users (e.g., metrics, statistical evaluation of the quality of the data).


WOD general QC tests

QUALITY CONTROL OF OBSERVED LEVEL DATA

1. Format conversion: checks in data units, instruments, significant figures, metadata development, etc
2. Check cast position/date/time
3. Assignment of cruise and cast numbers: Assigning casts, profiles (assigning granularity)
4. Cruise speed checks
5. Duplicate cast checks (e.g., Identical or nearly identical profiles, Identical casts, Overlapping Cruises)
6. Depth inversion and depth duplication checks
7. High-resolution pairs check (discrete vs continuous profiles)
8. Range checks on observed level data (Broad regional ranges)
9. Excessive negative, no-gradient, or positive vertical depth (pressure) gradient checks
10. Observed level density checks
11. Property-property plots and internal data consistency against other historical data

QUALITY CONTROL OF STANDARD LEVEL DATA

1. Vertical interpolation method (minimum requirements must be met including acceptable depth differences)
2. Standard level density check
3. Statistical analysis of data at standard depth levels for coastal, near-coastal, open ocean (e.g., decadal, pentadal, annual, seasonal, monthly mean, sdev, serr 1/10-deg, 1-deg, 5-deg)
4. Objective analysis (iterative process)
5. Corrections XBT depth-time equation error. All other data in WOD are unmodified.

Documentation about WOD quality control procedures and data documentation can be obtained from the following references:


Definition of WOD Quality Flags

(1) FLAGS FOR ENTIRE CAST (AS A FUNCTION OF VARIABLE)

<table>
<thead>
<tr>
<th>Flag</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>accepted cast</td>
</tr>
<tr>
<td>1</td>
<td>failed annual standard deviation check</td>
</tr>
<tr>
<td>2</td>
<td>two or more density inversions (Levitus, 1982 criteria)</td>
</tr>
<tr>
<td>3</td>
<td>flagged cruise</td>
</tr>
<tr>
<td>4</td>
<td>failed seasonal standard deviation check</td>
</tr>
<tr>
<td>5</td>
<td>failed monthly standard deviation check</td>
</tr>
<tr>
<td>6</td>
<td>failed annual and seasonal standard deviation check</td>
</tr>
<tr>
<td>7</td>
<td>bullseye from standard level data or failed annual and monthly standard deviation check</td>
</tr>
<tr>
<td>8</td>
<td>failed seasonal and monthly standard deviation check</td>
</tr>
<tr>
<td>9</td>
<td>failed annual, seasonal and monthly standard deviation check</td>
</tr>
</tbody>
</table>

(2) FLAGS ON INDIVIDUAL OBSERVATIONS

(a) Depth Flags

<table>
<thead>
<tr>
<th>Flag</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>accepted value</td>
</tr>
<tr>
<td>1</td>
<td>duplicates or inversions in recorded depth (same or less than previous depth)</td>
</tr>
<tr>
<td>2</td>
<td>density inversion</td>
</tr>
</tbody>
</table>

(b) Observed Level Flags

<table>
<thead>
<tr>
<th>Flag</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>accepted value</td>
</tr>
<tr>
<td>1</td>
<td>range outlier (outside of broad range check)</td>
</tr>
<tr>
<td>2</td>
<td>failed inversion check</td>
</tr>
<tr>
<td>3</td>
<td>failed gradient check</td>
</tr>
<tr>
<td>4</td>
<td>observed level “bullseye” flag and zero gradient check</td>
</tr>
<tr>
<td>5</td>
<td>combined gradient and inversion checks</td>
</tr>
<tr>
<td>6</td>
<td>failed range and inversion checks</td>
</tr>
<tr>
<td>7</td>
<td>failed range and gradient checks</td>
</tr>
<tr>
<td>8</td>
<td>failed range and questionable data checks</td>
</tr>
<tr>
<td>9</td>
<td>failed range and combined gradient and inversion checks</td>
</tr>
</tbody>
</table>

(c) Standard Level Flags

<table>
<thead>
<tr>
<th>Flag</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>accepted value</td>
</tr>
<tr>
<td>1</td>
<td>bullseye marker</td>
</tr>
<tr>
<td>2</td>
<td>density inversion</td>
</tr>
<tr>
<td>3</td>
<td>failed annual standard deviation check</td>
</tr>
<tr>
<td>4</td>
<td>failed seasonal standard deviation check</td>
</tr>
<tr>
<td>5</td>
<td>failed monthly standard deviation check</td>
</tr>
<tr>
<td>6</td>
<td>failed annual and seasonal standard deviation check</td>
</tr>
<tr>
<td>7</td>
<td>failed annual and monthly standard deviation check</td>
</tr>
<tr>
<td>8</td>
<td>failed seasonal and monthly standard deviation check</td>
</tr>
<tr>
<td>9</td>
<td>failed annual, seasonal and monthly standard deviation check</td>
</tr>
</tbody>
</table>

(d) Biological data flags (applied only to Comparable Biological Value - CBV Taxa code 27)

<table>
<thead>
<tr>
<th>Flag</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>accepted value</td>
</tr>
<tr>
<td>1</td>
<td>range outlier (outside of broad range check)</td>
</tr>
<tr>
<td>2</td>
<td>questionable value (“bullseye flag”)</td>
</tr>
</tbody>
</table>
Dr Garcia then summarized as follows:

- World Ocean database (WOD) is a scientifically quality-controlled database that can be used for documenting ocean variability. A fine tuned Primary Quality control procedure provides a data base of uniform quality for addressing variety of research questions. No QC/QA can address all possible questions.

- World Ocean database (WOD) and World Ocean Atlas (WOA) are made possible because of the data that scientists worldwide provide to national and World Data Centers.

- NODC/WDC is dedicated to providing all available data to without restriction consistent following IODE principles. All of the data in WOD and WOA are freely available at http://www.nodc.noaa.gov/.

Dr Garcia called the attention of the meeting to the OceanTeacher Digital Library section on Marine Data Quality Flags:
http://library.oceanteacher.org/OTMediawiki/index.php/Marine_Data_Quality_Flags

DISCUSSIONS

Dr Garcia, recalling his statement that 10-20% of the historical nutrient data in WOD are marked as questionable, clarified that these data might be questionable for making high-quality regional climatologies but could still be useful for other purposes as their variation might be due to e.g. eddies, El Niño. Developing a climatology could be seen as one additional QC procedure for data consistency.

2.1.9 Global Temperature and Salinity Profile Programme (GTSPP) Data Quality Tests – Charles Sun, Chair SG-GTSPP

Presentation available through

Dr Charles Sun (CS) recalled that GTSPP is a joint WMO-IOC program designed to provide improved access to the highest resolution, highest quality data as quickly as possible.

History

- In 1990, GTSPP was initiated jointly by IODE (International Oceanographic Data and Information Exchange) and IGOSS (Integrated Global Ocean Services System) as a pilot project (through Recommendation IODE-XIII.4.
- In 1996, GTSPP was transformed into a permanent operational programme under the co-sponsorship of IODE and IGOSS (IODE Recommendation IODE-XV.4.
- In 2001, JCOMM-I defined GTSPP as a program jointly sponsored by JCOMM and IODE.

Where to find GTSPP data?

