Upgrade Black Sea Scene

WP9: Data Quality Control guidelines for physical and chemical parameters

Version 1.3

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Contents

Abstract

The scope of this document is to provide the Upgrade-BSS project partners guidelines and recommended standards for management and quality control of physical and chemical oceanographic data. It has been produced by compiling guidelines, common sets of quality control procedures and best practices that are implemented in major European and International Projects (e.g. SeaDataNet, MyOcean, MEDAR/MEDATLAS, ESEAS, SIMORC, WOCE, JGOFS, GOSUD, Argo, GLOSS, etc), shared among National Oceanographic Data Centres (IODE/NODCs) and marine research organizations and recommended by IOC, ICES and EU for data access and exchange.

The document describes procedures that make extensive use of specific data quality flags, processing/archive formats and tools that developed in the framework of several research projects. In order to standardize the QC procedures and ensure data reability, consistency and interoperability with other systems, Upgrade-BSS project adopts the SeaDataNet standards, vocabularies, exchange formats, and tools for quality control.

The guidelines include the quality control procedures in real time and delayed mode which are carried out by the NODCs and research Institutes for vertical profiles, time series, trajectories and wave data. They do not include information for field data collection and laboratory methods.

The procedures are intended to cover the physical (temperature and salinity) and chemical (oxygen and nutrients) oceanographic data but there are obvious generalizations that can be made to other parameters measured from the same instruments.

1. Introduction

The Earth's natural systems are complex environments in which research is difficult in most instances and where many natural factors and events need to be taken into consideration. Especially complex are the aquatic environments which have specific research obstacles to overcome, namely deep, dark and often turbulent conditions. Good quality research depends on good quality data and good quality data depends on good quality control methods. Data can be considered 'trustworthy' after thorough processing methods have been carried out. At this stage they can be incorporated into databases or distributed to users via national or international exchange.

Data quality control essentially and simply has the following objective:

"To ensure the data consistency within a single data set and within a collection of data sets and to ensure that the quality and errors of the data are apparent to the user who has sufficient information to assess its suitability for a task."

(IOC/CEC Manual, 1993)

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

1. Maintaining Common Standards

   There is a minimum level to which all oceanographic data should be quality controlled. There is little point banking data just because they have been collected; the data must be qualified by additional information concerning methods of measurement and subsequent data processing to be of use to potential users. Standards need to be imposed on the quality and long-term value of the data that are accepted (Rickards, 1989). If there are guidelines available to this end, the end result is that data are at least maintained to this degree, keeping common standards to a higher level.

2. Acquiring Consistency

Data within data centres should be as consistent to each other as possible. This makes the data more accessible to the external user. Searches for data sets are more successful as users are able to identify the specific data they require quickly, even if the origins of the data are very different on a national or even international level.

3. Ensuring Reliability

Data centres, like other organisations, build reputations based on the quality of the services they provide. To serve a purpose to the research community and others their data must be reliable, and this can be better achieved if the data have been quality controlled to a 'universal' standard. Many national and international programmes or projects carry out investigations across a broad field of marine science which require complex information on the marine environment. Many large-scale projects are also carried out under commercial control such as those involved with oil and gas and fishing industries. Significant decisions are made, and theories formed, on the assumption that data are reliable and compatible, even when they come from many different sources.

(SIMORC,Data Quality Control Procedures, 2006)

2. Information (Metadata) compilation

Alongside the data, additional information (metadata) is needed not only for quality control and archiving, but also for exchanging data or integration of them into regional or global data sets.

For all types of data, information is required about:

- **Where** the data were collected: location (preferably as latitude and longitude) and depth/height
- **When** the data were collected (date and time in UTC or clearly specified local time zone)
- **How** the data were collected (e.g. sampling methods, instrument types, analytical techniques)
- **How** you refer to the data (e.g. station numbers, cast numbers)
- **Who** collected the data, including name and institution of the data originator(s) and the principal investigator
- **What** has been done to the data (e.g. details of processing and calibrations applied, algorithms used to compute derived parameters)
- **Watch points** for other users of the data (e.g. problems encountered and comments on data quality)

The ICES Working Group on Data and Information Management (WGDIM) has developed a number of data type guidelines which itemize these elements that are required for thirteen different data types (see table below). These Data Type Guidelines have been developed using the expertise of the oceanographic data centres of ICES Member Countries. They have been designed to describe the elements of data and metadata important to the ocean research community. These guidelines are targeted toward physical-chemical-biological data types collected on oceanographic research vessel cruises. Each guideline addresses the data and metadata requirements of a specific data type. This covers three main areas:

What the data collector should provide to the data centre (e.g. collection information, processing, etc)

How the data centre handles data supplied (e.g. value added, quality control, etc)

What the data centre can provide in terms of data, referral services and expertise back to the data collector.

ICES Data Type Guidelines		
CTD	Moored ADCP	Moored Current Meter
Shipborne ADCP	Seasoar (Batfish)	Surface (Underway)
Water Level	XBT	Net Tow (Plankton)
Surface Drifting Buoy	Profiling Float and Drifting Buoy	Discrete water sample data
Multibeam echosounder data		

The guidelines can be assessed from the ICES web site at the address: http://www.ices.dk/datacentre/guidelines/DataTypeGuidelines/DataTypeGuidelines.asp

For purposes of long term data viability and future access, this information should be documented in databases and always accompany the data. The SeaDataNet metadata catalogue system serves this principle and is being used for data discovery and data access (www.seadatanet.org/meta-data). The information is organized in six interrelated thematic metadatabases describing the data sets (EDMED), Common Data Index (CDI), Cruise Summary Reports (CSR), Research Projects (EDMERP), Marine Organizations (EDMO), and Monitoring Systems (EDIOS). The Black Sea discovery system has been extended and includes the Data Quality Control procedures in Black Sea, the Scientists, the Publications and the Socio-economic metadata bases. The use of common vocabularies in all metadatabases and data formats ensure consistency and interoperability. The SeaDataNet Vocabulary service (seadatanet.maris2.nl/v_bodc_vocab/welcome.aspx) is based upon the NERC DataGrid (NDG) vocabulary Web service (www.bodc.ac.uk/products/web_services/vocab/).

3. Metadata/Data Reformatting and QC Tools

Metadata

The ISO 19115 content model is the basis for the XML formats and exchange schema (XSD) for each of the metadata bases. The maintenance of each of the metadata directories is coordinated at a national level by the National Oceanographic Data Centre/Marine Data Centre, belonging to the UP-GRADE BS-SCENE (UBSS) project partnership. They collect references from institutes in their country and enter these into the directories.

For the maintenance and content upgrade from Version 0 to Version 1 there are available on-line (like **CMS** forms) and off-line tools (**MIKADO**) that produce XML ISO 19115 compliant exchange formats which have been developed by the SeaDataNet Technical Task Team.

A Data management plan with detailed information for the work division between NODC and other national partners per country, overviews on the available tools for maintenance, references to online manuals and formats for all UBSS metadata directories, can be found on the Project deliverable "d4-1_4-2_4-5_manual-directories.doc" (available at the Project Extranet, under directory UPGRADE BSS: Deliverables to EU)

Data

In general, the original measurement data formats cannot be used in data management and exchange because they have incomplete and not-standardized information and they are not compatible with QC and other processing tools. The data management format, the archiving and the transport (exchange) format may not be necessarily the same. The archiving format should:

- be independent from the computer (and libraries),
- insure that any isolated data includes enough meta-data to be processed (eg. Location and date)
- be compatible and include at least the mandatory fields (meta-data) requested for the greed exchange format(s)
- Include additional textual or standardized "history" or "comment" fields to prevent any loss of information
- Provide similar structure and meta-data for different data type such as vertical profiles and time series

The above rules are normally followed also for the exchange formats.

Seadatanet exchange formats:

- Obligatory formats
  - *NetCDF CF Compliant* (Binary) for gridded data and 3D observation data such as ADCP
  - *ODV4* spreadsheet for other data types (vertical profiles and time series)
- Optional
  - *ASCII SeaDataNet Medatlas*

Reformatting Tools:

- *MIKADO* javatool: Editing and generating XML metadata entries:
- *NEMO* javatool: Conversion of any ASCII format to the SeaDataNet ODV4 ASCII format
- *Med2MedSDN:* Conversion of the Medatlas format to the SeaDataNet Medatlas format

QC Tools:

- *Ocean Data View* (ODV): QC, analysis and visualization of data sets in ODV, Medatlas, WOCE, US NODC format
- *QCDAMAR:* archiving and quality control of oceanographic data in Medatlas format
- *MHI* tool for QC of oceanographic data in Medatlas format
- a *statistical tool* to filter datasets for outliers was developed *TU-Varna* (Bulgaria).

UBSS Partners can always use their own software tools as long as these are consistent with the same protocols and procedures which are described at this document.

4. Quality Control Flags

The SeaDataNet QC Flags scheme is based on on IGOSS/UOT/GTSPP & Argo quality flags and is available as L201 controlled list at the Seadatanet vocabulary web page (www.seadatanet.org):

Flag	Short description
Data quality flags	
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
Information flags	
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

5. Automatic checks (Real Time QC) for Temperature and Salinity

(MyOcean Project, 2010)

One central part of the functions to be implemented by an in-situ Thematic Assembly Centre of MyOcean Project, is the control of incoming decoded measurements. Since at this step data should be available in real time, the QC during that process is limited and automated. An agreement on the RTQC procedure recommendations needs to be achieved in order to guarantee good quality data as well as data consistency throughout the MyOcean in-situ RT database. This is a vital step to be taken before data exchange and scientific analysis can be initiated.

