

### **EMODnet Thematic Lot n° 4- Chemistry**

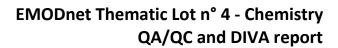
### Methodology for data QA/QC and DIVA products

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V8

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### Introduction

Data quality assurance and quality control (QA/QC) is an important issue in oceanographic data management, especially for the creation of multidisciplinary and comprehensive databases which include data from different and/or unknown origin covering long time periods. The data-collection methods involve a wide range of instruments, water sample analyses and accuracies. Historical data are often deprived of any detailed information on analytical procedures, calibrations and confidence intervals. The adoption of appropriate QA/QC methodology as well as feedback from the scientific community will contribute considerably to the validation of large data collections.

This report intends to be a reference manual for EMODnet Chemistry data QA/QC and the subsequent product generation. In fact, during the first data validation loop, each region adopted its own protocol and the results showed many inconsistent data quality flags and the need for coordination and harmonization of practices. A dedicated workshop was organized to review the different practices and agree on a common methodology for data QA/QC and Diva products generation for EMODnet Chemistry.



### 1. Common methodology for data QA/QC

Use Odv software to manage the data collection QA/QC activities.

In order to obtain the enriched metadata Odv collections, make use of the new Import function in Odv **Special Version 4.6.3.3** for SDN spreadsheet which will merge the SeaDataNet ODV data files together with CDI metadata csv files in order to create a metadata enriched SeaDataNet ODV data collection inside Odv software. This version is applicable for the regional data sets that have been harvested by MARIS (end of October 2014) and distributed to regional coordinators in EMODnet Chemistry during the last round and which have end of January 2015 as deadline for data-product generation. This will still have P01 terms internally in Odv.

Once the metadata enrichment is done, the official ODV <u>Version 4.6.4</u>, or later, must be used for aggregation and QA/QC activities. Regional coordinators will prepare an export from Odv for station data into metadata enriched SeaDataNet aggregated data collection file(s). These export files will include P35 parameters for all P01 which could be aggregated (and still remaining P01 parameters where not yet in P35 vocabulary). These resulting validated and aggregated SeaDataNet ODV data collections are to be used as input for the Diva analyses and data products generation. In addition, these resulting validated and aggregated SeaDataNet ODV data collections must be forwarded to MARIS together with a QA/QC report for storage and wider use by the visualization software processes that are being developed by technical partners.

P35 vocabulary is set up to aggregate various P01 terms with a common meaning into a unified aggregated term with a unique unit (P06). The Odv software has a built-in aggregation procedure, making use of the P35 vocabulary and also applying a number of business rules, such as for averaging and possible unit conversions. The P35 vocabulary is being populated by BODC with contributions from various chemical experts; the nutrient part is considered completed and ready to be used at September 2014 while progress is being made with contaminants.

Use SeaDataNet qualifier flags (L20 from BODC Vocab Library), where 0 = no quality control, 1 = good value, 2 = probably good value, 3 = probably bad value, 4 = bad value, 5 = changed value, 6 = value below detection (The accompanying value is the detection limit for the technique or zero if that value is unknown), 7 = value in excess, 8 = interpolated value, 9 = missing value, A = value phenomenon uncertain.

For data QA/QC, activities should focus only on imported data with SeaDataNet <u>quality flags QF = 0, 1,</u> 2, 6 which are considered as the initial collection.

Apply unit conversion and aggregation (using P35 and business rules as built in inside Odv software as explained above).

Set QF=9 for empty stations, set QF=9 for empty lines.

Search for duplicates and eliminate.



Search for out of "broad range" data with QF=1 and change their qualifier flag to QF=4

Perform the "broad range" check for all data with QF=0. The "broad range" check is understood as the comparison with a minimum and a maximum regional value. This results in changing the qualifier flag to QF=4 in case of failure or to QF=1.

Search for default values (e.g. 999.99, 999.999, ...) with QF=0 or QF=1 and set these to QF=9.

It is suggested to involve internal regional experts to review the aggregated data set before finalizing.

Keep track of QA/QC activities by means of a regional QA/QC report, following the EMODnet Chemistry agreement.

Export the final Odv results into a regional metadata enriched SeaDataNet aggregated data collection file for all regional station data (see above) which can then be used for the Diva product generation.

Provide a copy of the regional metadata enriched SeaDataNet aggregated data collection file to MARIS including the regional QA/QC report.

The same regional QA/QC report should also be sent to the data provider of erroneous data together with the corrected data in order to encourage an improvement of the overall quality at source level.

### Additional checks for Nutrients: N:P ratio

An additional criterion is here proposed, based on the relative proportion of Nitrogen to Phosphorus in seawater which, at least in open waters, far from continental inputs and in oxygenated waters, are fairly constant. In fact, it is well known that, under aerobic conditions, the assimilation and the regeneration of nutrients occur in constant ratios (Redfield ratio: N:P = 16:1; Redfield et al., 1963).

However, especially in coastal waters influenced by continental discharges, but also in oligotrophic open waters of the Mediterranean Sea, N:P can vary over a broad range, from ratios below 2:1 to over 500:1 (Lipizer et al., 2011; 1999; Socal et al., 2008; Degobbis et al., 2005). Particularly broad ranges are typical of the north Adriatic due to the much larger nitrogen river input in relationship with phosphorus.

In order to find an operative range to be used for QC purposes, the EMODnet community proposes to adopt different ranges for different marine regions.