- HTTP: http://www.nodc.noaa.gov/gtspp/
- HTTP: http://data.nodc.noaa.gov/gtspp/
- OPeNDAP: http://data.nodc.noaa.gov/opendap/gtspp/
- THREDDS: http://data.nodc.noaa.gov/thredds/catalog/gtspp/catalog.html
Data Quality tests

<table>
<thead>
<tr>
<th>STAGE NO.</th>
<th>TEST NO.</th>
<th>QUALITY CONTROL TEST</th>
<th>STAGE NO.</th>
<th>TEST NO.</th>
<th>QUALITY CONTROL TEST</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Stage 1: Location and Identification Tests</td>
<td></td>
<td></td>
<td>Stage 2: Profile Tests</td>
</tr>
<tr>
<td>1.1</td>
<td>01</td>
<td>Platform Identification</td>
<td>2.1</td>
<td>07</td>
<td>Global Impossible Parameter Values</td>
</tr>
<tr>
<td>1.2</td>
<td>02</td>
<td>Impossible Date/Time</td>
<td>2.2</td>
<td>08</td>
<td>Regional Impossible Parameter Values</td>
</tr>
<tr>
<td>1.3</td>
<td>03</td>
<td>Impossible Location</td>
<td>2.3</td>
<td>09</td>
<td>Increasing Depth</td>
</tr>
<tr>
<td>1.4</td>
<td>04</td>
<td>Position on Land</td>
<td>2.4</td>
<td>10</td>
<td>Global Profile Envelope</td>
</tr>
<tr>
<td>1.5</td>
<td>05</td>
<td>Impossible Speed</td>
<td>2.5</td>
<td>11</td>
<td>Constant Profile</td>
</tr>
<tr>
<td>1.6</td>
<td>06</td>
<td>Impossible Sounding</td>
<td>2.6</td>
<td>12</td>
<td>Freezing Point</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Stage 3: Climatology Tests</td>
<td></td>
<td></td>
<td>Stage 4: Profile Consistency Tests</td>
</tr>
<tr>
<td>3.1</td>
<td>17</td>
<td>Levitus Seasonal Statistics</td>
<td>4.1</td>
<td>21</td>
<td>Waterfall</td>
</tr>
<tr>
<td>3.2</td>
<td>18</td>
<td>Emery and Dewar Climatology</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.3</td>
<td>19</td>
<td>Asheville SST Climatology</td>
<td>5.1</td>
<td>22</td>
<td>Cruise Track</td>
</tr>
<tr>
<td>3.4</td>
<td>20</td>
<td>Levitus Monthly Climatology</td>
<td>5.2</td>
<td>23</td>
<td>Profiles</td>
</tr>
<tr>
<td>3.5</td>
<td>26</td>
<td>Levitus Annual Climatology</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

GTSSP Quality Control Code

<table>
<thead>
<tr>
<th>Code</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>No quality control (QC) has been performed on this element.</td>
</tr>
<tr>
<td>1</td>
<td>QC has been performed; element appears to be correct.</td>
</tr>
<tr>
<td>2</td>
<td>QC has been performed; element appears to be correct but is inconsistent with other elements.</td>
</tr>
<tr>
<td>3</td>
<td>QC has been performed; element appears to be doubtful.</td>
</tr>
<tr>
<td>4</td>
<td>QC has been performed; element appears to be erroneous.</td>
</tr>
<tr>
<td>5</td>
<td>The value has been changed as a result of QC.</td>
</tr>
<tr>
<td>6-8</td>
<td>Reserved for future use.</td>
</tr>
<tr>
<td>9</td>
<td>The value of the element is missing.</td>
</tr>
</tbody>
</table>
Data Quality Control Cruise Editor (QCED)

Features:

- Map of ship position for visual inspection of the cruise.
- Bar graph of the ship speeds between stations in the cruise.
- Waterfall plot of neighboring profiles.
- Profile plot overlaid on the World Ocean Atlas 2005 climatology and ETOPO5 Bathymetry plots.
- Temperature/Salinity plot when both are available.
- Formatted text display of all fields from the data file.
- Key metadata displayed in a scrolling list.
- Performs a suite of automated data quality tests and displays "trouble lights" to draw operator attention to questionable data.
- Operator may edit:
  - Time and Position.
  - QC flags for temperature or salinity values.

GTSPP ASCII Sample File

He reported that QNF$ and QNP$ are GTSPP Quality Control codes. The first letter, ‘Q’, in each quality control code stands for quality control. The letter, ‘N’, indicates the quality control test was performed by the U.S. National Oceanographic Data Center. Letters, ‘F’ and ‘P’, represent for QC tests ‘Failed’ or QC test performed, respectively. Both QNF$ and QNP$ codes are followed by an 8-digit hexadecimal number representing quality test result and code, respectively.

Interpretation of QC Test Codes and Results

The steps of interpretation of GTSPP QC test codes and results are as follows:

1. Convert the QC test codes (or results) from hexadecimal to decimal number.
2. Convert the decimal number to binary number.
3. Reverse the binary number in accordance with the order of the GTSPP QC test numbers.
4. Map the reversed bit numbers to the corresponding numbers of the QC tests in the ascending order and identify the test names and results, accordingly.

Decoding hexadecimal to decimal

- QNF$ = 00010000 (QC tests "Fail")
- QNP$ = 0021735E (QC tests "Performed")

Decoding the QNP$

Hex number: 0021735E
Tests 2,3,4,5, (NOT 6), 7, etc. until 26 have been performed

If this was QNFS, replace “performed” by “failed”

(equivalent to QP1$, QT1#, QP1#, QCPS, QCFS, QTE#, QPS#, QP9$, QT9#, QP9#)

**List of Data Quality Tests performed (in hight lighted bold face)**

1. 1.1 Platform Identification Location & Identification Tests
2. 1.2 Impossible Date/Time
3. 1.3 Impossible Location
4. 1.4 Position on Land
5. 1.5 Impossible Speed
6. 1.6 Impossible Sounding
7. 2.1 Global Impossible Parameter Value Profile Tests
8. 2.2 Regional Impossible Parameter Value
9. 2.3 Increasing Depth
10. 2.4 Profile Envelop
11. 2.5 Constant Profile
12. 2.6 Freezing Point
13. 2.7 Spike
14. 2.8 Top and Bottom Spike
15. 2.9 Gradient
16. 2.10 Density Inversion
17. 3.1 Levitus Seasonal Statistics Climatology Tests
18. 3.2 Emery and Dwar Climatology
19. 3.3 Asheville Climatology
20. 3.4 Levitus Monthly Climatology
21. 4.1 Waterfall Profile Consistency Test
22. 5.1 Visual Inspection of Cruise Track Visual Inspection
23. 5.2 Visual Inspection of Profiles
24. 2.11 Bathymetry Profile Tests (cont’d)
25. 2.12 Temperature inversion
26. 3.5 Levitus Annual Climatology

The GTSP group at the US National Oceanographic Data Center has developed a script written in PERL to assist users in interpretation of quality control tests and results.

**DISCUSSIONS**

*Dr Konovalov expressed his appreciation for the preservation of information on applied tests in the system. The list shown above is open and additional quality tests can be added. He had however some questions on the nature of some flags (e.g. value has been changed) which may not mean much to users.*

*Dr Sun explained that GTSP had published a GTSP data user guide to help users understand the meaning of QC flags and defines the sequence of QC flags are in the order of 1, 2, 5, 0, 3, and 4 (from good to bad data).*

*Dr Garcia stated that GTSP second level indexing scheme may not be practical for chemical data because of the number of chemical variables is much larger than the number of variables currently handled by GTSP. It was mentioned that the number of chemical variables, as an example, could be around 165. Dr Sun agreed that applying the GTSP second level indexing scheme could be very challenge for chemical data because of the large number of chemical variables.*
2.1.10 Quality Control of CTD data using proposed IODE QF scheme – Greg Reed, Andrew Walsh, RAN Hydrography and Metoc Branch


Mr Greg Reed reported on the assessment of the proposed IODE quality flag scheme applied to the quality control of CTD data.

Initial processing of the CTD data was described which includes gross range checks, removal of any corrupted or unrealistic data, correction of raw pressure readings for any offset error, extraction of a sequence of unique monotonic pressures, and computed salinity from conductivity, temperature and pressure using the PSS-78 scale.

Quality control includes viewing the location of the data on a chart, visual inspection of each profile of temperature and salinity and comparison with nearest neighbours and climatology. Quality flags are applied according to the proposed primary level quality flag codes (good, not evaluated, questionable/suspect, bad, missing data). Quality flags may apply at the whole profile level or individual pressure levels.