In the following, automated RTQC will be listed for different types of temperature and salinity measurements, i.e. vertical profiles as well as time series. The automated QC procedures described here have been developed for the QC for the Argo data management (Argo, 2009) and have been extended on other profile data and on time series. To improve the efficiency of some tests, specifications are incorporated into the validation process of regional measurements, depending on local water mass structures, statistics of data anomalies, the depth and gradient of the thermocline, as well as using regional enhanced bathymetry and climatology.

5.1 RTQC for vertical profiles: Argo, CTD, XBT

Automated tests for vertical profiles are presented here, i.e. temperature and salinity measurements from Argo floats, CTDs and XBTs.

1. Platform identification: (applies only to GTS data)

Every centre handling GTS data and posting them to the GTS will need to prepare a metadata file for each float and in this is the WMO number that corresponds to each float ptt (platform transmitter terminal). There is no reason why, except because of a mistake, an unknown float ID should appear on the GTS.

Action: If the correspondence between the float ptt cannot be matched to the correct WMO number, none of the data from the profile should be distributed on the GTS.

2. Impossible date test:

The test requires that the observation date and time from the profile data be sensible.

• Year greater than 1997

• Month in range 1 to 12

• Day in range expected for month

• Hour in range 0 to 23

• Minute in range 0 to 59

Action: If any one of the conditions is failed, the date should be flagged as bad data.

3. Impossible location test:

The test requires that the observation latitude and longitude from the profile data be sensible.

• Latitude in range −90 to 90

• Longitude in range −180 to 180

Action: If either latitude or longitude fails, the position should be flagged as bad data.

4. Position on land test:

The test requires that the observation latitude and longitude from the profile measurement be located in an ocean. Use can be made of any file that allows an automatic test to see if data are located on land. We suggest use of at least the 2-minute bathymetry file that is generally available. This is commonly called and can be downloaded from http://www.ngdc.noaa.gov/mgg/global/etopo2.html.

Action: If the data cannot be located in an ocean, the position should be flagged as bad data.

5. Impossible speed test: (applies only to GTS data)

Drift speeds for floats can be generated given the positions and times of the floats when they are at the surface and between profiles. In all cases we would not expect the drift speed to exceed 3 m/s. If it does, it means either a position or time is bad data, or a float is mislabelled. Using the multiple positions that are normally available for a float while at the surface, it is often possible to isolate the one position or time that is in error.

Action: If an acceptable position and time can be used from the available suite, then the data can be distributed. Otherwise, flag the position, the time, or both as bad data.

6. Global range test:

This test applies a gross filter on observed values for temperature and salinity. It needs to accommodate all of the expected extremes encountered in the oceans.

• Temperature in range −2.5°C to 40.0°C

• Salinity in range 2 to 41.0

Action: If a value fails, it should be flagged as bad data. If temperature and salinity values at the same depth both fail, both values should be flagged as bad.

7. Regional range test:

This test applies to only certain regions of the world where conditions can be further qualified. In this case, specific ranges for observations from the Mediterranean and Black Sea further restrict what are considered sensible values. The Black Sea is defined by the region 40.12N, 27.18E; 47.24N,41.54E and the Mediterranean Sea by the region 30N,6W; 30N,40E; 40N,35E; 42N,20E; 50N,15E; 40N,5E; 30N,6W.

Action: Individual values that fail these ranges should be flagged as bad data.

Black Sea

• Temperature in range -2.0 to 30.0°C

• Salinity in range 2 to 35.0

Mediterranean Sea

• Temperature in range 10.0°C to 40.0°C

• Salinity in range 2 to 40.0

8. Pressure increasing test

This test requires that the profile has pressures that are monotonically increasing (assuming the pressures are ordered from smallest to largest).

Action: If there is a region of constant pressure, all but the first of a consecutive set of constant pressures should be flagged as bad data. If there is a region where pressure reverses, all of the pressures in the reversed part of the profile should be flagged as bad data.

9. Spike test

Difference between sequential measurements, where one measurement is quite different than adjacent ones, is a spike in both size and gradient. The test does not consider the differences in depth, but assumes a sampling that adequately reproduces the temperature and salinity changes with depth. The algorithm is used on both the temperature and salinity profiles:

Test value = $| V2 - (V3 + V1)/2 | - | (V3 - V1) / 2 |$,

where V2 is the measurement being tested as a spike, and V1 and V3 are the values above and below.

Temperature: The V2 value is flagged when

• the test value exceeds 6.0°C for pressures less than 500 db or

• the test value exceeds 2.0°C for pressures greater than or equal to 500 db

Salinity: The V2 value is flagged when

• the test value exceeds 0.9 for pressures less than 500 db or

• the test value exceeds 0.3 for pressures greater than or equal to

500db

Action: Values that fail the spike test should be flagged as bad data. If temperature and salinity values at the same depth both fail, they should be flagged as bad data.

10. Bottom Spike test (XBT only):

This is a special version of the spike test, which compares the measurements at the end of the profile to the adjacent measurement. Temperature at the bottom should be not different from the adjacent measurement by more than 1°C.

Action: Values that fail the test should be flagged as bad data.

11. Gradient test:

This test is failed when the difference between vertically adjacent measurements is too steep. The test does not consider the differences in depth, but assumes a sampling that adequately reproduces the temperature and salinity changes with depth. The algorithm is used on both the temperature and salinity profiles:

Test value = $| V2 - (V3 + V1)/2 |$,

where V2 is the measurement being tested as a spike, and V1 and V3 are the values above and below.

Temperature: The V2 value is flagged when

- the test value exceeds 9.0°C for pressures less than 500 db or
- the test value exceeds 3.0°C for pressures greater than or equal to 500 db

Salinity: The V2 value is flagged when

- the test value exceeds 1.5 for pressures less than 500 db or
- the test value exceeds 0.5 for pressures greater than or equal to 500 db

Action: Values that fail the test (i.e. value V2) should be flagged as bad data. If temperature and salinity values at the same depth both fail, both should be flagged as bad data.

12. Digit rollover test:

Only so many bits are allowed to store temperature and salinity values in a sensor. This range is not always large enough to accommodate conditions that are encountered in the ocean. When the range is exceeded, stored values rollover to the lower end of the range. This rollover should be detected and compensated for when profiles are constructed from the data stream from the instrument. This test is used to be sure the rollover was properly detected.

- Temperature difference between adjacent depths > 10°C
- Salinity difference between adjacent depths > 5

Action: Values that fail the test should be flagged as bad data. If temperature and salinity values at the same depth both fail, both values should be flagged as bad data.

13. Stuck value test:

This test looks for all measurements of temperature or salinity in a profile being identical.

Action: If this occurs, all of the values of the affected variable should be flagged as bad data. If temperature and salinity are affected, all observed values are flagged as bad data.

14. Density inversion:

This test uses values of temperature and salinity at the same pressure level and computes the density (sigma0). The algorithm published in UNESCO Technical Papers in Marine Science #44, 1983 should be used. Densities (sigma0) are compared at consecutive levels in a profile, in both directions, i.e. from top to bottom profile, and from bottom to top.

Action: from top to bottom, if the density (sigma0) calculated at the greater pressure is less than that calculated at the lesser pressure, both the temperature and salinity values should be flagged as bad data. From bottom to top, if the density (sigma0) calculated at the lesser pressure is more than calculated at the greater pressure, both the temperature and salinity values should be flagged as bad data.

15. Grey list: (Argo only)

This test is implemented to stop the real-time dissemination of measurements from a sensor that is not working correctly.

The grey list contains the following 7 items:

- Float Id
- Parameter : name of the grey listed parameter
- Start date : from that date, all measurements for this parameter are flagged as bad and probably bad
- End date : from that date, measurements are not flagged as bad or probably bad
- Flag : value of the flag to be applied to all measurements of the parameter
- Comment : comment from the PI on the problem
- DAC : data assembly center for this float

Each DAC manages a black list, sent to the GDACs. The merged black-list is available from the GDACs. The decision to insert a float parameter in the grey list comes from the PI.

16. Gross salinity or temperature sensor drift (Argo only):

This test is implemented to detect a sudden and significant sensor drift. It calculates the average salinity on the last 100 dbar on a profile and the previous good profile. Only measurements with good QC are used.

Action: if the difference between the two average values is more than 0.5 psu then all measurements for this parameter are flagged as probably bad data (flag '3'). The same test is applied for temperature: if the difference between the two average values is more than 1°C then all measurements for this parameter are flagged as probably bad data (flag '3').

17. Frozen profile test:

This test can detect an instrument that reproduces the same profile (with very small deviations) over and over again. Typically the differences between two profiles are of the order of 0.001 for salinity and of the order of 0.01 for temperature.

A. Derive temperature and salinity profiles by averaging the original profiles to get mean values for each profile in 50 dbar slabs (Tprof, T_previous_prof and Sprof, S_previous_prof). This is necessary because the instruments do not sample at the same level for each profile.

B. Substract the two resulting profiles for temperature and salinity to get absolute difference profiles:

- deltaT = abs(Tprof − T_previous_prof)
- deltas = abs(Sprof − S_previous_prof)

C. Derive the maximum, minimum and mean of the absolute differences for temperature and salinity:

- mean(deltaT), max(deltaT), min(deltaT)
- mean(deltaS), max(deltaS), min(deltaS)

D. To fail the test, require that:

- max(deltaT) < 0.3
- min(deltaT) < 0.001

- mean(deltaT) < 0.02
- max(deltaS) < 0.3
- min(deltaS) < 0.001
- mean(deltaS) < 0.004

Action: if a profile fails this test, all measurements for this profile are flagged as bad data (flag ‘4’). If the float fails the test on 5 consecutive cycles, it is inserted in the grey-list.