#### Mediterranean Sea

For the North Adriatic, the broadest ranges are to be used, considering as QF 1 N:P ratios ranging between 1 and 600 (according to the range reported by Socal et al., 2008), as QF 2 N:P ratios up to 1600 (according to the values reported by Maestrini et al., 1997) and over that limit it is proposed to use QF = 4. For the rest of the Adriatic and for the Mediterranean Sea, N:P ratios between 1 to 43 can be considered as QF 1. Outside these limits it is proposed to use QF = 4 (Krom et al., 2004; 2014; Pujo-Pay et al., 2011).



#### Black Sea

For the Black Sea a broad range of N:P ratio will be used, considering as QF=1 ranges between 2 to 800 for the Western Black Sea (Cociasu et al, 1997) and between 2 to 38 for the rest of the Black Sea (BSC, 2008).

#### Baltic Sea

N:P ratio in the open sea, not close to the coast, ranges from 10:1 to 30:1.

#### Atlantic Sea

N:P ratio in the open sea (regions deeper than 150m), not close to the coast, ranges from 5:1 to 30:1.

### Additional checks for Nutrients: inorganic to total N or P

Another criterion proposed is the comparison between inorganic and total N or P, with the following suggestion for setting of flags:

**Table 1:** QF flags suggested according to inorganic to total N or P.

Ratio of inorganic to total	QF value	Description				
1 – 1.05	2	<10% difference, data could be correct within				
		uncertainty of measurements				
1.15 – 2	3	Data are very probably incorrect for inorganic or total				
		measurement				
>2	4	Some of the data are likely incorrect				

<sup>\*</sup>Note: if the threshold is exceeded it is still necessary to determine which of the two parameters (inorganic or total) has a problem and only flag the problematic one

Where ratio of inorganic to total is defined as:

 $R_P = OP/TP$  (ortho phosphate/total phosphorus)

 $R_N = (NH4+NOx [+other N-inorganic species as e.g. Urea])/TN$ 

### Values under detection limits and 0 values

Values under detection limit (namely with QF=6) but having as measured value "0" are regarded as incorrect. Several experts suggested to replace data flagged as "6" with values corresponding to  $\frac{1}{2}$  of the detection limit of the applied analytical method, however a general consensus on the treatment of data flagged as QF=6 was not reached. The common agreement is not to change original data but just flag the measurement with flag QF=6.



**Table 2:** Detection limits indicated by AU-DCE (accredited methods) as valid for laboratories collecting data in the **North Sea area**:

Nutrient	Detection limit	Expected Relative	
		standard deviation	
NO2	0.04 μmol/ l	7%	
NO3	0.1 μmol//l	7%	
NOx	0.1 μmol/l	7%	
NH4	0.3 μmol/l	7%	
TN	1 μmol/l	12.5%	
OP	0.06 μmol/l	5%	
TP	0.1 μmol/l	10%	
SiO4	0.2 μmol/l	4%	

A general value of 0.05 for inorganic N-species could be applied (0.5 for TN), and 0.03/0.05 for P.

**Table 3:** Detection limits indicated by SMHI (accredited methods) as valid for laboratories collecting data in the **Baltic Sea area**:

Nutrient	Detection limit	Expected	Relative	
		standard deviation		
NO2	0.02 μmol/l	6%		
NO3	0.1 μmol/l	4%		
NOx	0.1 μmol/l	6%		
NH4	0.2 μmol/l	4%	4%	
TN	5.0 μmol/l	7%		
OP	0.02 μmol/l	6%		
TP	0.10 μmol/l	9%		
SiO4	0.1 μmol/l	4%		

**Table 4:** Detection limits indicated by the Portuguese NODC (EDMO\_CODE=590) as valid for laboratories collecting data for the **NE Atlantic area**:

P35 parameter	Detection limit
Ammonium	0.96 – 0.7 – 1 μmol/l
Silicate	0.1 – 0.3 μmol/l
Phosphate	0.03 – 0.07 – 0.2 μmol/l
Nitrate+Nitrite	0.24 – 0.5 – 0.51 μmol/l
Nitrite	0.027 – 0.03 – 0.1 μmol/l
Nitrate	0.7 μmol/l



**Table 5:** Detection limits indicated by IFREMER (accredited methods) as valid for data collected in the framework of the Quadrige monitoring program in the **Atlantic and Mediterranean Seas\***:

P01 parameter	parameter name + method	Detection limit
CPHLZZXX	chl-a	0.05
CPHLFLPZ	chl-a_fluorometry	0.01
CPHLSPPZ	chl-a_LorSpec	0.05
DOXYPE01	dissO2_insitu-pulsed-electrode	0.10
DOXYWITX	dissO2_Winkler-titration	0.02
AMONZZXX	NH4	0.05
AMONAADZ	NH4_Filt_ColAA	0.05
AMONAADZ	NH4_Filt_ColAA	0.02
NTRZAADZ	NO3andNO2_Filt_ColAA	0.1
NTRZMADZ	NO3andNO2_Filt_ColMan	0.1
PHOSAADZ	PO4_Filt_ColAA	0.02
PHOSMADZ	PO4_Filt_ColMan	0.02
ODSDM021	Sal	0.5
SLCAMAZX	SiO4_ColMan	0.1
SLCAAADZ	SiO4 Filt ColAA	0.1

<sup>•</sup> As data are provided by several laboratories, different detection limits have been indicated.