Temperature and salinity profiles are compared against a three standard deviation envelope from a regional climatology (CSIRO-Atlas of Regional Sea). Profiles or segments of profiles with data outside the envelope are flagged using the secondary flag to indicate the result of this test and data is flagged 0 (passed), 1 (failed) or 2 (not performed).

The raw data file is converted to netCDF before quality control. The netCDF file follows the CF-netCDF conventions v1.6 and attribute names are from the recommended Unidata "NetCDF Attribute Convention for Dataset Discovery". The Data Parameter names used are from the CF Standard Names list.

Mr Reed provided examples of a netCDF implementation of the proposed quality flag scheme.

**Primary Flags**

The primary level flags (1=good; 2=not evaluated or unknown; 3=questionable/suspect; 4=bad; 9=missing) are applied to temperature, salinity, pressure, time, position. In this example the primary level flags are applied to the salinity data.

```
byte salinity_qc_flag(pressure);

salinity_qc_flag:long_name = "quality control flag for salinity (primary Level 1 flag)";
salinity_qc_flag:standard_name = "sea_water_salinity status_flag";
salinity_qc_flag:quality_control_convention = "Proposed IODE qc scheme March 2012";
salinity_qc_flag:valid_min = 1;
salinity_qc_flag:valid_max = 9;
salinity_qc_flag:flag_values = 1b, 2b, 3b, 4b, 9b;
salinity_qc_flag:flag_meanings = "good not_evaluated_or_unknown suspect bad missing";
salinity_qc_flag:coordinates = "time latitude longitude pressure";
```

**Secondary Flags**

The secondary level flags demonstrated (0=passed; 1=failed; 2=not performed) are applied to the results of the three standard deviation test for salinity.

```
byte salinity_sd_test(pressure);

salinity_sd_test:long_name = "qc flag for monthly salinity 3 standard deviation test (secondary Level 2 flag)";
salinity_sd_test:quality_control_convention = "Proposed IODE qc scheme March 2012";
salinity_sd_test:valid_min = 0;
salinity_sd_test:valid_max = 2;
salinity_sd_test:flag_values = 0b, 1b, 2b;
salinity_sd_test:flag_meanings = "passed failed unknown";
salinity_sd_test:coordinates = "time latitude longitude pressure";
```
Mr Reed stated that the proposed flag scheme is easy to implement as there are only a small number of primary level flags but there is the ability to define additional tests at the secondary level. Data users may only want to assess the quality using the primary flags, which are easy to understand. If a user requires more detailed information about the quality of the data, the secondary level flags provide this information.

The use of netCDF for data exchange provides a standardized format including standard data parameter names from the CF Standard Names list. As netCDF is a self-describing format, all information about primary and secondary flags and the tests applied is included in the data file. It is also possible to implement the proposed flag scheme using an ASCII format.

**DISCUSSIONS**

Dr Sun posed the question whether they ran into any issues where they wanted to represent something but could not, when they tried to use the QC flags as proposed. Mr Reed answered that no issues came up: when they wanted to use a quality flag that was not available in this could be added to the list of secondary flags. The first level should be simple and anyone should understand immediately what it means. The second level is more for the experts who want to know more about the quality tests applied to the data. As netCDF is a self-describing format the descriptions of the test is documented.

Dr Garcia stated that it is important or more practical that the information about the quality of the data go along with the data. Mr Reed responded that this is the big advantage of using NetCDF. All metadata describing the quality tests is included in a single file with the data. As netCDF is an international standard, there are no difficulties in exchanging the data.

Dr Moncoiffé asked how difficult it would be to translate the NetCDF file into ASCII format. Mr Reed responded that a CDL representation of the NetCDF file provides a human-readable version. Ms Moncoiffé then asked the same question about CSV. Mr Reed answered that this would be more difficult. It would probably be necessary to write a script that converts into CSV.

**2.1.11 SeaDataNet QC, Flags and Emodnet Chemistry experience – Matteo Vinci, Alessandra Giorgetti, OGS NODC, Trieste, Italy**


Mr Vinci started with a brief introduction to SeaDataNet, an efficient distributed Marine Data Management Infrastructure for the management of large and diverse sets of data deriving from in situ and remote observation of the seas and oceans. The development and adoption of common communication standards and adapted technology ensure the platforms interoperability.

**SeaDataNet-QC- from last DQC procedures report of May 2010**

WHY a Quality Check?


- “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.”

Quality control, if done well, brings about a **number of key advantages**:
• Maintaining standards
• Consistency
• Reliability

SeaDataNet - QC

The first step of the quality control is:

TO COMPLETE DATA WITH INFORMATION! For all types of data!

• Where the data were collected;
• When the data were collected;
• How the data were collected;
• Who collected the data;
• What has been done to the data;

Comments for users of the data (e.g. problems encountered and comments on data quality).

SeaDataNet - AUTOMATIC QUALITY CONTROL CHECKS performed for ALL datatypes

• Date and time of an observation has to be valid (Year 4 digits, month between 1 and 12 …); QF→5
• -Latitude and longitude have to be valid (Latitude in range -90 to 90…); QF→5
• -Position must not be on land;
• -Check for duplicates (Cruises or stations within a cruise using a space-time radius (e.g., for duplicate cruises: 1 mile, 15min or 1day if time is unknown))…
• Global range (expected extremes encountered in the oceans); QF→4
• -Regional range (expected extremes encountered in particular regions); QF→4
• -Deepest pressure (…profile does not contain pressures higher than the highest value expected); QF→4
• -Spike (…large differences between adjacent values); QF→3
• -Gradient (vertically adjacent salinity and temperature measurements too steep);
• -Density inversion (…a higher pressure in a profile is less than the calculated density at an adjacent lower pressure); QF→4
• -Pressure increasing (Pressures from the profile monotonically increasing). QF→4

QC references

• NODC procedures (e.g. France, Greece, Italy, Norway, Spain, Sweden, UK)
• EU MEDAR-MEDATLAS procedures and SCOOP software
• EU SIMORC project (Met-ocean data QC)
• EU ESEAS (sea level) and IOC GLOSS documents
• GTSP QC (IOC Manuals and Guides No. 22)
• Argo Quality Control Manual (Real Time and Delayed Mode)
• GOSUD Real-time quality control
• IODE’s OceanTeacher
• ICES WG Marine Data Management Data Type Guidelines
• JPOTS Manual, 1991
• WOCE manuals
• JGOFS Protocols
• World Ocean Database Quality Control documentation
• TOGA/COARE Handbook of Quality Control Procedures for Surface Meteorology Data
• BODC-WOCE Sea Level Data Assembly Centre Quality Assessment
• AODC Quality Control Cookbook for XBT Data
• Chapman, A. D. 2005. Principles and Methods of Data Cleaning – Primary Species and Species-Occurrence Data, version 1.0.
• ‘Ocean biodiversity informatics’: a new era in marine biology research and management (Mark J. Costello, Edward Vanden Berghe)
• QARTOD (Quality Assurance of Real-Time Oceanographic Data)

“Scientific” quality control

Further quality control is carried out on the data sets, and may be dependent on the data type. There is often a subjective element in this process (eg. profiles visual QC).

Regional Quality Checks:

Performed at Regional level with specific climatologies. (eg. Regional range checks for specific sections of the Adriatic Sea: North, Middle, South. Seasonal climatology (mean vertical profile and standard deviation) is computed from MEDAR/MedAtlas II data

SeaDataNet - QF schema – L201 vocab

Flag Short description
0 No quality control
1 The value appears to be correct
2 The value appears to be probably good
3 The value appears probably bad
4 The value appears erroneous
5 The value has been changed
6 Below detection limit
7 In excess of quoted value
8 Interpolated value
9 Missing value
A Incomplete information

Some are not applied by OGS (6,7,8,A)

EMODNET

A pilot component for a final operational European Marine Observation and Data Network, launched by DG MARE that aims to assemble fragmented and inaccessible marine data into interoperable, continuous and publicly available data streams;

Lot 3 – Chemical data

The contract started in June 2009, with a duration of three years.