18. Deepest pressure test (Argo only):

This test requires that the profile has pressures that are not higher than DEEPEST_PRESSURE plus 10%. DEEPEST_PRESSURE value comes from the meta-data file of the instrument.

Action: If there is a region of incorrect pressures, all pressures and corresponding measurements should be flagged as bad data.

5.2 RTQC for vertical profiles: Gliders and AUVs

Automated tests for vertical temperature and salinity profiles as measured by Gliders are presented here and automatic QC should be applied as listed below.

1. Platform identification: (Slocum Gliders)

Every centre handling float data and posting them to the GTS will need to prepare a metadata file for each float and in this is the WMO number that corresponds to each float ptt. There is no reason why, except because of a mistake, an unknown float ID should appear on the GTS.

Action: If the correspondence between the glider ptt cannot be matched to the correct WMO number.

2. Impossible date test:

The test requires that the observation date and time from the profile data be sensible.

- Year greater than 1997
- Month in range 1 to 12
- Day in range expected for month
- Hour in range 0 to 23
- Minute in range 0 to 59

Action: If any one of the conditions is failed, the date should be flagged as bad data.

3. Impossible location test:

The test requires that the observation latitude and longitude from the profile data be sensible.

- Latitude in range −90 to 90
- Longitude in range −180 to 180

Action: If either latitude or longitude fails, the position should be flagged as bad data.

4. Position on land test:

The test requires that the observation latitude and longitude from the profile measurement be located in an ocean. Use can be made of any file that allows an automatic test to see if data are located on land. Since glider deployments are also performed on the shelf and Autonomous underwater vehicles (AUV) work in shallow waters, we suggest to use the high resolution 30” second bathymetry file that is generally available. This is commonly called STRM30+ and can be downloaded from http://topex.ucsd.edu/WWW_html/srtm30_plus.html.

Action: If the data cannot be located in an ocean, the position should be flagged as bad data.

5. Impossible speed test:

Gliders usually work in upper layers and have their own speed (~0.4 m/s) and thus remain in areas where currents are strong. Drift speeds for gliders can be generated given the positions and times of the glider. In all cases we would not expect the drift speed to exceed 3.5 m/s plus the maximum platform speed of the glider or the propelled AUVs. If it does, it means either a position or time is bad data.

Action: If an acceptable position and time can be used from the available suite, then the data can be distributed. Otherwise, flag the position, the time, or both as bad data.

6. Global range test:

This test applies a gross filter on observed values for temperature and salinity. It needs to accommodate all of the expected extremes encountered in the oceans.

- Temperature in range −2.5°C to 40.0°C
- Salinity in range 2 to 41.0

Action: If a value fails, it should be flagged as bad data. If temperature and salinity values at the same depth both fail, both values should be flagged as bad.

7. Regional range test:

This test applies to only certain regions of the world where conditions can be further qualified. In this case, specific ranges for observations from the Mediterranean and Red Seas further restrict what are considered sensible values. The Black Sea is defined by the region 40.12N,27.18E; 47.24N,41.54E and the Mediterranean Sea by the region 30N,6W; 30N,40E; 40N,35E; 42N,20E; 50N,15E; 40N,5E; 30N,6W.

Action: Individual values that fail these ranges should be flagged as bad data.

Black Sea

- Temperature in range -2.0 to 30.0°C
- Salinity in range 2 to 35.0

Mediterranean Sea

- Temperature in range 10.0°C to 40.0°C
- Salinity in range 2 to 40.0

8. Instrument sensor range test :

The test before have checked if the measurements lie inside the oceanographic limits. This test requires that the profile lies inside the instrument sensor limits.

- Temperature in range -2.5°C to 40.0°C
- Salinity in range 2 to 41.0
- Conductivity in range 1.9 mS/cm to 79.7 mS/cm

Action: If a value fails, it should be flagged as bad data.

<u>9. Spike test</u>

Difference between sequential measurements, where one measurement is quite different than adjacent ones, is a spike in both size and gradient. The test does not consider the differences in depth, but assumes a sampling that adequately reproduces the temperature and salinity changes with depth. The algorithm is used on both the temperature and salinity profiles:

Test value = | V2 − (V3 + V1)/2 | − | (V3 − V1) / 2 | ,

where V2 is the measurement being tested as a spike, and V1 and V3 are the values above and below.

Temperature: The V2 value is flagged when

- the test value exceeds 6.0°C for pressures less than 500 db or
- the test value exceeds 2.0°C for pressures greater than or equal to 500 db
- Salinity: The V2 value is flagged when
- the test value exceeds 0.9 for pressures less than 500 db or
- the test value exceeds 0.3 for pressures greater than or equal to
- 500db

Action: Values that fail the spike test should be flagged as bad data. If temperature and salinity values at the same depth both fail, they should be flagged as bad data.

<u>10. Gradient test:</u>

This test is failed when the gradient of the measurements is too steep with respect to the depth gradient. This test considers the difference in depth to take into account irregular sampling of the platform. The gradient is computed using forward and backward differences on the two edges of the profile, and centered differences elsewhere. The algorithm is used on both the temperature and salinity profiles:

Grad (V) = [V(2) – V(1), V(3:end) – V(1:end-2) / 2, V(end) – V(end-1)];

Test value = | Grad(V) / Grad(depth) | ,

where V is the measurement being tested for a gradient, and depth are the depth related to V values.

Temperature: The V value is flagged when

- the test value exceeds 9.0°C for pressures less than 500 db or
- the test value exceeds 3.0°C for pressures greater than or equal to 500 db

Salinity: The V value is flagged when

- the test value exceeds 1.5 for pressures less than 500 db or
- the test value exceeds 0.5 for pressures greater than or equal to 500 db

Action: Values that fail the test should be flagged as bad data. If temperature and salinity values at the same depth both fail, both should be flagged as bad data.

11. Stuck value test:

This test looks for all measurements of temperature or salinity in a profile being identical.

Action: If this occurs, all of the values of the affected variable should be flagged as bad data. If temperature and salinity are affected, all observed values are flagged as bad data.

12. Frozen profile test:

This test can detect an instrument that reproduces the same profile (with very small deviations) over and over again. Typically the differences between two profiles are of the order of 0.001 for salinity and of the order of 0.01 for temperature.

A. Derive temperature and salinity profiles by averaging the original profiles to get mean values for each profile in 50 dbar slabs (Tprof, T_previous_prof and Sprof, S_previous_prof). This is necessary because the instruments do not sample at the same level for each profile.

B. Substract the two resulting profiles for temperature and salinity to get absolute difference profiles:

- deltaT = abs(Tprof − T_previous_prof)
- deltas = abs(Sprof − S_previous_prof)

C. Derive the maximum, minimum and mean of the absolute differences for temperature and salinity:

- mean(deltaT), max(deltaT), min(deltaT)
- mean(deltaS), max(deltaS), min(deltaS)

D. To fail the test, require that:

- max(deltaT) < 0.3
- min(deltaT) < 0.001
- mean(deltaT) < 0.02
- max(deltaS) < 0.3
- min(deltaS) < 0.001
- mean(deltaS) < 0.004

Action: if a profile fails this test, all measurements for this profile are flagged as bad data (flag '4'). If the float fails the test on 5 consecutive cycles, it is inserted in the grey-list.

13. Deepest pressure test:

This test requires that the profile has pressures that are not higher than vehicle safe depth range plus 10%. The deepest depth range value comes from the meta-data file of the instrument.

Action: If there is a region of incorrect pressures, all pressures and corresponding measurements should be flagged as bad data.

5.3 RTQC for time series

Automated tests for time series are presented here. Recommended tests for time series have been chosen based on RTQC of Argo data and RTQC of the M3A mooring site (Basana et al., 2000). Specifications are given if tests differ from those already described in section 5.1.

1. Impossible date test

2. Impossible location test

3. Global range test

4. Regional range test

5. Pressure increasing test

6. Spike test

7. Frozen Profile test

8. Rate of change in time:

The aim of the check is to verify the rate of the change in time. It is based on the difference between the current value with the previous and next ones. Failure of a rate of the change test is ascribed to the current data point of the set.

Action: Temperature and salinity values are flagged if

$|V_i - V_{i-1}| + |V_i - V_{i+1}| \leq 2*(2*\sigma V)$,

where V_i is the current value of the parameter, V_{i-1} is the previous and V_{i+1} the next one. σV is the standard deviation of the examined parameter. If the one parameter is missing, the relative part of the formula is omitted and the comparison term reduces to $2* \sigma V$. The standard deviation is calculated from the first month of significant data of the time series.

5.4 RTQC for Ferryboxes

Automated tests for ferrybox measurements are presented here. Recommended tests are based on RTQC for time series (see section 4.3), but somehow modified due to the geospatial coverage of measurements. Specifications are given if tests differ from those already described in section 4.1.

1. Impossible date test

2. Impossible location test

3. Frozen date/location/speed test

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

<u>4. Speed range test</u>

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

<u>5. Pump test</u>

If applicable (and it should), a test checking the state of the pump should be performed.

<u>6. Pump history test</u>

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

<u>7. Global range test</u>

<u>8. Regional range test</u>

<u>9. Gradient test</u>

Horizontal gradient tests must take into account the distance between adjacent measurements. This will depend on ship speed and data logging frequency. Moreover, only adjacent data measured at expected interval should be taken into account in the test. This test includes testing of spikes. Threshold values are likely to depend very much on regional specifications.