**Table 6:** Detection limits indicated for data collected by OGS Laboratory of Marine Chemistry (accredited methods) in the **Adriatic Sea**:

Nutrient	Detection limit	Expected Relative	
		standard deviation	
NO2	0.01 μmol/l	10%	
NO3	0.01 μmol/l	3%	
NOx	0.01 μmol/l	7%	
NH4	0.04 μmol/l	12%	
TN	1 μmol/l	1%	
OP	0.02 μmol/l	5%	
TP	0.02 μmol/l	8%	
SiO4	0.016 μmol/l	3%	

**Table 7:** Detection limits indicated by several laboratories (accredited methods) providing data for the **Mediterranean Sea:** 

Organization	Parameter	Detection Limit (μmol/l)	Notes
Institute of Marine	Ammonium	0.05	
Sciences, Middle East Technical University	Nitrite	0.01	
,	Ammonium	0.034	



Institute of	Nitrite	0.0015	
Oceanography and	Nitrate	0.010	
Fisheries-Croatia	Phosphate	0.020	
	Silicate	0.016	
	Phosphate	0.008	
Israel Marine Data	Nitrate	0.08	
Center (ISRAMAR)	Nitrite	0.08	
	Silicates	0.05	
	Phosphate	0.003	From 2010.
	Nitrate		In case of HCMR oxygen data, zero
LICARD	Nitrite	0.01	values are detected and are considered
HCMR	Silicates	0.05	acceptable (QF ≠6)
	Ammonium	0.03	
	Nitrate+Nitrite	0.04	

**Table 8:** Detection limits suggestions from HCMR (accredited methods, valid from 2010 and after) as valid for laboratories collecting data in the **Eastern Mediterranean Sea area**:

Nutrient	Detection limit	Expected Relative
		standard deviation
NO2	0.01μmol/l	3%
NO3	Is not suggested	
NOx	0.04 μmol/l	10%
NH4	0.03 μmol/l	20%
TN	0.04 μmol/l	10%
OP	0.01 μmol/l	10%
TP	0.01 μmol/l (adopted from Baltic Sea)	10%
PHOS	0.003μmol/l	-
SiO4	0.05 μmol/l	20%

**Table 9:** Detection limits indicated by NIMRD (accredited methods) as valid for laboratories collecting data in the **Black Sea area**:

Nutrient	Detection limit	Expected Relative
		standard deviation
NO2	0.03 μmol/l	9%
NO3	0.1 μmol/l	7%
NOx	0.1 μmol/l	10%
NH4	0.1 μmol/l	4%
TN	5.0 μmol/l (adopted from Baltic Sea)	7%
OP	0.02 μmol/l (adopted from Baltic Sea)	6%
TP	0.10 μmol/l (adopted from Baltic Sea)	9%
SiO4	0.2 μmol/l	4%

Measured values 0 with QF =1 or 2: set QF=6.



#### How to replace zero values in ODV

As a general rule, the EMODnet Chemistry Steering Committee decided to keep the zero values (even if flagging in 6) and not to change the zero values.

However, upon agreement with the originator there is the possibility to replace zero values with the detection limit. As **the version of the data sets should be the same between the local copies and the aggregated data sets**, the regional leaders should therefore proceed with the replacement only when they have checked and confirmed that the local data sets have been also changed by the originators.

Below there is a method or replacing 0 (zero) values with the LOD, where LOD= "detection limit".

#### **Procedure**

To avoid multiple repeats and for simplicity, the method below is recommended to be applied at the end of the variable aggregation as well as at the end of the QC. The aggregated data file (or collection) includes then only 1, 2, 6 qc flags.

The method is based on the derived variables which by default carry the ODV flag scheme. The derived SDN qc flags 1,2 are turned to 0. The SDN qc flag 6 is turned to 1. So, it is important during export at step 2 below, not to exclude 0 qc flag, so it is safer not to filter the data but export all the qc flags of the derived variables.

The method below is applied for each EDMO separately, unless a global regional LOD is known/suggested in the bibliography. Also the time range is used as station selection filter together with the EDMO filter. This results from the providers comments (see table above).

Let's say that the final QCed aggregated data set is named *SiO4\_aggr.txt*. (You can also work with an ODV collection)

#### Step 0: Make a copy of your final aggregated and QCed data files

#### Step 1: Create macro file(s)

- 1. Open ODV4.6.5 or later versions,
- 2. Tools> Macro Editor > Create new macro
  - Label = dSiO4
  - Units = μmol/l
  - O Digits = 3
  - Comments (optional)
  - Input Variables: write a name in the 'New' field and then press <<</li>
    - New = dSiO4
  - Expression in Post fix Notation
    - #1 0.000 <= x.xxxx#1IFTE, where x.xxxx= LOD</p>
  - Save as (e.g. Macrofile\_SiO4\_269 (where 269=EDMO))



Here you can create more than one macro files, depending on the number of variables you have to replace zeros.