Chemistry Lot already presented by Anders W. (NERI→DMU)
during the GE-BICH meeting January 2011

“QA/QC-guidelines” presented
Chemical lot pilot project: Parameters selection: Choice based on MSFD requirements; Selected from 8 groups of compounds; 3 matrices: water, biota, sediment; 17 selected parameters for product generation.

<table>
<thead>
<tr>
<th>Chemical group</th>
<th>Parameter</th>
<th>Chemical group</th>
<th>Parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pesticides</td>
<td>Dichlorodiphenyltrichloroethane (DDT)</td>
<td>Hydrocarbons</td>
<td>Anthracene (C14H10)</td>
</tr>
<tr>
<td>Pesticides</td>
<td>Hexachlorobenzene (HCB)</td>
<td>Hydrocarbons</td>
<td>Fluoranthene (C14H10)</td>
</tr>
<tr>
<td>Antitubercants</td>
<td>Tribromphenol (TBP)</td>
<td>Radionuclides</td>
<td>Cesium 137</td>
</tr>
<tr>
<td>Pharmaceuticals</td>
<td>Oxytetracycline (C22H24N6O8)</td>
<td>Radionuclides</td>
<td>Plutonium 239</td>
</tr>
<tr>
<td>Heavy metals</td>
<td>Mercury (Hg)</td>
<td>Fertilisers/Nitrogen</td>
<td>Nitrate (NO3)</td>
</tr>
<tr>
<td>Heavy metals</td>
<td>Cadmium (Cd)</td>
<td>Fertilisers/Nitrogen</td>
<td>Phosphate (PO4)</td>
</tr>
</tbody>
</table>

Chemical lot PP - HOW: Infrastructure set up based on SeaDataNet V1

Principle of “ADOPTED AND ADAPTED”

- **SDN Standards for metadata, data and products:**
  - metadata ➔ CDI (xml ISO 19115),
  - Standard Vocabs (P021,P011,P061...) for common terms.
  - for background data exchange à ODV data format.

- **Infrastructure:**
  - CDI mechanism, SDN Security Services, SDN Products viewing services...

- **Softwares:**
  - MIKADO xml generator, NEMO data formatting tool, DIVA software, ODV software...

- **Extension of SDN Common Vocabularies:**
  - P021 for CDI generation (metadata)
  - P061 for units (data)
  - P011 for ODV generation (data)
    - Specific implementation of Services: eg. Ocean Browser products viewing service

Chemical lot PP – Challenges:

- **Data Complexity:**
  - from 8 groups of compounds;
  - 3 matrices (sediment, water column and biota);
  - 17 selected parameters for products generation;

- **Heterogeneity:**
• Of the sampling/data distribution (coastal points time series Vs homogenous sampling at basins level);

• Of measurement methods (instrument, method, target species, target basis, grain sizes).

RESULTS OF DATA COLLECTION

<table>
<thead>
<tr>
<th>MSFD categories</th>
<th>entry_jump_2021</th>
<th>Total COL numbers</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>North Sea</td>
<td>Black Sea</td>
</tr>
<tr>
<td>Antifoulants</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Concentration of other organic contaminants in biota</td>
<td>24</td>
<td></td>
</tr>
<tr>
<td>Concentration of other organic contaminants in sediment samples</td>
<td>1636</td>
<td>177</td>
</tr>
<tr>
<td>Concentration of other organic contaminants in suspended particulate material</td>
<td>630</td>
<td></td>
</tr>
<tr>
<td>Concentration of other organic contaminants in the water column</td>
<td>1590</td>
<td>2142</td>
</tr>
<tr>
<td>Organo metallic species concentration parameters in biota</td>
<td>129</td>
<td></td>
</tr>
<tr>
<td>Organo metallic species concentration parameters in sediments</td>
<td>540</td>
<td></td>
</tr>
<tr>
<td>Ammonium concentration parameters in the water column</td>
<td>85375</td>
<td>5450</td>
</tr>
<tr>
<td>Dissolved inorganic nitrogen concentration in the water column</td>
<td>1440</td>
<td>65</td>
</tr>
<tr>
<td>Dissolved total and organic nitrogen concentrations in the water column</td>
<td>1770</td>
<td></td>
</tr>
<tr>
<td>Dissolved total or organic phosphorus concentration in the water column</td>
<td>1141</td>
<td></td>
</tr>
<tr>
<td>Nitrate concentration parameters in the water column</td>
<td>101316</td>
<td>10599</td>
</tr>
<tr>
<td>Nitrite concentration parameters in the water column</td>
<td>43223</td>
<td>10286</td>
</tr>
<tr>
<td>Nutrient concentrations in sediment pore waters</td>
<td>16</td>
<td></td>
</tr>
<tr>
<td>Phosphate concentration parameters in the water column</td>
<td>109900</td>
<td>22059</td>
</tr>
<tr>
<td>Heavy metals</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dissolved metal concentrations in the water column</td>
<td>3399</td>
<td>412</td>
</tr>
<tr>
<td>Inorganic chemical composition of sediment or rocks</td>
<td>1190</td>
<td>603</td>
</tr>
<tr>
<td>Metal concentrations in biota</td>
<td>2577</td>
<td></td>
</tr>
<tr>
<td>Particulate metal concentrations in the water column</td>
<td>981</td>
<td></td>
</tr>
<tr>
<td>Total metal concentrations in water bodies</td>
<td>609</td>
<td>514</td>
</tr>
<tr>
<td>Concentration of other hydrocarbons in the water column</td>
<td>230</td>
<td>1677</td>
</tr>
<tr>
<td>Concentration of polycyclic aromatic hydrocarbons (PAHs) in biota</td>
<td>536</td>
<td></td>
</tr>
<tr>
<td>Concentration of polycyclic aromatic hydrocarbons (PAHs) in sediment samples</td>
<td>3422</td>
<td></td>
</tr>
<tr>
<td>Concentration of polycyclic aromatic hydrocarbons (PAHs) in suspended particulate material</td>
<td>10531</td>
<td></td>
</tr>
<tr>
<td>Concentration of polycyclic aromatic hydrocarbons (PAHs) in the water column</td>
<td>323</td>
<td></td>
</tr>
<tr>
<td>Hydrocarbons</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Carbon concentrations in sediment</td>
<td>2100</td>
<td></td>
</tr>
<tr>
<td>Carbon concentrations in suspended particulate material</td>
<td>3159</td>
<td></td>
</tr>
<tr>
<td>Concentration of organic matter in sediments</td>
<td>26</td>
<td></td>
</tr>
<tr>
<td>Dissolved organic carbon concentration in the water column</td>
<td>236</td>
<td></td>
</tr>
<tr>
<td>Dissolved organic carbon concentrations in sediment pore waters</td>
<td>16</td>
<td></td>
</tr>
<tr>
<td>Nitrogen concentrations in sediment</td>
<td>461</td>
<td></td>
</tr>
<tr>
<td>Nitrogen concentrations in suspended particulate material</td>
<td>3752</td>
<td></td>
</tr>
<tr>
<td>Particulate total and organic carbon concentrations in the water column</td>
<td>9193</td>
<td>20</td>
</tr>
<tr>
<td>Particulate total and organic nitrogen concentrations in the water column</td>
<td>85434</td>
<td>1956</td>
</tr>
<tr>
<td>Particulate total and organic phosphorus concentrations in the water column</td>
<td>91477</td>
<td>2034</td>
</tr>
<tr>
<td>Organic matter</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Alkalinity, acidity and pH of the water column</td>
<td>12689</td>
<td>4968</td>
</tr>
<tr>
<td>Concentration of suspended particulate material in the water column</td>
<td>9286</td>
<td>924</td>
</tr>
<tr>
<td>Dissolved oxygen parameters in the water column</td>
<td>189270</td>
<td>35680</td>
</tr>
<tr>
<td>Raw oxygen sensor output</td>
<td>5151</td>
<td></td>
</tr>
<tr>
<td>Suspended particulate material grain size parameters</td>
<td></td>
<td>72</td>
</tr>
<tr>
<td>Total dissolved inorganic carbon (TIC) concentration in the water column</td>
<td>25</td>
<td>19</td>
</tr>
<tr>
<td>Concentration of polychlorinated biphenyls (PCBs) in biota</td>
<td>233</td>
<td></td>
</tr>
<tr>
<td>Concentration of polychlorinated biphenyls (PCBs) in sediment samples</td>
<td>1325</td>
<td></td>
</tr>
<tr>
<td>Concentration of polychlorinated biphenyls (PCBs) in suspended particulate material</td>
<td>163</td>
<td></td>
</tr>
<tr>
<td>Concentration of polychlorinated biphenyls (PCBs) in the water column</td>
<td>323</td>
<td>384</td>
</tr>
<tr>
<td>Pesticides</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pesticide concentrations in biota</td>
<td>709</td>
<td></td>
</tr>
<tr>
<td>Pesticide concentrations in sediment</td>
<td>1039</td>
<td>233</td>
</tr>
<tr>
<td>Pesticide concentrations in water bodies</td>
<td>213</td>
<td>904</td>
</tr>
<tr>
<td>Radionuclides</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Radioactivity in the water column</td>
<td>773</td>
<td>1195</td>
</tr>
</tbody>
</table>