6. Scientific checks (Delayed Mode QC) for Temperature, Salinity, Oxygen and Nutrients

(Medar/Medatlas, 2000)

6.1 Vertical Profiles: CTD, XBT, MBT, Water Bottle Data, etc

In conformity with the UNESCO/IOC and MAST recommendations, the QC includes automatic and visual procedures. Theses checks are performed on each profile/time series separately and also on profiles grouped by cruises. The result of QC is to add a quality flag to each numerical value, but the values of the observations are not modified. In case of outlier on recent data sets, the originator is contacted to validate/correct/eliminate the value.

The principle of the QC of any parameter is to compare the observations with the available statistics of the same parameter. These statistics vary from a region to another, and the checks are adjusted accordingly.

The flags are then validated or corrected manually, taking into account the overall coherence of the data within the cruise, which is somehow subjective but not arbitrary, and the remarks of the data originator. Using pre-existing knowledge on the region makes automatic checks: extreme values for broad range checks (corresponding to high error level), and previous climatological profiles for narrow range checks; there is also some subjectivity in the tuning of these parameters. It is expected not to get any flag different from In case of outlier, the originator, if available and known, will be contacted to see where is the problem and if the data point has to be corrected or rejected. An early data submission facilitates the QC.

1. Check of the format

Detects anomalies like wrong platform codes or names, parameters name or units, missing mandatory information like reference to a cruise or observation system, source laboratory, sensor type.

No further control should be made before the correction and validation of the archive format.

2. Check of the date and location

The following tests are performed automatically first and the results displayed on a screen to perform the manual check. As these checks concerns location and date, they may be followed with a correction in case of obvious errors like sign errors or time assign to 24 hours. If this is not the case, the profile is eliminated with a global flag to 4 (false).

Check for duplicates:

I. Duplicate cruises: This is one the main difficulty of the archiving and for which the cruise information is very important. The links between stations of the same cruise is used to compare with similar data sets. The check for duplicates includes:
   - check for no pre-existing same cruise identifier
   - check for cruises with same dates for beginning and end
   - for same year, same country: visual check for superposed stations
   - for each month, visual check of superposed stations (local position maps)

II. Duplicate profiles:
   - automatic check for same profile identifiers
   - automatic check for same stations positions (within 1 mile, 1 hour) within a) the same cruise and b) out of the cruise
   - visual check of the position maps of cruises having duplicate profiles

In case of duplicate: the *observed* data set is preferred compared to the *reduced* (standard level) data set, or the most complete (or a combination), or the *latest* and the corresponding cruise summary

Check the date:

- The day must be between 1 and the number of days of the month.
- The year of the profile must be the same as included in the cruise reference

- The month must be between 1 and 12
- The end of cruise must be later than the beginning
- The date and time of the profile must be within the cruise duration.

If this is not the case the values are modified and the changes are recorded. Obvious errors like time= 24 hours are corrected with time=0 and day=day+1 flag=5. In this case the new calculated ship velocity must be acceptable.

Check the ship velocity:

If the ship velocity > maximum velocity of the ship (default is 15 knots) between two consecutive profiles, find the erroneous data (date or location), correct and flag= 5 (changed after QC) the modified value. Always keep the initial values in the data file before any modification.

Check the bottom sounding:

- If the bottom depth sounding is not reported flag=9 (missing value)
- If the bottom depth is out of the regional scale flag= 4 (bad)
- If the sounding is within the minimum (- 20%) and maximum (+ 20%) of 9 reference values, the flag = 1 (good). If the bottom depth is outside this interval flag = 3 (questionable).

The references values are the ETOPO 5 gridded (5' x 5') bottom depth at the station location and at the 9 nearest points.

Screening Procedure and manual validation

All the previous checks are reviewed:

- Check for position over the sea
- Check the ship velocity between the consecutive stations
- Check the bottom depth (mainly deep basin / shelf water)

In order to facilitate the QC, the following should be displayed on the computer screen:

- Cruise identifier and name (permanent) and complete headers
- Coastal lines and bathymetry ETOPO5 (4) and GEBCO (5)
- Stations locations (linked or not)

In case of necessity, the values are modified and the changes are recorded. If it is not possible to get an acceptable date or position, global flag =4 (bad).

3. Check of the parameters

The higher severity checks are performed first, because there is no reason to perform for example narrow range checks, if a value is already out of the regional broad range scale. Only the vertical density check is performed at the end because it makes use of the results of the other checks and it is more difficult to implement (4 values are taken into account).

When a parameter is fully checked, a «global parameter flag» is attributed, depending on the percentage of flagged values (20%). It can be discussed if the number of values on the vertical, for examples profiles with less than 3 good levels the vertical, has to be taken into account to give the global flags. It has been chosen here not to attribute any quality index to this number, first because this test can be automatically recomputed, also because the interest of such «gappy» profiles depends on the potential further scientific analysis for example time series of coastal stations or deep sea geostrophic computations.

Check for acceptable data

- The reference parameter must be present: if the vertical co-ordinate (pressure or depth) is not present, reject the whole profile.
- If the vertical co-ordinate exists but no other parameters, reject the profile.

Check for increasing pressure

The reference parameter must be increasing

- If the pressure is not continuously increasing: flag = 4 (bad) for the first redundant data.
- If the complete profile is in the reverse order, prepare it properly.

In the particular following cases, this check returns too many problematic data and the data are processed before further QC:

- the profile is in reverse order beginning from the bottom: it is transcended in increasing order;
- an important part is duplicated (the cast down of the CTD is interrupted to raise it a hundred meter before continuing the down cast): the first duplicated segments are rejected;
- if the profile includes more than one value per decibar, the values are filtered to about one decibar.

Check for constant profiles

A parameter cannot be constant on the vertical. If all the temperatures or all the salinities are constant then: data points flags = 4 (bad)

Check for impossible regional values

For each data, if the parameter is out of the regional scales (minimum and maximum), the data flag = 4 (bad). The deep layer and the upper layers can have different scales of variation.

These min-max values are adjusted on the vertical.

<u>Regional Parameterisation</u>

For simplicity, Mediterranean and Black Sea regions have been subdivided in rectangle geographical sub-domains, whose geographical limits and maximum depth value are given in the following table and are available on: http://www.ifremer.fr/medar/htql/liste_region.htql

CODE	NAME	LAT. MIN.	LAT. MAX	LON. MIN.	LON. MAX	MAX DEPTH.
DF1	ALGERIAN BASIN NORTH	N39 18.00	N42 00.00	E004 30.00	E009 18.00	2900
DF2	GULF OF LIONS	N42 00.00	N43 36.00	E002 48.00	E006 18.00	2732
DF3	LIGURIAN SEA WEST	N42 00.00	N44 30.00	E006 18.00	E009 24.00	2964
DF4	LIGURIAN SEA EAST	N42 48.00	N44 18.00	E009 24.00	E010 48.00	1632
DF5	BERRE POND	N43 20.00	N43 42.00	E004 57.00	E005 15.00	100
DH1	AEGEAN SEA	N35 15.00	N41 12.00	E022 30.00	E027 18.00	4500
DH2	CRETAN PASSAGE	N31 00.00	N35 15.00	E022 30.00	E027 18.00	4220
DH3	LEVANTINE BASIN	N30 42.00	N37 04.00	E027 18.00	E036 30.00	4620
DI1	SARDINIA STRAIT	N36 48.00	N39 18.00	E008 24.00	E010 00.00	2857
DI3	SICILIA STRAIT	N36 00.00	N38 00.00	E010 00.00	E014 00.00	1585
DJ1	ADRIATIC NORTH	N41 54.00	N45 54.00	E012 11.00	E015 07.00	250
DJ2	ADRIATIC MIDDLE	N40 36.00	N44 54.00	E015 07.00	E018 02.00	1362
DJ3	ADRIATIC SOUTH	N40 00.00	N42 48.00	E018 02.00	E019 54.00	1375
DJ4	IONIAN 1 (NE)	N38 00.00	N40 00.00	E018 00.00	E022 30.00	3725
DJ5	IONIAN 2 (SOUTH)	N30 06.00	N36 00.00	E010 00.00	E022 30.00	4465
DJ6	IONIAN 3 (NW)	N38 00.00	N40 36.00	E016 07.80	E018 00.00	2826
DJ7	IONIAN 4 (MIDDLE)	N36 00.00	N38 00.00	E014 00.00	E022 30.00	5121
DK0	BLACK SEA AND SEA OF ASOV	N40 12.00	N47 24.00	E027 18.00	E041 54.00	2313
DK1	BLACK SEA NORTH WEST SHELF	N45 20.00	N46 50.00	E029 30.00	E033 50.00	1000
DK2	BLACK SEA NORTH SLOPE	N44 00.00	N45 20.00	E030 00.00	E039 00.00	1500
DK3	BLACK SEA WEST SLOPE	N42 00.00	N45 20.00	E027 30.00	E030 00.00	1500
DK4	BLACK SEA WEST ABYSSAL	N42 00.00	N44 00.00	E030 00.00	E033 00.00	2313
DK5	BLACK SEA CENTRAL ABYSSAL	N42 00.00	N44 00.00	E033 00.00	E036 00.00	2313
DK6	BLACK SEA EAST ABYSSAL	N42 00.00	N44 00.00	E036 00.00	E039 00.00	2313
DK7	BLACK SEA SOUTH SLOPE	N40 55.00	N42 00.00	E030 00.00	E039 00.00	1500
DK8	BLACK SEA SOUTH-EAST SLOPE	N40 50.00	N44 10.00	E039 00.00	E041 40.00	1500
DK9	BLACK SEA ADJACENT TO BOSPHORUS	N41 05.00	N42 00.00	E028 00.00	E030 00.00	1500
DL0	MARMARA SEA	N40 12.00	N41 05.00	E026 50.00	E030 00.00	1000
DL1	SEA OF AZOV	N45 20.00	N47 20.00	E033 50.00	E039 20.00	200