#### Step 2: zerovalues substitution in a derived variable

- 3. Import in ODV4.6.5 or later versions, the SiO4\_aggr.txt (or open the collection)
- 4. Station Selection Criteria (by right click on map) >
  - a. Meta Data > EDMO code:
    - i. type 269 twice as Acceptable Range and click OK
  - b. Date / Time;
    - i. choose the appropriate time range e.g Jan/01/2010 to today
- 5. right click on the Current Sample Window popup menu and click on Derived Variables:
  - Derived Variables > Expressions, Derivatives, Integrals
    - Macro File > Add 9and select the macro file 'Macrofile\_SiO4\_269.mac'. By clicking open you will be asked to
    - identify: dSiO4. Then choose 'Water body silicate [μmol/l]' and click OK
    - Export > Station Data > ODV Spreadsheet file (e.g. dSiO4\_aggr\_269.txt),
      - select the derived variable instead the 'Water body silicate'.
      - Data filter: export all data
         Now, for the specific EDMO\_code, a derived variables dSiO4 [μmol/l] has been created and zero values have been replaced by LOQ/2
    - Station Selection Criteria (by right click on map) >
      - Meta Data > Relax Criteria, and press OK
      - Date / Time > Relax Criteria, and press OK
- Repeat above steps 4 and 5 for the next EDMO code
- 7. Now export all data: Export > Station Data > ODV Spreadsheet file: e.g. dSiO4 aggr all.txt

#### Step 3: Re-set the P35 variable name

- 8. With a text editor, edit files dSiO4\_aggr\_all.txtand dSiO4\_aggr\_269.txtand change the derived variable name from dNO3 to 'Water body silicate' at the <dataVariable> block and the Column Header Row:
  - at line 72: //<DataVariable>label="Water body silicate [μmol/l]"
  - o end of line 74

If the file size is big and the editor cannot open it, you can use the following command in cygwin to change the P35 variable name:

- \$ sed -e 's/zeros/Water body silicate/g' dSiO4\_aggr\_269.txt>tmp.txt
- \$ mv tmp.txt dSiO4\_aggr\_269.txt

#### Step 4: Change the qc flag scheme of the derived variable and re-set the qc values of 6



- 9. Open ODV 4.6.5 or later versions,
- 10. Import the dSiO4\_aggr\_269.txt
- 11. Collection > Properties > Data Variables >
  - o select 'Water body silicate' and Edit
  - change the QF Scheme from ODV to SEADATANET
  - You will be asked if 'Really want to change the collection variables and re-write the collection?
  - Press Yes
- 12. Tools> Find Outliers (Range Check)> Water body silicate [μmol/l]
  - Select a very narrow range e.g from –(LOD)/10 to (LOD)/10
  - o as Action select 'find values inside range' and press OK
  - o save somewhere the outliers.lst file
  - o a box will appear indicating the number of outliers found:
    - Click 'View outlier list'
    - Click 'Inspect and edit outliers'
    - Press OK

This number is actually the number of the substituted with LOD zero value.

- The list will appear in one window and in the Outlier Action window click 'Flag as' and choose 'value below detection'
- Apply to All (if you agree with the content of the outliers.list)
- Confirm your action
- 13. Export > Station Data > ODV spreadsheet file (e.g. SiO4 aggr 269.txt)

#### Step 5: Change the qc flag scheme of the whole data set of derived variable

14. Repeat step 4 for the dSiO4 aggr all.txt file and export as SiO4 aggr all.txt

#### Step 6: Merging aggregated data from different providers

- 15. Open ODV4.6.5 or later versions
- 16. Import SiO4 aggr all.txt
- 17. Import SiO4 aggr 269.txt.
- 18. When you asked to 'Confirm Station Replace' Press 'Yes to All'
- 19. Export > Station Data> ODV spreadsheet file e.g SiO4 agg.txt



This is the final file that we have to:

- sent to MARIS and
- o use in DIVA for the products preparation

#### Step 7 (Optional)

20. Instead of separate ODV txt files per variable, you can merge the results of step 19 above into one unique txt file and sent it to MARIS and in DIVA. This can be done by importing the SDN aggregated txt files per variable of step 19 into a new SDN aggregated ODV collection. Then export all data into a ODV spreadsheet file e.g. NO3.txt



### Broad-range check values in the European sea basins:

#### Mediterranean

The broad-range check values in the Mediterranean were defined within EU-MAST/MEDAR/MEDATLAS II project (Mediterranean Data Archeology and Rescue of temperature, salinity and bio-chemical parameters, 1998-2001).

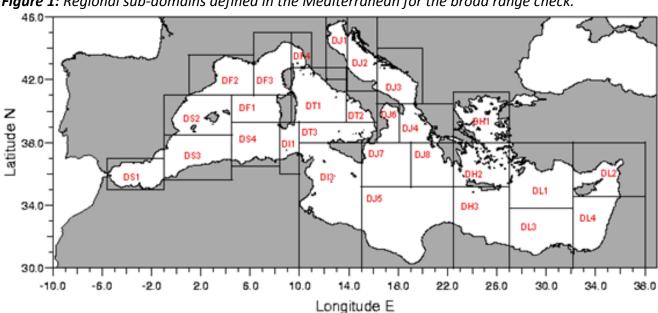


Figure 1: Regional sub-domains defined in the Mediterranean for the broad range check.

Table 10: Geographical limits of the central Mediterranean regions for broad range scale definition and the corresponding maximum depth.