Chemical lot PP - Quality check

Emodnet Chemistry lot PP was based on a subset of NODCs coming from SeaDataNet.

The NODCs harvested data at national level performing the quality checks.

Each Partner (NODC) who was delivering data to the project was responsible for the quality control of its own data.

This means that the data that were assembled at the Regional Pools were carrying the qc flags coming from the previous quality control.

Further quality checks were also performed by Regional Leaders that collected data for data-products generation. Example for the Mediterranean case (input from Sissy Iona HCMR):

• water column, nutrients:
with the use of ODV tool performed the outliers detection (broad range check). Some extremes were creating artificial features not consistent to the bibliography, to the published and known min-max values for the regions and these extremes were not used at the further analysis with DIVA.

DIVA tool used also for the automatic outlier detection (by comparing the data analysis residual and the expected standard deviation) to eliminate them from the analysis. This option was used in few cases where the merging of data from the beginning of the century with recent ones highlighted very noisy and inhomogeneous results.

- water column, metals:

no further assessment on the quality was done. The raw data were used as they were given for the products generation.

- Biota and Sediment matrixes:

as the data were insufficient no further qc other than the originators was applied to these data.

For Water column we managed mainly 2 subsets of data:

- “Classic” parameters (fertilizers and organic matter) → the same QC and QF procedures of SDN;
- “Exotic” parameters (eg: contaminants) → still to find an ad hoc QC to flag them.

For Sediment and Biota matrix we had not enough data to perform a quality check at NODC level, only Originators QC was done.

“Exotic” parameters:

- How to apply Range checks? Not enough data availability for a climatology;
- How to apply Spike checks? The contaminants are more related to an “event” logic… hi-values could be related to events, not necessary to spikes!
- Often measures under detection limits… we have to keep them or not!?

Chemical lot PP - …some of the lessons learned…

- The complexity of the measurements covering 8 groups of parameters collected on 3 matrices → need to have wide metadata description and continue with adapting process of SDN standards;

…

- The “exotic parameters” (contaminants) → need an ad hoc QC protocol (no spikes, difficult to apply ranges);

**DISCUSSIONS**

Dr Vinci noted that in the case of SeaDataNet and the EMODnet chemical lot, often very little quality or even no information was received from the data originators. Dr Konovalov added that the data are obtained from national data centres and there is no additional information to justify or understand the reason that QC flags were applied.
3. AN OVERVIEW OF THE PROPOSED STANDARD QF SCHEME

3.1 Justification of the need for QF/QC standard for data exchange

This agenda item was introduced by Sergey Konovalov and considering the justification of the need for the QF/QC standard for data exchange.

- Managing access, discovery, and exchange of multi-disciplinary oceanographic data on marine ecosystems requires scanning across multiple observing systems and temporal and spatial scales.
- Quality checks and quality flagging have been recognized to be of primary importance for oceanographic and marine meteorological data management.
- All major programmes and data centres have been developing and applying various systems of data quality verification and flagging.
- These systems are well developed and established for individual national and international programmes for marine meteorological and physical oceanographic data using a relatively homogenous data structure.
- When it comes to inter-disciplinary data exchange between national and international scientific programs, data centres, and other data management projects and organizations, established quality flagging systems often result in conflicts or quality information loss.

3.2 The standard proposal

A standard proposal was prepared: Proposal to adopt a quality flag scheme standard for data exchange in oceanography and marine meteorology. Version 1.2 was prepared in March 2012. It was submitted by Sergey Konovalov (co-chair IODE GE-BICH), Hernan Garcia (co-chair IODE GE-BICH), Reiner Schlitzer, Laure Devine, Cyndy Chandler, Gwen Moncoiffé, Toru Suzuki, and Alex Kozyr.

This is a proposal to recommend that a modified quality flag (QF) scheme standard be adopted to facilitate the exchange of multi-disciplinary oceanographic and marine meteorological data and the generation of data bases using data from different programs and sources.

The proposal is intended for the exchange of oceanographic and marine meteorological data by national and international programs and projects.

The proposed standard does not oblige currently established programs or projects to change their quality flag systems for the proposed standard, but it can serve as a proposed standard for future programs.

The utility of the proposed QF scheme is obvious when data of different origins or natures are exchanged or combined into a joint data base;

The proposed standard makes it possible to combine various quality flags into one scheme, preserve original information on quality flags, add the results of additional quality checks, and effectively serve users of different levels and experience.

Some flag schemes are limited to data quality (e.g., ODV, OceanSITES) and provide limited or no information on data processing history and/or quality tests applied. Other flag schemes include
references to applied tests and their results (e.g., WOD) and/or data processing history rather than only
data quality (e.g., GTSP, SeaDataNet).

Two-level quality flag scheme

The first or **primary level** is composed of five quality codes and their definitions.

The second level complements the first level by reporting the results of QC tests performed and data
processing history.

If a data user only wants data flagged “good”, then this person will only use the primary level.

If the user needs information identifying and justifying the primary level flags, then the secondary
level provides complete information on the quality test applied and their results. In this way the data
user can accept or reject any data based on level 1 or make an informed choice based on level 2.

Primary-level quality flag codes and definitions. Any quality control tests must be well
documented in the metadata that accompany the data.

<table>
<thead>
<tr>
<th>Code</th>
<th>Primary-level flag’s short name</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Good</td>
<td>passed documented required QC tests</td>
</tr>
<tr>
<td>2</td>
<td>Not evaluated, not available or unknown</td>
<td>used for data when no QC test performed or the information on quality is not available</td>
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<tr>
<td>3</td>
<td>Questionable/suspect</td>
<td>failed non-critical documented metric or subjective test(s)</td>
</tr>
<tr>
<td>4</td>
<td>Bad</td>
<td>failed critical documented QC test(s) or as assigned by the data producer</td>
</tr>
<tr>
<td>9</td>
<td>Missing data</td>
<td>used as place holder when data are missing</td>
</tr>
</tbody>
</table>

The reason for a specific quality flag for a data point at the first level is justified by the list and results
of applied quality tests, with details proclaimed in the second level. While different tests can be
applied and qualified as required, the critical and non-critical tests for data sets of different nature and
origin and information on the tests and their results is completely preserved at the second level.