DS1	GIBRALTAR STRAIT	N33 00.00	N37 42.00	W009 00.00	W005 36.00	3000
DS2	BALEARIC SEA	N38 30.00	N42 00.00	W000 24.00	E004 30.00	2700
DS3	ALGERIAN BASIN SW	N35 36.00	N38 30.00	W001 00.00	E004 30.00	2800
DS4	ALGERIAN BASIN SE	N36 30.00	N39 18.00	E004 30.00	E008 24.00	3000
DS5	ALBORAN NW	N36 00.00	N37 30.00	W005 36.00	W003 00.00	2000
DS6	ALBORAN SW	N35 00.00	N36 00.00	W005 36.00	W003 00.00	2000
DS7	ALBORAN NE	N36 00.00	N37 30.00	W003 00.00	W001 00.00	2700
DS8	ALBORAN SE	N35 00.00	N36 00.00	W003 00.00	W001 00.00	2800
DT1	TYRRHENIAN (NW) 1	N39 18.00	N42 48.00	E009 18.00	E013 48.00	3162
DT2	TYRRHENIAN (NE) 2	N39 18.00	N41 18.00	E013 48.00	E016 6.00	3128
DT3	TYRRHENIAN 3	N38 30.00	N39 18.00	E010 00.00	E016 18.00	3146
DT4	TYRRHENIAN 4	N38 00.00	N38 30.00	E010 00.00	E015 00.00	1513
DT5	TYRRHENIAN 5 (MESSINA)	N38 00.00	N38 30.00	E015 00.00	E016 00.00	1022

Broad Range Control Values for the parameters

The minimum and maximum values for each parameter in the sub-regions defined in the previous table can be accessed at: http://www.ifremer.fr/medar/htql/liste_param.htql.

The broad range control values for the core physical and chemical parameters for the Black Sea (global) and its regions (regional values) are listed in Appendix I.

Check for spikes

This test is difficult and may be adjusted for continuous or discrete profiles. It requires at least 3 consecutive acceptable values. When selecting 3 consecutive acceptable values:

- If flag of the value = default value the value is not acceptable, take the following
- If flag of the value = 4 the value is not acceptable, take the following

Search the spiky values:

The IOC check is the following:

If (|V2-(V3+V1)/2 | - |V1-V3|/2) > THRESHOLD VALUE ---> flag (V2) = 3 (dubious)

However this test does not always work properly for data not regularly collected on the vertical, as it is often encompass with bottle casts. There are also difficulties with more than one value on the spike. In this case, a better algorithm to detect the spikes, taking into account the difference in gradients instead of the difference in values is:

| |(V2-V1)/(P2-P1)-(V3-V1)/(P3-P1)| - |(V3-V1)/(P3-P1)| |> THRESHOLD VALUE

In general the spike test requires manual validation.

Bottom Spike test

This is a special version of the spike test, which compares the measurements at the end of the profile to the adjacent measurement:

(V2-V1)/(P2-P1)>THRESHOLD VALUE

Compare with the pre-existing statistics - check for pressure

The available reference statistics are the same as for the bottom depth sounding (ETOPO5):

- If the bottom depth sounding is recorded in the header and flag = 1(good)

  If Pressure > sounding + 5%, flag = 4 (bad)

- If the bottom depth sounding is recorded in the header and flag = 2 (inconsistent with statistics)

  If Pressure > sounding + 5%, flag = 3 (questionable)

- If bottom depth sounding is not recorded

  If Pressure > the pressure must be within 0.5 and 2 times the reference statistics

If this is not the case, flag =3 (questionable)

Narrow range check for the data: Compare with the pre-existing climatological statistics

Comparing the data points with the existing statistics performs the narrow range check. Current available selections:

For temperature and salinity:

- MEDATLAS 1997,averaged on 1x1 square degree

For oxygen and nutrients:

- Brickman and Petrie 2003, World Ocean Atlas 2009, Hydrobase, GLODAP, Gouretski and Koltermann 2004, Oceanographic Atlas for the Black and Azov seas 2009, MEDATLAS 1997

These statistical profiles are defined in a limited number of standard levels, and the automatic comparison is made by linearly interpolating them at the level of the observation. The allowed distance to the reference depends varies between respectively 3, 4 and 5 standard deviations, depending on the type of station: over the shelf (depth < 200 m), the slope and straits regions (200< depth < 400 m), the deep sea (> 400 m).

Procedure

- Select the nearest mean statistic profile of the same month (default same season, default same year) and the standard deviation
- Interpolate the reference profile and the standard deviation at the observed pressure level
- Recall the bottom sounding DEPH (default the ETOPO5 depth of the location) and compute the acceptable range of variation:

  If bottom DEPH <= 200 then range = 5 x standard deviation

  If bottom 200 < DEPH <= 400 then range = 4 x std. deviation

  If bottom 400 < DEPH then range = 3 x std. deviation

- Compute the absolute value of the difference between the data point and the (interpolated) reference at the same level. with this range:

  If difference > range then flag =2, else flag =1

Density inversion test

This test requires two consecutive acceptable levels of values. The automatic check is mainly used to assist the operator, the decision to flag one of the 4 values (temperature and salinity at the two levels) is always validated manually. A level of noise is attributed for the density.

- acceptable noise level for density:

  EPS= 0.03 (increased to 0.05 near the surface, in coastal areas for bottle sampling)

- selection of two consecutive acceptable level:

  if (pressure, temperature or salinity flag) = 4 or 9 the level is not acceptable

- compute the potential (unless deep density anomalies will be found) density anomaly from the equations of state of sea water (FOFONOFF and MILLARD, 1983 (9) and MILLERO and POISSON, 1981(10)) at each selected level:

  TETA= Potential temperature (PRES, TEMP, SAL, PRES0=0)

  D = density anomaly = sigma (PRES, TETA, PSAL)

- Perform the check each two consecutive densities:

  IF D2 + EPS > D1 then the stratification is stable, the temperature and salinity flags are unchanged

  IF D2 + EPS < D1 then the stratification is unstable

- In case of instability, find out which is the bad value: checks for other anomalies detected by previous checks at one of the two levels, and modify the flag to bad:

  IF FLAG (SAL1) > 1 MODIFY FLAG (SAL1) = 4

  IF FLAG (SAL2) > 1 MODIFY FLAG (SAL2) = 4

  IF FLAG (TEMP1) > 1 MODIFY FLAG (TEMP1) = 4

  IF FLAG (TEMP2) > 1 MODIFY FLAG (TEMP2) = 4

  If the doubt is on the pressure, flag all the parameters

  IF FLAG (PRES1) > 1

  MODIFY FLAG (PRES1) = 4, FLAG (TEMP1) = 4 , FLAG(SAL1) = 4

  IF FLAG (PRES2) > 1

  MODIFY FLAG (PRES2) = 4, FLAG(TEMP2) = 4 , FLAG(SAL2) = 4

- In case of instability, if no anomaly has been previously detected (all flags = 1 at levels PRES1 and PRES2) then arbitrarily modify the flag on the level 2 only to facilitate the visualization and the further manual correction of the flags:

  FLAG (PRES2)= 4, FLAG(TEMP2) = 4 , FLAG(SAL2) = 4

Test of the Redfield ratio for nutrients

An additional test is the Redfield ratio: the ratio of the oxygen, nitrate and alkalinity (carbonates) concentration over the phosphate concentration has been estimated respectively to 172, 16 and 122 by Takahashi & al. (13) in the Atlantic and Indian Ocean. New studies are made in the frame of MEDAR and CYCLOPS projects and these values will be adjusted for the Mediterranean in a near future.

These estimates allow a visual check on the corresponding nutrients, by checking the dispersion around the reference curve.

Screening Procedure and validation of the flagging

The coherence and continuity of the observations within a cruise is only checked subjectively, and allow making manual corrections of the flags especially:

- in coastal water where the control values are poorly estimated
- when there is a doubt on the climatological reference, or if these values are missing
- in the thermo cline where very strong gradients are assimilated with spiky values
- when the standard deviation is missing or poorly estimated (frequently, the value is two low)
- to validate the vertical stability check.

These checks are implemented by using the following displays for each parameter, including the density (which is not archived, but give additional information):

- Separate and superposed profiles of vertical variations; the reference profile of the current profile is plotted with the envelope of «good» values when this envelope can be computed;
- waterfall diagrams;
- superposed and waterfall temperature/salinity diagrams

The data points are plotted separately or joined by straight lines between two consecutive points, and coloured according to the computed flags. During these checks, it is always useful to check the location of the profile on the map, and the cruise identifier and name will be displayed permanently during the visual inspection

Superposing the profiles of another cruise of the same region checks external coherency of the data.

6.2 Time Series of fixed moorings: Current Meter, ADCP, Sediment Traps, etc

Specifications are given if checks differ from those already described in 6.1

1. Check of the format

2. Check of the date and location

Additionally to the quality control procedures mentioned above for vertical profiles in 6.1, in case of time series some additional checks are applied:

- **Control of start date:** start date and time (year, month, hour, minute and seconds) in the header has to be the same or earlier than the date and time of the first (start) data record.