Code	Region Name	Lat. min	Lat. max	Lon. min	Lon. max	Max depth
DJ1	Adriatic North	42 00.00'	46 00.00'	12 10.00'	13 50.00'	150
DJ2	Adriatic Middle	41 18.00'	46 00.00'	13 50.00'	16 16.00'	270
DJ3	Adriatic South	40 36.00'	44 00.00'	16 16.00'	20 00.00'	1350
DJ4	Ionian NE	38 00.00'	40 36.00'	18 00.00'	22 30.00'	3650
DJ5	Ionian South	30 00.00'	35 10.00'	15 00.00'	22 30.00'	4300
DJ6	Ionian NW	38 00.00'	40 36.00'	16 16.00 '	18 00.00'	2770
DJ7-8	Ionian Middle	35 10.00'	38 00.00'	15 00.00'	22 30.00'	5100
DI3	Sicily Strait	30 00.00'	38 00.00'	10 00.00'	15 00.00'	1550
DI1	Sardinia Strait	36 00.00'	39 18.00'	8 24.00'	10 00.00'	2660
DT1	Tyrrhenian 1 NW	39 18.00'	42 48.00'	9 18.00'	13 48.00'	3100



Code	Region Name	Lat. min	Lat. max	Lon. min	Lon. max	Max depth
DT2	Tyrrhenian 2 NE	39 18.00'	41 18.00'	13 48.00'	16 16.00'	3100 m
DT3	Tyrrhenian 3 South	38 00.00'	39 18.00'	10 00.00'	16 16.00'	3100 m
DF3	Ligurian W	41 00.00'	45 00.00'	6 18.00'	9 18.00'	2900 m
DF4	Ligurian E	42 48.00'	45 00.00'	9 18.00'	11 00.00'	1050 m

**Table 11:** Minimum and maximum control values for the two layers (0-200 m, 201-bottom) in the Central Mediterranean regions as used for the broad-range check of hydrological core parameters.

Code-Region Name		Oxygei	n (ml/l)			Nitrate	(µmol/l)	
	0 - 2	00 m	201 m -	201 m - bottom		0 - 200 m		- bottom
DJ1 - Adriatic North	3.0	10.0	/	/	.0	16.0	/	/
DJ2 - Adriatic Middle	3.0	9.0	2.0	9.0	.0	9.0	.0	9.0
DJ3 - Adriatic South	3.0	9.0	3.0	8.0	.0	9.0	.0	9.0
DJ4 - Ionian NE	3.0	8.0	3.0	6.0	.0	9.0	.0	9.0
DJ5 - Ionian South	3.0	8.0	3.0	6.0	.0	9.0	.0	11.0
DJ6 - Ionian NW	3.0	8.0	3.0	6.0	.0	9.0	.0	9.0
DJ7 - Ionian Middle	3.0	8.0	3.0	6.0	.0	9.0	.0	9.0
DI3 - Sicily Strait	3.0	8.0	3.0	6.0	.0	9.0	.0	12.0
DI1 - Sardinia Strait	3.0	8.0	3.0	6.0	.0	9.0	.0	12.0
DT1 - Tyrrhenian NW	3.0	8.0	3.0	3.0	.0	9.0	.0	9.0
DT2 - Tyrrhenian NE	3.0	8.0	3.0	3.0	.0	9.0	.0	9.0
DT3 - Tyrrhenian South	3.0	8.0	3.0	3.0	.0	9.0	.0	11.0
DF3 - Ligurian W	3.0	8.0	3.0	6.0	.0	7.0	.0	9.0
DF4 - Ligurian E	3.0	8.0	3.0	6.0	.0	7.0	.0	9.0

Code-Region Name	Phosphate (μmol/l) Silicate (μmol/						(μmol/l)	
	0 - 2	0 - 200 m		201 m - bottom		0 - 200 m		bottom
DJ1 - Adriatic North	.0	1.5	/	/	.0	60.0	/	/
DJ2 - Adriatic Middle	.0	1.0	.0	1.0	.0	20.0	.0	26.0
DJ3 - Adriatic South	.0	1.0	.0	1.0	.0	11.0	.0	25.0
DJ4 - Ionian NE	.0	1.0	.0	1.0	.0	10.0	.0	16.0
DJ5 - Ionian South	.0	1.0	.0	1.0	.0	9.0	.0	11.0
DJ6 - Ionian NW	.0	1.0	.0	1.0	.0	9.0	.0	11.0
DJ7 - Ionian Middle	.0	1.0	.0	1.0	.0	9.0	.0	11.0
DI3 - Sicily Strait	.0	1.0	.0	1.0	.0	9.0	.0	12.0
DI1 - Sardinia Strait	.0	1.0	.0	1.0	.0	9.0	.0	12.0
DT1 - Tyrrhenian NW	.0	1.0	.0	1.0	.0	9.0	.0	10.0
DT2 - Tyrrhenian NE	.0	1.0	.0	1.0	.0	9.0	.0	10.0
DT3 - Tyrrhenian South	.0	1.0	.0	1.0	.0	9.0	.0	12.0
DF3 - Ligurian W	.0	1.0	.0	1.0	.0	9.0	.0	11.0
DF4 - Ligurian E	.0	1.0	.0	1.0	.0	9.0	.0	11.0