**The second-level quality flags** are variable in their quantity and quality, summarizing information on
the applied quality tests (e.g., excessive spike check, regional data range check) and data processing
history (e.g., interpolated values, corrected value).

This scale makes it possible to join the gained experience and information from established programs
and projects (e.g., Argo, GTSP, OceanSites, Qartod, SeaDataNet, IMOS, MMI, WOD) and provides
a possibility for an additional, currently unforeseen second-level quality tests and procedures.
Advantages of the 2-level scheme

- Small and fixed number of unambiguous flags at the primary level, which are identified and justified by the list and results of tests at the second level;

- Primary-level code values are numeric and ordered such that increasing quality flag values indicate a decreasing level of quality. This supports the identification of all data that meet a minimum quality level and facilitates automatic data analysis and filtering;

- The monotonic primary scale facilitates the inheritance of quality flags for derived or calculated variables. For example, when temperature and salinity values are used to calculate density, the density value will inherit the flag of the datum with the lowest quality;

DISCUSSIONS

Dr Giorgetti recalled that the SDN infrastructure is developed for data sharing and exchange. There is no difference whether this scheme is used for data exchange. EMODnet is developed as a network. QC schemas seem to have been split into 2 levels which are incorporating the same: originator QC is important but is still absent. Ms Chandler pointed out that we would not lose originator but rather get a system that represents each originator. Now we are proposing a common framework.

Dr Vinci stated that what is being proposed is something that can be laid over other QC schemas and can be mapped with other QC schemas. So, the other schema can remain and can be mapped 1-1. He then asked how SDN and EMODnet will supply the new quality flag schema to the existing infrastructure?

Dr Konovalov responded that any programme can keep their quality flagging and quality assessment scheme. If they find their system is not that good then they can consider this proposal and modify it as to their needs. So we are not expecting anyone to change their system.

Dr Vinci stated that a problem was now being looked at from different sides: the proposal for a 2-level scheme is very interesting when considering a problem they face in the EMODnet chemical lot: data coming from physical oceanographers gave some problems when applying tests like range checks, spikes, etc. When giving the flag “good” it is not always clear what “good” implies.

Dr Konovalov stated that a programme can easily decide to map their existing flag scheme to the proposed scheme. Ms Chandler added that such crosswalks have already been prepared. Dr Konovalov stated further than SDN currently uses a one layer flag scheme which implies that no information is available on the reasons a flag was given to the data. Dr Konovalov recalled that the 1st level should be limited to quality flags. We cannot limit the number of quality tests in the 2nd level so the 2nd level is kept open.

Dr Garcia summarized the discussions as follows: there are many different quality and quality control flags being used. The idea put forward in our proposal was to be on top of this and
allowing for the exchange of data while preserving quality flags and quality control that each institution has put in place. So it should be seen as a way forward to facilitate the exchange of data.

3.3 Comments by the ad hoc ODS group

This agenda items was introduced by Dr Charles Sun. He referred to the discussions held by the ETDMP at its 3rd Session, the previous week. He recalled that he had attended IODE-XXI and was invited by former Co-Chair to review the proposal as part of the expert review. In May 2011 there was an announcement for the community review. Dr Sun was involved in this as well. Around November 2011, when Dr Sun was attending the Argo meeting in Seoul, he discussed the matter with Argo, GTSPP, OceanSites and others. People started sending comments back to the IODE Secretariat. Mr Pissierssens then invited Dr Sun to summarize the discussions until that time. A summary had been prepared and submitted to the IODE Secretariat and to the co-authors. This was done early 2012. Briefly before the SG-ODS meeting in April version 1.2 of the proposal was released. The SG-ODS then reviewed release 1.2. Subsequently Dr Sun then sent version 1.2 for community review inviting comments with deadline of 30 June 2012. No comments were received. Upon the expiry of the deadline Dr Sun sent reminders and again no responses were received. Recently comments were received from Australia and Canada. He then summarized the comments received as follows:

1. The proposal reviewers support the concept of two levels of quality flags, with the first providing an overall indication of the quality of a data point and the second level providing more information on how the quality assessment was made. With suitable flag definitions, this second flag could also contain information on the history of the data point. The reviewers feel however that there is not enough detail on the second level for the proposal to be adopted as is. There would need to be significant work undertaken to define this level before it could be termed a standard; and

2. Table 1 of the paper advocates the use of the value “2” to indicate “not evaluated, not available or unknown”. This is a significant departure from common practice with no explanation of the merits of this. If there is no good reason to change then we strongly feel that any standard should stay as close as possible to current practice, which typically has flag value 0 for “not evaluated, not available or unknown” and the flag values 1 through 4 for decreasing levels of confidence in the data value (as used by Argo and GTSPP, for example).

3.4 Current situation and further steps

On behalf of the two co-chairs of the ETDMP ODS-TT, Dr Sun continued to debrief the meeting attendees about the discussions taken in place at the ETDMP-III. They recommended the following:

1) Ask the authors to modify the proposal as suggested by the ad hoc ODS SG (PO, YM, CS)

2) Circulate the revised V1.3(?) to the IODE Member States for comments (PO, YM)

3) Publish the primary level of the QC flagging system as a standard with clearly defined meanings of QC flag, (ODS, IODE office)

4) Publish the secondary level of QC flagging system as a best practice of the proposed ODSBP, if wish. (ODS, IODE office)

(note: PO=Paul Oloo; YM=Yutaka Michida; CS: Charles Sun).
DISCUSSIONS

Dr Garcia referred to (3) and (4) above and inquired if these would be published separate? Dr Sun affirmed this. Dr Sun commented that our definition of best practice implies that the method has been successfully used by a large group. This is not the case for the proposed practice (4).

Dr Garcia expressed his high appreciation for the work put into the reviewing of the proposal. He opened the floor for comments.

Mr Reed asked about (3) above. He stated that splitting the publication into two separate publications would be confusing.

Mr Pissierssens stated that version 1.2 is too verbose and does not clearly identify the advantages and reasons for the proposed scheme. He referred to the discussions of the previous day when these advantages were given clearly. He invited the meeting to recall these.

Dr Giorgetti expressed agreement to have two levels but for the first level she suggested to use 0 and 2 flagging as it is used in Argo, GTSP and SDN. For the second level she expressed agreement with Dr Sun that it is not detailed enough. Lists of codes should be more complete and should cover possibilities we now have. It should be a commonly agreed coding.

Dr Vinci, referring to level 2 observed that this reminded him of common vocabularies of SDN. There are standard vocabularies used by SDN. So, the idea of an open list would be good for level 2 but it needs to be controlled by someone.

Mr Reed noted that the level 2 codes will grow with use so having control is a good idea. Maybe the ODSBP could be tasked to control the list. Regarding quality flag 0 Mr Reed noted that the most widely used software for ocean data is ODV. ODV uses quality flag 0 for good data. How does SDN use ODV with mismatched quality flags? So why is using 2 such a big issue?

Dr Giorgetti responded that: ODV is an oceanographic data analysis software which uses its own flag scale internally. ODV maps all existing flag scale to its own scale for colour plotting and further analysis but the ODV flag scale is not exported nor used for data exchange.

Ms Chandler stated that most of the people in this room seem clear on what we are trying to propose but we have not been able to communicate this effectively. Comments seem to be in 3 areas: the 2 level seems to be acceptable but there are two residual issues: what is the idea behind the level 1 flags 0 and 2. This seems counter-intuitive. So we need to say monotonic: good to less good. We need to make this more clear. The other issue is that level 2 is not specific enough but that was exactly the purpose: it should be flexible and can be extended as needed. Because we are proposing this as a standard, may be we must be more specific.

Dr Sun continued to lead the discussion and advised that the QC flag proposal should address the justification and intended audiences of the proposal and felt that the proposed primary (first) level is primary for data users and suggested that the proposal should reflect it to avoid any confusion raised by any data manager.