- **Control of end date:** end date and time in the header has to be the same or later than the date and time of the last (end) data record. In case of lacking of the end date in the header, last date of end record is written instead and the correspondent quality flag is changed to 5.

- **Control of end position:** if the distance between start and end positions > 1 nautical mile the flag is changed to 4; in case of no value of final position, it's changed to the start position value and its correspondent flag takes value 5.

For cases of movement, i.e. when latitude and longitude are present as parameters of a time serie, end position in the header is compared to the end time series record position.

- **Control of "SENSOR DEPTH":** if its value is greater than DEPTH the flag = 4.

- **Control of "DISTANCE TO THE BOTTOM":** if the sum of "SENSOR DEPTH" +

"DISTANCE TO THE BOTTOM" differs greatly from "DEPTH" the flag = 4.

- **Control of duration:** if the duration in the header is less than that calculated from data records, the flag = 4. If the duration value in the header is absent, real calculated duration is written down instead and the flag is changed to 5. Default value = -9

3. Check of the data

- **Acceptable data sets:** Time must exists in the file either as YEAR MNTH DAYX TIME or YEAR DATE TIME. There must be at least one other parameter than the reference.

If the time series is a current meter we need to have: either HCSP and HCDT (current speed and direction) or EWCT and NSCT (current components).

- **Date and time control:** all time series records must be consecutive in time, i.e. each next record must have date and time equal to that of previous record plus time interval of the series data. On the contrary the flag for all parameters of erroneous record is put to 4 and further analysis is stopped.

- **Pressure/Depth parameter control:** if absolute value of the difference between pressure/depth in each record and "SENSOR DEPTH" is greater than a value established by the user, the flag is changed to 3.

- **Broad range:** if parameter values don't enter in the established diapason, correspondent flag is = 4.

- **Constant profile:** same as for the vertical profiles.

- **Delta check (spike and gradient detection):** for this detection we apply first a LANZOS filter on the time series to avoid the effect of the tide and of internal waves.

The LANZOS filter will be applied on the time series only if:

The duration of the series is > 10 days

The interval between 2 consecutive measurements is < 1 day

The spike detection algorithm is the same than the one used for CTD for the current meters, the thermistor strings and the tide measurements, and the same than the one used for the bottle in the case of sediment trap time series: if absolute value of the difference between consecutive data records of any parameter is greater than limit established for that difference, the flag = 3.

- **Statistics checks:** for each time series, we calculate the mean and the standard deviation. These values are plotted on the screen. The standard deviation is multiplied by a factor of 5.

- **Position parameters check:** if velocity calculated between consecutive records when latitude and longitude parameters are present (case of movement) is greater than established maximum ship velocity (15,-20 knots), the flag is set to 3.

6.3 Time series: Sea Level Data

(Eseas document, 2005)

Specifications are given if checks differ from those already described in 6.2

1. Check of the format

2. Check of the date and location

3. Data Quality Control

As part of the "scientific" or delayed mode quality control, a more detailed processing of sea level data is performed, applied to longer time series (typically 1 year) that include not only the steps described in 6.2, but also the filtering to hourly values, computation of annual harmonic constants, residuals, extremes and means. The results of this process are themselves useful products from the station, but also the examination of their quality is crucial for the detection of problems and malfunction in the tide gauge. The primary quality control of sea level is based on the inspection of both recorded data and meteorological residuals; inspection of residuals is especially useful for detecting instrumental faults such as timing errors, datum shifts and spikes.

On the other hand, the harmonic constants may be severely corrupted if the site is characterized by highly nonlinear tides, influence of rivers or estuaries and particularly complex basin configuration. To produce more accurate predicted tides, it is advisable to compute 'fresh' tidal constants from recent data and not simply rely upon historical values. Tidal analysis can be performed by means of the software packages developed by the University of Hawaii Sea Level Center (UHSLC) and Puertos del Estado (PE), Spain, that facilitate the use of the Foreman tidal analysis and prediction programs of the Institute of Ocean Sciences, Victoria, British Colombia (Foreman, 1977) or by the PSMSL/Proudman Oceanographic Laboratory (POL TASK2000 Package) and the Australian National Tidal Facility, which utilise the TIRA tidal analysis programs (Murray, 1964). **Tidal constants used in tide predictions should never be mixed between different packages.**

Suspect tidal profiles should be checked against records of a nearby site, to see if the suspect values are due to a tide gauge fault or to station conditions. In case of a fault, data should be corrected or interpolated (if possible), otherwise must be kept as they are, taking note of the event. If possible, more than one instrument should be operated at the same site in order to allow direct comparison, and on occasion to fill gaps.

Filtering to hourly values

Raw data are normally registered at time intervals between 1 minute and 1 hour, the most common being 5, 6 and 10 minutes; only in regions where “seiches” occur frequently, or where phenomena such as tsunamis are to be detected, are the sea level registered at less than 1 minute intervals. Apart from the convenience of keeping higher frequency signals for other purposes, it is always necessary to obtain filtered hourly values before going on the sea level processing.

The filtering process will eliminate higher frequencies dependent on the frequency cut-off. Pugh (1987) describes useful filters that can be applied to the sea level data at intervals of 5, 10 or 15 minutes to obtain the hourly heights whilst preserving the tidal phenomena. In Godin (1972) there is an extensive discussion on tidal filters.

Harmonic analysis

A common procedure is to compute the harmonic constants for each year of observed data. Some of these constants may be particularly affected by meteorological conditions, and so will show important variations from one year to the next. This occurs for example for the longer term harmonic constituents as Sa and Ssa. Sometimes also the presence of problems in the data series appears as strange values of the normally stable harmonics (e.g. clock errors). In any case, an inspection of the variation through the years of the harmonic constants is interesting both for detecting problems and also for having information about changes on the station. For example, changes in the configuration of a harbour can affect the tide parameters, and this occurs very often.

A common practice in order to choose adequate harmonic constants for tide prediction is to perform the vector mean and statistics of the annual values for several years (provided they are computed for nearly complete years and so the same number of constituents have been resolved) and selecting for prediction only the mean of those constituents which do not present a variability that is over a fixed and reasonable tolerance.

Computation of prediction and meteorological residuals

As mentioned before the inspection of meteorological residuals is a very useful tool for the quality control process. All fundamental types of errors that a sea level series can present are easily detected in the residual plot.

Of course, the presence of a spike is also very obvious in the residual series, which is why some of the automatic algorithms for the detection of spikes are based on both the original and the residual data.

Correction of clock malfunction

This type of error is very easy to correct if there is a constant time shift. The problem arises when there is a drift in the lag between observed and predicted tide.

Apart from the inspection of the residuals, a constant lag can be exactly determined by means of lag-correlation analysis between observed and predicted data (lag of maximum correlation), or by comparing the values of the phase of M2 harmonic before and after the shift. Once determined, the part of the series that it is affected must be shifted accordingly to correct the error; if the lag is a multiple of the time interval, the shift is just a movement of data in time; if not, an interpolation to the correct time has to be performed.

This type of correction is not automatic for any of the software currently available, although the UHSLC Sea Level Software includes a program to make the correction in case of constant lags multiple of the time interval.

Gap filling

Depending on the application filling gaps in a series may or may not be reasonable. During the first stage of the quality control, very short gaps of several minutes or spikes are linearly interpolated in the higher frequency data. Gap filling for hourly values is less clear. The UHSLC interpolates gaps of less than 24 hours before computing daily and monthly means; this is done by computing the residual series, linearly interpolating by using the meteorological residual values at the extremes of the gap, and adding on the astronomical prediction to the interpolated values. The maximum length of data that is reasonable to fill should not be more than 24 hours depending on the meteorological conditions of the station. Interpolation of this kind should be undertaken with great caution, and the data values flagged accordingly.

Detection of reference changes

Improper maintenance operation, an accident, or even a natural phenomenon such as an earthquake may produce a sudden jump in the reference level. Most of these jumps are readily identifiable in hourly residual plots if the magnitude is large enough. Once detected, a proper way of correction is through the inspection of the scatter diagram of the tide staff or electric sound readings and corresponding tide gauge values, taken during the maintenance campaigns.

As it will be shown later, these jumps can also be detected by plotting the differences between daily and monthly means from adjacent stations or from redundant sensors. As a rule, the UHSLC considers changes greater than 1.5 cm as significant and worthy of an investigation to guarantee level stability.

A change in reference level must only be corrected and documented when firm confirmation has been established. Data values should be flagged accordingly.

Statistics

Basic statistics from historical data are computed or updated annually and some of these parameters are used for the quality control process. For example:

- upper and lower limits or historical extremes (for range check).
- tidal and observed sea level ranges
- extremes, mean and standard deviation of hourly values, meteorological residuals, ranges or mean sea levels
- tables of monthly and annual extremes
- density function for hourly values, tide predictions and residuals

4. Further quality control and process of historical data

When working with historical data, even if the station is well documented, check sheets may not be available with which to perform a confident quality check on the reference level. Furthermore, system measurement problems, changes in the instrumentation or in the environment surrounding the station can generate a discontinuity, which may appear as a datum shift or a trend. In this case some additional checks should be performed to obtain a unique reference. The normal procedure for this kind of higher level quality control is to work with several daily or monthly means sea level series from nearby stations and then reconstruct the time series of the heights.