	A	Alkalinity	μmol/ l	<i>)</i>	A	mmoniu	m (μmol/	<b>(I)</b>
	0 - 2	00 m	201 m -	bottom	0 - 2	00 m	201 m -	bottom
DJ1 - Adriatic North	2000	3000	/	/	.0	30.0	/	/
DJ2 - Adriatic Middle	2500	3000	2500	3000	.0	10.0	.0	7.0
DJ3 - Adriatic South	2500	3000	2500	3000	.0	10.0	.0	7.0
DJ4 - Ionian NE	2500	3000	2500	3000	.0	10.0	.0	7.0
DJ5 - Ionian South	2500	3000	2500	3000	.0	2.0	.0	1.0
DJ6 - Ionian NW	2500	3000	2500	3000	.0	2.0	.0	1.0
DJ7 - Ionian Middle	2500	3000	2500	3000	.0	2.0	.0	1.0
DI3 - Sicily Strait	2500	3000	2500	3000	.0	2.0	.0	1.0
DI1 - Sardinia Strait	2500	3000	2500	3000	.0	2.0	.0	1.0
DT1 - Tyrrhenian NW	2500	3000	2500	3000	.0	2.0	.0	2.0
DT2 - Tyrrhenian NE	2500	3000	2500	3000	.0	2.0	.0	2.0
DT3 - Tyrrhenian South	2500	3000	2500	3000	.0	2.0	.0	2.0
DF3 - Ligurian W	2500	3000	2500	3000	.0	2.0	.0	2.0
DF4 - Ligurian E	2500	3000	2500	3000	.0	2.0	.0	2.0

Code-Region Name	Chlorophyll-a (μ			(I)		Nitrite (	μmol/l)	
	0 - 2	0 - 200 m		201 m - bottom		0 - 200 m		bottom
DJ1 - Adriatic North	.0	20.0	/	/	0	10	/	/
DJ2 - Adriatic Middle	.0	2.0	.0	.5	0	3	0	3
DJ3 - Adriatic South	.0	2.0	.0	.5	0	2	0	2
DJ4 - Ionian NE	.0	2.0	.0	.5	0	1	0	0.5
DJ5 - Ionian South	.0	1.0	.0	.5	0	1	0	0.5
DJ6 - Ionian NW	.0	1.0	.0	.5	0	0.5	0	0.2
DJ7 - Ionian Middle	.0	1.0	.0	.5	0	0.5	0	0.2
DI3 - Sicily Strait	.0	1.0	.0	.5	0	0.5	0	0.5
DI1 - Sardinia Strait	.0	1.0	.0	.5	0	0.5	0	0.5
DT1 - Tyrrhenian NW	.0	1.0	.0	.5	0	0.5	0	0.2
DT2 - Tyrrhenian NE	.0	1.0	.0	.5	0	0.5	0	0.2
DT3 - Tyrrhenian South	.0	1.0	.0	.5	0	0.5	0	0.2
DF3 - Ligurian W	.0	3.0	.0	.5	0	1	0	0.5
DF4 - Ligurian E	.0	1.0	.0	.5	0	1	0	0.5

Code-Region Name	Tot	tal Nitrog	gen (µmo	01/1)	Total Phosphorus (μmol/l)				
	0 - 2	0 - 200 m 201 m - bottom		0 - 2	00 m	201 m - bottom			
DJ1 - Adriatic North	4.0	15	/	/	.0	1.5	/	/	
DJ2 - Adriatic Middle	4	15	6	15	.0	1.0	.0	1.0	
DJ3 - Adriatic South	4	30	6	30	.0	1.0	.0	1.0	
DJ4 - Ionian NE	4	20	6	20	.0	1.5	.0	1.0	
DJ5 - Ionian South	4	20	6	20	.0	1.0	.0	1.0	
DJ6 - Ionian NW	4	20	6	20	.0	1.0	.0	1.0	



DJ7 - Ionian Middle	4	20	6	20	.0	1.0	.0	1.0
DI3 - Sicily Strait	4	9	6	12	.0	1.0	.0	1.0
DI1 - Sardinia Strait	4	9	6	12	.0	1.0	.0	1.0
DT1 - Tyrrhenian NW	4	9	6	9	.0	1.0	.0	1.0
DT2 - Tyrrhenian NE	4	9	6	9	.0	1.0	.0	1.0
DT3 - Tyrrhenian South	4	9	6	9	.0	1.0	.0	1.0
DF3 - Ligurian W	4	7	6	9	.0	1.0	.0	1.0
DF4 - Ligurian E	4	7	6	9	.0	1.0	.0	1.0

Code-Region Name		р	Н	
	0 - 2	00 m	201 m -	bottom
DJ1 - Adriatic North	6.0	9.0	/	/
DJ2 - Adriatic Middle	7.0	9.0	7.0	9.0
DJ3 - Adriatic South	7.0	9.0	7.0	9.0
DJ4 - Ionian NE	7.5	9.0	7.5	9.0
DJ5 - Ionian South	7.5	9.0	7.5	9.0
DJ6 - Ionian NW	7.5	9.0	7.5	9.0
DJ7 - Ionian Middle	7.5	9.0	7.5	9.0
DI3 - Sicily Strait	7.5	9.0	7.5	9.0
DI1 - Sardinia Strait	7.5	9.0	7.5	9.0
DT1 - Tyrrhenian NW	7.5	9.0	7.5	9.0
DT2 - Tyrrhenian NE	7.5	9.0	7.5	9.0
DT3 - Tyrrhenian South	7.5	9.0	7.5	9.0
DF3 - Ligurian W	7.5	9.0	7.5	9.0
DF4 - Ligurian E	7.5	9.0	7.5	9.0

**Table 12**. Geographical limits of the Eastern Mediterranean regions for broad range scale definition and the corresponding maximum depth

Code	Region Name	Lat. min	Lat. max	Lon. min	Lon. max	Max depth
DH1	Aegean North	38 00'	41 12'	22 30'	27 00'	1747 m
DH2	Aegean South	35 10'	38 00'	22 30'	27 00'	4424 m
DH3	Cretan Passage	30 00'	35 10'	22 30'	27 00'	4007 m
DL1	Levantine North	33 50'	38 00'	27 00'	32 10'	4227 m
DL2	Levantine North-East	34 35'	38 00'	32 10'	38 00'	2452 m
DL3	Levantine South	30 00'	33 50'	27 00'	32 10'	3133 m
DL4	Levantine South-East	30 00'	34 35'	32 10'	38 00'	2650 m



**Table 13**. Minimum and maximum control values for the two layers (0-200 m, 201-bottom) in the Eastern Mediterranean regions as used for the broad-range check of nutrients parameters.