The meeting then decided to establish a sessional working group with the objective of revising the proposal and make it more clear. The membership was Ms Cyndy Chandler, Ms Laure Devine, Dr Sergey Knovalov, Mr Peter Pissierssens and Mr Greg Reed.

The meeting discussed the revised proposal under Agenda item 5.
4. QUALITY TESTS AND QUALITY FLAGS

4.1 Assignment and relationship between quality flag (QF) and measured or calculated data (data fit for purpose)

Dr Garcia opened the section with two questions: 1) what is a quality flag and 2) who assigns QF?

**What is a quality flag?** A quality flag provides basis (quantitative or qualitative, data processing history, provenance) information useful to help assess data fit for purpose. Data originators (e.g., data investigators)

**Who assigns QF?**

Data managers at NODCs

Data managers at operational data programs of data project offices

Order:

Data Originators provide QF codes and descriptors (1st and 2nd level)

Operational data programs provide QF codes and descriptors (1st, and 2nd level) and in the absence of the above, NODC provide QF as an output as requested (1st and 2nd level)

4.2 Minimum recommended list of SL flag codes and working towards and documented approach

The group suggested a list of QC tests that could be applied to a wide range of chemical, physical, and biological profile, underway, and moored data. However, the applicability and definition of each QC test will depend on the specific application of the data (fit for purpose) and specific project program or NODC data control requirements

1. Broad data range or globally impossible values check
2. Regional data range check
3. Excessive data gradient check
4. Excessive spike check
5. No data gradient check

The group recommended providing specific bibliographic citations to QF, and QC tests descriptions of individual programs, NODCs, etc if they exist.

4.3 Relationship between existing QF and results of additional quality tests (closed vs open SL flag list)

Dr. Garcia suggested that IODE GE-BICH, on behalf of the community, will maintain a centralized catalogue of available 1st and associated 2nd level QC tests for individual programs (SeaDataNet, WOD, GTSP, BODC, QUARTOD, etc). The group recommended that each program identified provide a POC for maintaining and keeping the catalogue of codes up-to-date. The group also indicated that there should be a data validation step to verify mapping between the first and the second level flags for each program. When a program decides to change the second level flagging system, for example, Leslie Richards could represent BODC on behalf of SeaDataNet, H. Garcia for WOD, Charles Sun for GTSP, Alex Kozy for CDIAC, etc
5. WRAP-UP SESSION

Dr Konovalov reported on the outcome of the sessional working group.

Dr Konavalov reported a change of the proposal title to “Quality Flag Scheme for the Exchange of Oceanographic and Marine Meteorological Data”. It is a scheme that we can suggest for data exchange or future projects. The revised proposal includes a few sections, including INTENDED AUDIENCE and JUSTIFICATION.

The scheme is intended for individual researchers, research groups or oceanographic/marine meteorological data centres who manage and/or exchange oceanographic/marine meteorological data. The scheme does not require existing programs or projects to change their quality flag systems, but aims to provide a scheme for the exchange of data between existing programs.

The proposal was then discussed.

DISCUSSIONS

Dr Garcia asked whether the intent was now that the document will not go to the ODS procedure. Mr Pissierssens responded that if the group agrees the proposal can be re-submitted to the ODS. If we still get a lot of negative comments, we can publish it as an IODE information document, IOC manuals and guides, or IOC technical series. We simplified the structure of the proposal to identify: why, what, and for whom. If it is agreed to submit to the ODS then the document can be restructured to comply with the ODS template.

The meeting agreed that the objective remains for the proposal to be re-submitted to the ODS.

Dr Konovalov continued to lead the discussion on the revised proposal. The group went through the proposal paragraph by paragraph. The revised proposal clearly addresses that the primary level flags are intended for data users to map the quality flags from the existing program of their interest to the new QC primary level flag as a guideline and can be used by the future programs.

The revised proposal is attached as Annex III

Dr Giorgetti and Dr Vinci, on behalf of SeaDataNet, continued to express their objections to the proposal. They rejected the proposal because the primary scale (the quality flag scale) gives a different meaning to the flag “2” with respect to what already used by SDN, GTSP, Argo and the changing will generate problems on the mapping (the flag 2 that in SDN means a value out of climatological check and is defined as a “probably good value” should be mapped as simply good=1 or probably bad=3, which is a loss of information even if the specification of the check can be included into the secondary level).

The meeting requested the Secretariat to circulate the draft report of the meeting within two weeks and send it to Dr Konovalov and Dr Garcia for further edits. They will then return the report to the Secretariat. The secretariat will then circulate the report to the participants for their final comments and edits.

6. CLOSING OF THE MEETING

The meeting was closed on Thursday 24 October at 14h15. The meeting requested the Secretariat to distribute the draft report for corrections during the next week and to publish the report not later than 15 November 2012.
ANNEX I

AGENDA OF THE MEETING

1. OPENING OF THE MEETING
   1.1 INTRODUCTIONS OF PARTICIPANTS
   1.2 ADOPTION OF THE AGENDA
   1.3 INTRODUCTION OF WORKING DOCUMENTS

2. AN OVERVIEW OF OCEANOGRAPHIC QUALITY CONTROL AND QUALITY ASSESSMENT SCHEMES AND THE BASIS FOR A STANDARD QF SCHEME
   2.1 PRESENTATIONS BY PARTICIPANTS
      2.1.1 DOKUZ EYLÜL UNIVERSITY, INSTITUTE OF MARINE SCIENCES AND TECHNOLOGY: NIHAYET BIZSEL
      2.1.2 EXAMPLES OF DATA QUALITY INDICATORS FOR DATA CONTRIBUTED TO BCO-DMO: MS CYNDY CHANDLER
      2.1.3 QUALITY CONTROL ON BIOLOGICAL DATA BEFORE AND AFTER DATA INTEGRATION: KLAAS DENEUDT, VLIZ, BELGIUM
      2.1.4 QUALITY CONTROL OF BOTTLE DATA AT INSTITUT MAURICE-LAMONTAGNE - FISHERIES AND OCEANS CANADA QUÉBEC REGION - LAURE DEVINE AND CAROLINE LAFLEUR
      2.1.5 THE QUALITY ASSURANCE/QUALITY CONTROL (QA/QC) PROCEDURE (GLODAP EXAMPLE) – ALEX KOZYR
      2.1.6 QUALITY CONTROL AND QUALITY FLAG OF PACIFICA – TORU SUZUKI, MARINE INFORMATION RESEARCH CENTER, JAPAN
      2.1.7 UKRAINIAN NODC (MARINE HYDROPHYSICAL INSTITUTE AND INSTITUTE OF BIOLOGY OF THE SOUTHERN SEAS, SEVASTOPOL) – SERGEY KONOVALOV, ALEXEY KHALIULIN (MHI), VOLODYMYR VLADYMYROV (IBSS)
      2.1.8 WORLD OCEAN DATABASE DATA QUALITY CONTROL - HERNAN GARCIA, NOAA NATIONAL OCEANOGRAPHIC DATA CENTER, SILVER SPRING, MD 20910, USA
      2.1.9 GLOBAL TEMPERATURE AND SALINITY PROFILE PROGRAMME (GTSPP) DATA QUALITY TESTS – CHARLES SUN, CHAIR SG-GTSPP /
      2.1.10 QUALITY CONTROL OF CTD DATA USING PROPOSED IODE QF SCHEME – GREG REED, ANDREW WALSH, RAN HYDROGRAPHY AND METOC BRANCH
      2.1.11 SEADATANET QC, FLAGS AND EMODNET CHEMISTRY EXPERIENCE – MATTEO VINCI, ALESSANDRA GIORGETTI, OGS NODC, TRIESTE, ITALY