Different algorithms are explained below that can help to detect this type of discontinuity or reference problems in historical data. All of them normally require the quality assessment of an expert before taking the final decision to correct the data. Apart from the more immediate computation of differences between levels of adjacent stations, which may clarify about the existence of a problem, there are other possibilities as described below.

Correlations

Correlations can be computed both between data from different stations or sensors and between different parameters at the same station (wind, atmospheric pressure, etc). In any case this is a valuable tool for detecting problems. The correlation analysis is also useful for filling gaps. This can be done as follows:

1. Calculate the Pearson's correlation coefficient between residual series

2. Select nearby stations with correlation coefficients above 0.7

3. Calculate the linear regression between them and fill the gaps. (Only fill gaps within the time series; not at the beginning or end of the series)

Standard Normal Homogeneity Test

Several tests have been described in the literature, which can be used to detect inhomogeneities in data series. Alexanderson (1986) developed the Standard Normal Homogeneity Test (SNHT) which is widely used in climatic time series studies. The SNHT gives the points where an inhomogeneity exists and provides information about the probable break magnitude. However, the inhomogeneity could be due to an error or to an anomalous, but real, behaviour of the variable. For this reason, the series are only corrected following comparison with other series in the same climatic region and supported by historical information about the incidences on the tide gauge.

EOF Analysis

The Empirical Orthogonal Functions (EOFs) analysis applies to a group of time series stations can be used not only to find special coherent signals or regional variability but also to detect possible errors in the time series. In fact, relevant differences on the variance of the first EOF may indicate errors in one or more time series. This technique is well documented in “Development of a Quality Checked Tide Gauge Data Set (A.G.P Shaw[1], M.N. Tsimplis[1], et all)” and in “Consistency of long sea-level time series in the northern coast of Spain (M. Marcos, D. Gomis, et all)

6.4 Wave Data

(Simorc, document, 2006)

Glossary

- **Hs : Significant wave height** - measure of the average height of the highest one third of waves during the record in metres
- **Tz: Zero upcrossing period** - the mean wave period (taken as the average time between consecutive crossings of the mean sea level line in an upwards direction) in seconds
- **Tmax: Maximum wave height** - maximum recorded wave height in metres
- **Tcrest: Crest period** - time taken between consecutive crossings of wave crests
- **Tpeak:** Peak period also known as dominant wave period - it is the period corresponding to the frequency band with the maximum value of spectral density.

Specifications are given if checks differ from those already described in 6.2

1. Check of the format

2. Check of the date and location

3. Data Quality Control

<u>Data Screening:</u>

The time series plots can be used to identify:

- Instrument failure test (10 or more consecutive points of identical value)
- Wandering mean test (interval between successive upcrossings of >25 seconds)
- Check that Tz falls within the range 2-16 seconds
- Check that Tpeak falls within the range 3 -20 seconds
- Check that Tz not less than Tcrest
- Check that Tpeak not less than Tz
- Value in excess of 4 times standard deviation (assumes a basically random process with approximately normal distribution).
- cDefinition of calm and appropriate flagging
- Changes in wave height/time slopes in excess of 1:10 which is unrealistically steep (NB this is only possible if we have full resolution data ie 1Hz or better; unlikely that we will get this, so far data submissions have been 20 minute sampling intervals)
- Check for stationarity: assuming that the wave field is not rapidly evolving or decaying, records of wave height and period should be broadly similar from one record to the next

<u>Scatter Plots:</u>

Scatter plots of wave height against (zero upcrossing or crest) period can show unrealistically steep waves with a slope of more than 1:10. They can also show outliers from the cluster of Tz vs. Hs values. Similarly, wind speed versus wave height scatter plots can be used to identify outliers from the clusters (NB make allowances for swell waves which will show higher than expected wave heights for a given wind speed).

Checks will be made for:

- Definition of unacceptable steepness and appropriate flagging (ratio of Hs/Tz)
- Outliers of clusters of Ts/Hz and of Ts versus wind speed

<u>Frequency Plots:</u>

The tail ends of the requency distributions of significant wave heights can be analysed to identify where instrument noise becomes detectable and a threshold or filter set accordingly.

<u>1D and Directional Wave Spectra:</u>

- Check slope of energy density spectrum – should follow a set slope due to transfer of energy from lower to higher frequencies (?)
- Check that energy in the spectrum at frequencies below 0.04 Hz is not more than 5% of the total spectral energy
- Check that energy in the spectrum at frequencies above 0.6 Hz is not more than 5% of the total spectral energy
- Check mean direction at high frequencies, which should correspond to the wind direction (assuming coincident meteorological data).
- For 1D spectra, calculate zeroth spectral moment from spectral variance densities and check that it corresponds to the given value
- For 1D spectra, calculate Te as the zeroth divided by first negative spectral moment and check that it correlates with (peak or zero upcrossing) period

7. IODE Workshop on Quality Control of Chemical Oceanographic Data Collections

An IODE workshop on quality control (QC) of chemical oceanographic data collections held at the IOC Project Office for IODE in Oostende, Belgium between 8 and 11 February 2010 met with the objective of evaluating existing procedures and define a minimum set of QC tests and criteria for dissolved inorganic nutrients (phosphate, silicate, nitrate+nitrite, nitrate, nitrite, and ammonium) and dissolved oxygen in seawater (IOC Workshop Report No. 228). The meeting issued a number of recommendations which will be taken forward in post-workshop activities in consultation and in interaction with the wider international community. These included: (1) metadata terminology for reporting measured variables and their units as well as (2) a work plan to recommend a minimum set of numerically defined QC tests that could be adjusted to reflect broad regional to basin scales conditions. These guidelines and recommendations will be assembled on the GE-BICH wiki for peer-review before being published as a technical white paper or guideline document.

Using the GTSPP quality control checks as a starting point, the workshop recommended the following four quantifiable data QC checks for variables as a minimum:

(1) data range checks;

(2) excessive gradient;

(3) excessive spike;

(4) no gradient.

In this context, quantifiable tests are a mean to assign a metric to qualify measured data quality. These tests need to be applicable to both vertical profiles and time-series/horizontal distributions. They are described in detail in the workshop report. The group noted that at present there is no simple way to determine the accuracy of nutrient and oxygen data already available at data centres without independent means (e.g., using certified reference material for nutrients and oxygen data).

In addition to the minimum outlined above, the group recommended the following:

- to develop data ranges at different spatial scales ranging from basin to regions to improve QC checks (objective tests).
- to use property-property plots such as nitrate versus phosphate, nitrate vs. temperature, oxygen vs. temperature, depth or time plots as a mean to visually check the data (subjective tests).
- when available we recommend the use of local climatologies as a quantitative or visual guide.
- to seek community-wise effort to develop less subjective tests.
- to compile a list of available statistical and objectively analyzed climatologies available such as Brickman and Petrie 2003, World Ocean Atlas 2009, Hydrobase, GLODAP, Gouretski and Koltermann 2004, the Baltic Atlas of long term inventory and climatology, Oceanographic Atlas for the Black and Azov seas 2009, MEDAR/MEDATLAS, etc.

8. References

- NODC procedures (e.g. France, Greece, Italy, Norway, Spain, Sweden, UK)
- “Medar-Medatlas protocol, Part I: Exchange format and quality checks for observed profiles”, V3, 2001
- SCOOP User Manual, V4.2, 2000
- Coriolis Data Centre, In-situ data quality control, V1.3, 2005
- QCDAMAR-Quality Control of Oceanographic Data (María Jesús García, Andrei Nikouline) (http://indamar.ieo.es/productos/software/qcdamar-guide.pdf)
- EU SIMORC project (Met-ocean data QC)
- IOC GLOSS documents
- QUALITY CONTROL OF SEA LEVEL OBSERVATIONS”, ESEAS-RI, V1.0, 2006

- Manual of Quality Control Procedures for Validation of Oceanographic Data, UNESCO, IOC - Manuals & Guides, 1993, Manual And Guides 26
- GTSPP Real-Time Quality Control Manual, 2009 (IOC MANUALS AND GUIDES #22)
- Argo Quality Control Manual, V2.1,2005 (Real Time and Delayed Mode)
- GOSUD Real-time quality control
- Data Type guidelines - ICES Working Group of Marine Data Management (12 data types)
- JPOTS Manual, 1991
- WOCE manuals
- JGOFS Protocols
- QUALITY CONTROL PROCESSING OF HISTORICAL OCEANOGRAPHIC TEMPERATURE, SALINITY, AND OXYGEN DATA. Timothy Boyer and Sydney Levitus, 1994. National Oceanographic Data Centre, Ocean Climate laboratory
- 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.
- Chapman, A. D. 2005. *Principles of Data Quality*, version 1.0. Report for the Global Biodiversity Information Facility, Copenhagen.
- ‘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)
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- Wilson, J.R. 1998. Global Temperature-Salinity Profile Programme (GTSPP) - overview and future, Intergovernmental Oceanographic Commission technical series 49, SC-98/WS/59.
- WMO. 1995. WMO Manual on Codes No. 306.
- UNESCO. 1991. Manual on International Oceanographic Data Exchange, IOC/ICSU Manual and Guides # 9, Revised Edition.
- Emery, W.J. and R. E. Thomson. 1998. Data Analysis Methods in Physical Oceanography, Pergamon.
- Karl, David, Luis Tupas, Fernando Santiago-Mandujanu, Craig Nosse, Dale Hebel, Eric Firing and Roger Lukas. 1996. Hawaii Ocean Time-Series Data Report 7:1995, SOEST 96-09, University of Hawaii.
- UNESCO. 1988. The acquisition, calibration and analysis of CTD data. A report of SCOR WG 51. Tech. Pap. Mar Sci., 54: 59pp.