Code-Region Name		Oxyge	n (ml/l)		Nitrate (μmol/l)				
	0 - 2	0 - 200 m 2		201 m - bottom		00 m	201 m - bottor		
DH1 - Aegean North	3.0	6.0	3.0	7.0	.0	7.0	.0	7.0	
DH2 - Aegean South	3.0	6.0	3.0	7.0	.0	7.0	.0	10.0	
DH3 - Cretan Passage	3.0	6.0	3.0	7.0	.0	7.0	.0	10.0	
DL1 - Levantine North	3.0	6.0	3.0	7.0	.0	5.0	.0	10.0	
DL2 - Levantine NE	3.0	6.0	3.0	7.0	.0	5.0	.0	10.0	
DL3 - Levantine South	3.0	6.0	3.0	7.0	.0	5.0	.0	10.0	
DL4 - Levantine SE	3.0	6.0	3.0	7.0	.0	5.0	.0	10.0	

Code-Region Name	Phosphate (μmol/l) Silicate (μmol/					(μmol/l)		
	0 - 2	0 - 200 m 2		201 m - bottom		00 m	201 m - bottom	
DH1 - Aegean North	.0	7.0	.0	2.0	.0	15.0	.0	25.0
DH2 - Aegean South	.0	2.0	.0	2.0	.0	15.0	.0	20.0
DH3 - Cretan Passage	.0	1.0	.0	2.0	.0	10.0	.0	15.0
DL1 - Levantine North	.0	1.0	.0	1.0	.0	10.0	.0	15.0
DL2 - Levantine NE	.0	1.0	.0	1.0	.0	10.0	.0	15.0
DL3 - Levantine South	.0	0.5	.0	1.0	.0	5.0	.0	11.0
DL4 - Levantine SE	.0	1.0	.0	1.0	.0	20.0	.0	11.0

Code-Region Name	Alkalinity (μmol/l) Amm				mmoniu	nmonium (μmol/l)			
	0 - 2	0 - 200 m   201 m - bottom		0 - 200 m		201 m - bottom			
DH1 - Aegean North	2000	3000	2000	3000	.0	50.0	.0	10.0	
DH2 - Aegean South	2000	3000	2000	3000	.0	10.0	.0	10.0	
DH3 - Cretan Passage	2000	3000	2000	3000	.0	1.5	.0	1.5	
DL1 - Levantine North	2000	3000	2000	3000	.0	1.0	.0	1.0	
DL2 - Levantine NE	2000	3000	2000	3000	.0	1.0	.0	1.0	
DL3 - Levantine South	2000	3000	2000	3000	.0	1.0	.0	1.0	
DL4 - Levantine SE	2000	3000	2000	3000	.0	1.0	.0	1.0	

Code-Region Name	Chlorophyll-a (μg/l) Nitri					Nitrite (	e (μmol/l)		
	0 - 2	0 - 200 m 2		201 m - bottom		0 - 200 m		bottom	
DH1 - Aegean North	.0	1.5	.0	2.0	0	1.0	0	0.5	
DH2 - Aegean South	.0	1.5	.0	2.0	0	1.0	0	1.0	
DH3 - Cretan Passage	.0	1.0	.0	1.0	0	1.0	0	1.0	
DL1 - Levantine North	.0	1.0	.0	1.0	0	0.5	0	0.5	
DL2 - Levantine NE	.0	1.0	.0	1.0	0	1.0	0	2.0	
DL3 - Levantine South	.0	1.0	.0	1.0	0	0.5	0	0.5	
DL4 - Levantine SE	.0	1.0	.0	1.0	0	0.5	0	0.5	



Code-Region Name	Tot	al Nitrog	gen (μmo	1/1)	Total Phosphorus (μmol/l)				
	0 - 2	00 m	201 m - bottom		0 - 200 m		201 m - bottom		
DH1 - Aegean North	4.0	10	5.0	9.0	.0	1.5	.0	1.5	
DH2 - Aegean South	4.0	10	5.0	9.0	.0	1.0	.0	1.0	
DH3 - Cretan Passage	4.0	10	4.0	9.0	.0	1.0	.0	1.0	
DL1 - Levantine North	4.0	10	4.0	9.0	.0	1.5	.0	1.0	
DL2 - Levantine NE	4.0	10	4.0	9.0	.0	1.0	.0	1.0	
DL3 - Levantine South	4.0	10	4.0	9.0	.0	1.0	.0	1.0	
DL4 - Levantine SE	4.0	10	4.0	9.0	.0	1.0	.0	1.0	