3. AN OVERVIEW OF THE PROPOSED STANDARD QF SCHEME
   3.1 JUSTIFICATION OF THE NEED FOR QF/QC STANDARD FOR DATA EXCHANGE
   3.2 THE STANDARD PROPOSAL
   3.3 COMMENTS BY THE AD HOC ODS GROUP
   3.4 CURRENT SITUATION AND FURTHER STEPS

4. QUALITY TESTS AND QUALITY FLAGS
   4.1 ASSIGNMENT AND RELATIONSHIP BETWEEN QUALITY FLAG (QF) AND MEASURED OR CALCULATED DATA (DATA FIT FOR PURPOSE)
   4.2 MINIMUM RECOMMENDED LIST OF SL FLAG CODES AND WORKING TOWARDS AND DOCUMENTED APPROACH
4.3 RELATIONSHIP BETWEEN EXISTING QF AND RESULTS OF ADDITIONAL QUALITY TESTS (CLOSED VS OPEN SL FLAG LIST)

5. WRAP-UP SESSION

6. CLOSING OF THE MEETING
ANNEX II

LIST OF PARTICIPANTS

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ANNEX III

QUALITY FLAG SCHEME FOR THE EXCHANGE OF OCEANOGRAPHIC AND MARINE METEOROLOGICAL DATA

INTRODUCTION

This document describes a two-level quality flag scheme (QF) that will facilitate the exchange and integration\(^1\) of multi-disciplinary oceanographic and marine meteorological data.

The primary level defines the data quality flags only, while the secondary level provides the justification for the quality flags, based on quality control tests or data processing history.

INTENDED AUDIENCE

The scheme is intended for individual researchers, research groups or oceanographic/marine meteorological data centres who manage and/or exchange oceanographic/marine meteorological data.

The scheme does not require existing programs or projects to change their quality flag systems, but aims to provide a scheme for the exchange of data between existing programmes. It may also serve as a quality flag scheme for new projects and programmes.

JUSTIFICATION

Quality flag schemes are used to record results of quality control and quality assessment checks and enable users to filter data based upon known quality criteria.

If the proposed scheme was in place, it would enable users to merge different data sets, retain previous quality information, add new information on data quality and processing history, and make informed decisions to accept or reject data depending on the particular application or research question.

In this way users can work with data that meet their quality requirements.

When data from different sources are combined in one data base, existing information on quality of data can be lost because different quality flag schemes are used by different data centres and there is rarely one-to-one mapping.

It is important to include detailed information on quality test results if such information exists, and one-level quality flag schemes do not support this capability.

Advantages of this two-level scheme:

- Small and fixed number of unambiguous flags at the primary level that can be justified by the details in the second level;
- Primary-level flag values are numeric and ordered such that increasing quality flag values indicate a decreasing level of quality. This supports the identification of all data that meet a minimum quality level and assignment of quality flags to calculated parameters;
- The scheme is universal; it can be applied to all types of data enabling exchange and integration of multi-disciplinary data;
- Existing QF schemes can be mapped to the proposed scheme with no information loss. This is specifically true when information on the applied tests is delivered by data providers;

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\(^1\) “integration” in this context covers the combination of data from two or more sources into one database as well as using the combined database for the development of data products.
Data sets with different QF schemes can be merged into one data set, preserving all existing quality flags and making it possible to apply new quality tests and add the results.

The flag scheme was designed based upon an extensive review of existing quality flag schemes (See Annex). None of the reviewed schemes met all advantages stated above. A detailed comparison between 15 widely used flagging schemes is available from [http://odv.awi.de/fileadmin/user_upload/odv/misc/ODV4_QualityFlagSets.pdf](http://odv.awi.de/fileadmin/user_upload/odv/misc/ODV4_QualityFlagSets.pdf)

**THE QUALITY FLAG SCHEME**

A two-level quality flag scheme is proposed.

**Primary Level**

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

**Table 3: Primary level**

<table>
<thead>
<tr>
<th>Value</th>
<th>Primary-level flag’s short name</th>
<th>Definition</th>
</tr>
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</tr>
<tr>
<td>9</td>
<td>Missing data</td>
<td>used as place holder when data are missing</td>
</tr>
</tbody>
</table>

*Note: The quality of verified "Good" (flag 1) is considered higher (smaller flag value) compared to "Not evaluated" (flag 2), as the latter could turn out to be of any quality from good to bad, once the quality checks have been performed. Consequently, the neutral "Not evaluated" (flag 2) is placed between verified "Good" and verified "Questionable/suspect".*

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.

The primary level flags are such that increasing flag values indicate decreasing data quality. This is an important property that facilitates data quality filtering and/or processing, including inheritance of quality flag values for derived variables. The quality of a calculated value inherits the lowest quality qualifier of the variables used in the calculation. For example, when we calculate density from temperature (T) and salinity (S), then if T is of “good” quality and S is of “unknown” quality, then density should inherit the “unknown quality”.

**Mapping**

Mappings for existing and future programmes, including those in Annex A, will be invited and maintained on the ODS web site ([http://www.oceandatastandards.org](http://www.oceandatastandards.org)) and by GE-BICH.
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 4: An example of quality control tests and data processing history

<table>
<thead>
<tr>
<th>Example Quality control test / data processing history (description)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Globally impossible value</td>
</tr>
<tr>
<td>Monthly climatology standard deviation test</td>
</tr>
<tr>
<td>excessive spike check</td>
</tr>
<tr>
<td>excessive offset/bias when compared to a reference data set</td>
</tr>
<tr>
<td>excessive data uncertainty</td>
</tr>
<tr>
<td>unexpected X/Y ratio (e.g., chemical stoichiometry or property-property X to T, S, density, among others)</td>
</tr>
<tr>
<td>excessive spatial pattern check (“bullseyes”)</td>
</tr>
<tr>
<td>above detection limit of method</td>
</tr>
<tr>
<td>interpolated value (not measured)</td>
</tr>
<tr>
<td>data offset corrected value relative to a reference data</td>
</tr>
<tr>
<td>expert review</td>
</tr>
</tbody>
</table>

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 the values 0 (for passed), 1 (for failed) or 2 (for not performed).

Example: implementation of secondary level

The example below is derived from the NODC World Ocean Database, the test is identified by a code and the possible outcomes of the test are represented in “values” and their “meanings”. Test for an individual observation that fails QC checks for broad data range and a depth inversion.

Test description: WOD uses a hierarchy of QC tests. Broad data range range checks are used to screen the data for extreme values as a function of depth and oceanic basins for each variable in WOD. The range for a variable, in each region, is set large enough to encompass variations for all seasons and years. Ranges were determined using frequency distributions, statistical analysis, literature values, and atlases. Depth inversions and duplication of depths were found in some profiles. A depth inversion occurs when an observation has a shallower depth than the observation directly preceding it. A depth duplicate is a reading which has the same depth as the reading immediately before. See Boyer et al. 2009. World Ocean Database 2009. S. Levitus, Ed., NOAA Atlas NESDIS 66, U.S. Gov. Printing Office, Wash., D.C., 216 pp., and Johnson et al 2009. World Ocean Database 2009 Documentation. Edited by Sydney Levitus. NODC Internal Report 20, NOAA Printing Office, Silver Spring, MD, 175 pp.)

NODC WOD QC flags for observed levels

<table>
<thead>
<tr>
<th>Code</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>Accepted value</td>
</tr>
</tbody>
</table>
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

Value: In WOD, a single integer digit value is assigned only if the observation fails a particular test or a combination of QC tests. In the case of a value that fails both range outlier and a depth inversion check, a single digit value of “6” is assigned to the individual value as shown in the above table of NODC WOD QC flags for observed levels. This WOD secondary QF value of “6” maps to a QF of “3” in the proposed primary QF level (Table 3). We note that WOD also preserves QF values provided by the originator of the data if available.

Mapping

Existing and future programmes will be invited to provide their Secondary Level Table (including chosen codes, description of Quality control tests / data processing history, values and meanings) which will be maintained on the ODS web site (http://www.oceandatastandards.org).
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