- UNESCO, 1991. Processing of Oceanographic Station Data, JPOTS Editorial Panel.
- First IODE Workshop on Quality Control of Chemical Oceanographic Data Collections, IOC Project Office for IODE, Oostende, Belgium, 8-11 February 2010 Paris, UNESCO, 25 March 2010 (IOC Workshop Report No. 228) (English)

Useful links:

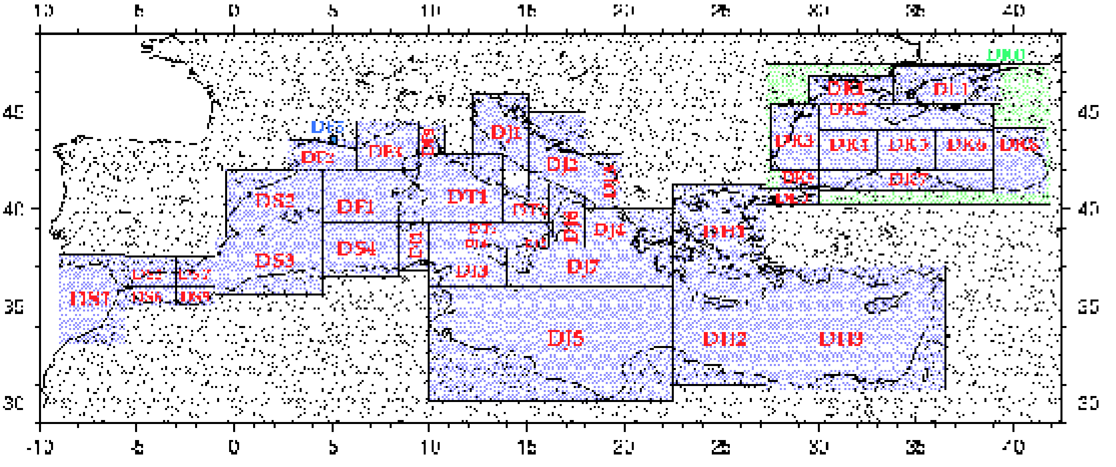
- http://www.seadatanet.org
- http://www.ifremer.fr/medar
- http://www.blackseascene.net/
- http://www.ices.dk
- http://www.iode.org
- http://www.oceanteacher.org/
- http://odv.awi.de/

Appendix I

BROAD RANGE CHECK & REGIONAL PARAMETERIZATION

(MEDAR/MEDATLAS Protocol, 2000)

http://www.ifremer.fr/medar



Core Parameters

(P091 MEDATLAS Parameter Usage Vocabulary)

CODE	NAME	UNIT
DOX1	DISSOLVED OXYGEN	ml/l
DOXY	DISSOLVED OXYGEN	millimole/m3
TPHS	TOTAL PHOSPHORUS (P) CONTENT	millimole/m3
NTOT	TOTAL NITROGEN (N) CONTENT	millimole/m3
HSUL	HYDROGEN SULPHIDE (H2S)	millimole/m3
TEMP	SEA TEMPERATURE	Celsius degree
PRES	SEA PRESSURE sea surface=0	decibar=10000 pascals
PSAL	PRACTICAL SALINITY	P.S.U.
NTRA	NITRATE (NO3-N) CONTENT	millimole/m3
NTRI	NITRITE (NO2-N) CONTENT	millimole/m3
AMON	AMMONIUM (NH4-N) CONTENT	millimole/m3
PHOS	PHOSPHATE (PO4-P) CONTENT	millimole/m3
SLCA	SILICATE (SIO4-SI) CONTENT	millimole/m3
CPHL	CHLOROPHYLL-A TOTAL	milligram/m3
PHPH	PH	pH unit
DOX2	DISSOLVED OXYGEN	micromole/kg
NTRZ	NITRATE + NITRITE CONTENT	millimole/m3
ALKY	ALKALINITY	millimole/m3

Global Limits of Parameters for Black Sea (DK0)

PARAMETER CODE	MIN PRES	MAX PRES	MIN PARAMETER	MAX PARAMETER
ALKY	0	2313	1000	4600
AMON	0	2313	0	100
DOXY	0	2313	0	600
DOX1	0	2313	0	13,3
NTRA	0	2313	0	33
NTRI	0	2313	0	15
PHOS	0	2313	0	13
PHPH	0	2313	7	9,1
PSAL	0	2313	0	24
SLCA	0	2313	0	330
TEMP	0	2313	-1	29

Regional Limits of Parameters for Black Sea North West Shelf (DK1)

PARAMETER CODE	MIN PRES	MAX PRES	MIN PARAMETER	MAX PARAMETER
ALKY	0	1000	1200	4300
AMON	0	1000	0	15
DENS	0	1000	10	30
DOXY	0	1000	0	600
DOX1	0	1000	0	13,3
NTRA	0	1000	0	33
NTRI	0	1000	0	6
PHOS	0	1000	0	6
PHPH	0	1000	7,4	9,1
PSAL	0	1000	0	21
SLCA	0	1000	0	160

Regional Limits of Parameters for Black Sea North Slope (DK2)

PARAMETER CODE	MIN PRES	MAX PRES	MIN PARAMETER	MAX PARAMETER
ALKY	0	1500	1400	4500
AMON	0	1500	0	70
DOXY	0	1500	0	570
DOX1	0	1500	0	12,7
NTRA	0	1500	0	24
NTRI	0	1500	0	3
PHOS	0	1500	0	10
PHPH	0	1500	7,2	8,9
PSAL	0	1500	4	23
SLCA	0	1500	0	200
TEMP	0	1500	2	28

Regional Limits of Parameters for Black Sea West Slope (DK3)

PARAMETER CODE	MIN PRES	MAX PRES	MIN PARAMETER	MAX PARAMETER
ALKY	0	1500	2800	4200
AMON	0	1500	0	96
DOXY	0	1500	0	580
DOX1	0	1500	0	12,8
NTRA	0	1500	0	20
NTRI	0	1500	0	1,5
PHOS	0	1500	0	10
PHPH	0	1500	7,5	8,9
PSAL	0	1500	7	23
SLCA	0	1500	0	310
TEMP	0	1500	3	27

Regional Limits of Parameters for Black Sea West Abyssal (DK4)

PARAMETER CODE	MIN PRES	MAX PRES	MIN PARAMETER	MAX PARAMETER
ALKY	0	2313	2900	4500
AMON	0	2313	0	98
DOXY	0	2313	0	450
DOX1	0	2313	0	10
NTRA	0	2313	0	15
NTRI	0	2313	0	,8
PHOS	0	2313	0	10
PHPH	0	2313	7,4	8,9
PSAL	0	2313	12	24
SLCA	0	2313	0	330
TEMP	0	2313	5	27

Regional Limits of Parameters for Black Sea Central Abyssal (DK5)

PARAMETER CODE	MIN PRES	MAX PRES	MIN PARAMETER	MAX PARAMETER
ALKY	0	2313	2800	4500
AMON	0	2313	0	100
DOXY	0	2313	0	380
DOX1	0	2313	0	8,4
NTRA	0	2313	0	13
NTRI	0	2313	0	,8
PHOS	0	2313	0	11
PHPH	0	2313	7,5	9
PSAL	0	2313	16	23
SLCA	0	2313	0	330
TEMP	0	2313	5	27

Regional Limits of Parameters for Black Sea East Abyssal (DK6)

PARAMETER CODE	MIN PRES	MAX PRES	MIN PARAMETER	MAX PARAMETER
ALKY	0	2313	2700	4600
AMON	0	2313	0	105
DOXY	0	2313	0	480
DOX1	0	2313	0	10,6
NTRA	0	2313	0	13
NTRI	0	2313	0	1
PHOS	0	2313	0	12
PHPH	0	2313	7,5	8,7
PSAL	0	2313	15	23
SLCA	0	2313	0	320
TEMP	0	2313	6	28

Regional Limits of Parameters for Black Sea South Slope (DK7)

PARAMETER CODE	MIN PRES	MAX PRES	MIN PARAMETER	MAX PARAMETER
ALKY	0	1500	2700	4200
AMON	0	1500	0	94
DOXY	0	1500	0	400
DOX1	0	1500	0	8,8
NTRA	0	1500	0	10
NTRI	0	1500	0	,5
PHOS	0	1500	0	10
PHPH	0	1500	7,6	8,7
PSAL	0	1500	13	24
ALKY	0	1500	2700	4200
AMON	0	1500	0	94

Regional Limits of Parameters for Black Sea South-East Slope (DK8)

PARAMETER CODE	MIN PRES	MAX PRES	MIN PARAMETER	MAX PARAMETER
ALKY	0	1500	1900	4500
AMON	0	1500	0	100
DOXY	0	1500	0	520
DOX1	0	1500	0	11,5
NTRA	0	1500	0	21
NTRI	0	1500	0	15
PHOS	0	1500	0	13
PHPH	0	1500	7,5	8,9
PSAL	0	1500	4	23
SLCA	0	1500	0	310
TEMP	0	1500	6	29

Regional Limits of Parameters for Black Sea adjacent to Bosphorus (DK9)

No Regional Limits defined for the parameter
Global limits are taken for QC of the parameters

Regional Limits of Parameters for Marmara Sea (DL0)

No Regional Limits defined for the parameter
Global limits are taken for QC of the parameters

Regional Limits of Parameters for Sea of Azov (DL1)

No Regional Limits defined for the parameter
Global limits are taken for QC of the parameters