Code-Region Name	рН					
	0 - 200 m		201 m -	bottom		
DH1 - Aegean North	7.5	9.0	7.5	9.0		
DH2 - Aegean South	7.5	9.0	7.5	9.0		
DH3 - Cretan Passage	7.5	9.0	7.5	9.0		
DL1 - Levantine North	7.5	8.5	7.5	8.5		
DL2 - Levantine NE	7.5	8.5	7.5	8.5		
DL3 - Levantine South	7.5	8.5	7.5	8.5		
DL4 - Levantine SE	7.5	8.5	7.5	8.5		

**Table 14**. Geographical limits of the Western Mediterranean regions for broad range scale definition and the corresponding maximum depth

Code	Region Name	Lat. min	Lat. max	Lon. min	Lon. max	Max depth
DF1	Algero-Provencal	39 18'	41 00'	4 30'	9 18'	2791 m
DF2	Gulf of Lions	41 00'	43 36'	1 00'	6 18'	2642 m
DS1	Alboran Sea	35 00'	37 30'	-5 36'	-1 00'	2583 m
DS2	Balearic Sea	38 30'	41 00'	-1 00'	4 30'	2653 m
DS3	Algerian Basin SW	35 36'	38 30'	-1 00'	4 30'	2728 m
DS4	Algerian Basin SE	36 30'	39 18'	4 30'	8 24'	2799 m

**Table 15**. Minimum and maximum control values for the two layers (0-200 m, 201-bottom) in the Western Mediterranean regions as used for the broad-range check of nutrients parameters.

Code-Region Name	Oxygen (ml/l) Nitrate (					(μmol/l)		
	0 - 2	00 m	201 m - bottom		0 - 2	00 m	201 m - bottom	
DF1 - Algero-Provencal	3.0	6.0	3.0	7.0	.0	15.0	.0	30.0
DF2 - Gulf of Lions	3.0	6.0	3.0	7.0	.0	50.0	.0	10.0
DS1 - Alboran Sea	3.0	6.0	3.0	7.0	.0	15.0	.0	15.0
DS2- Balearic Sea	3.0	6.0	3.0	7.0	.0	10.0	.0	10.0
DS3 - Algerian Basin SW	3.0	6.0	3.0	7.0	.0	10.0	.0	10.0
DS4 - Algerian Basin SE	3.0	6.0	3.0	7.0	.0	10.0	.0	10.0



Code-Region Name	F	Phosphat	e (µmol/	<b>(</b> )	Silicate (µmol/l)				
	0 - 200 m		201 m - bottom		0 - 200 m		201 m - bottom		
DF1 - Algero-Provencal	.0	1.0	.0	1.0	.0	25.0	.0	25.0	
DF2 - Gulf of Lions	.0	2.0	.0	1.5	.0	40.0	.0	15.0	
DS1 - Alboran Sea	.0	2.0	.0	1.0	.0	20.0	.0	20.0	
DS2- Balearic Sea	.0	1.0	.0	1.0	.0	10.0	.0	15.0	
DS3 - Algerian Basin SW	.0	1.0	.0	1.0	.0	10.0	.0	12.0	
DS4 - Algerian Basin SE	.0	1.0	.0	1.0	.0	10.0	.0	10.0	

	Alkalinity (μmol/l)				Ammonium (μmol/l)					
	0 - 2	0 - 200 m		201 m - bottom		0 - 200 m		bottom		
DF1 - Algero-Provencal	2000	3000	2000	3000	.0	50.0	.0	10.0		
DF2 - Gulf of Lions	2000	3000	2000	3000	.0	6.0	.0	6.0		
DS1 - Alboran Sea	2000	3000	2000	3000	.0	10.0	.0	10.0		
DS2- Balearic Sea	2000	3000	2000	3000	.0	2.0	.0	2.0		
DS3 - Algerian Basin SW	2000	3000	2000	3000	.0	0.5	.0	0.1		
DS4 - Algerian Basin SE	2000	3000	2000	3000	.0	10.0	.0	10.0		

	C	Chlorophyll-a (μg/l)				Nitrite (μmol/l)			
	0 - 2	0 - 200 m		201 m - bottom		0 - 200 m		bottom	
DF1 - Algero-Provencal	.0	1.0	.0	.5	0	2.0	0	2.0	
DF2 - Gulf of Lions	.0	3.0	.0	.5	0	3.0	0	2.0	
DS1 - Alboran Sea	.0	1.0	.0	.5	0	2.0	0	2.0	
DS2- Balearic Sea	.0	1.0	.0	.5	0	2.0	0	2.0	
DS3 - Algerian Basin SW	.0	1.0	.0	.5	0	2.0	0	2.0	
DS4 - Algerian Basin SE	.0	1.0	.0	.5	0	2.0	0	2.0	

	Total Nitrogen (μmol/l)				Total Phosphorus (μmol/l)			
	0 - 2	0 - 200 m		201 m - bottom		0 - 200 m		bottom
DF1 - Algero-Provencal	4.0	10	4.0	9	.0	1.5	.0	1.5
DF2 - Gulf of Lions	4.0	7	4.0	9	.0	1.0	.0	1.0
DS1 - Alboran Sea	4.0	10	4.0	9	.0	1.0	.0	1.0
DS2- Balearic Sea	4.0	10	4.0	9	.0	1.0	.0	1.0
DS3 - Algerian Basin SW	4.0	10	4.0	9	.0	1.0	.0	1.0
DS4 - Algerian Basin SE	4.0	10	4.0	9	.0	1.0	.0	1.0

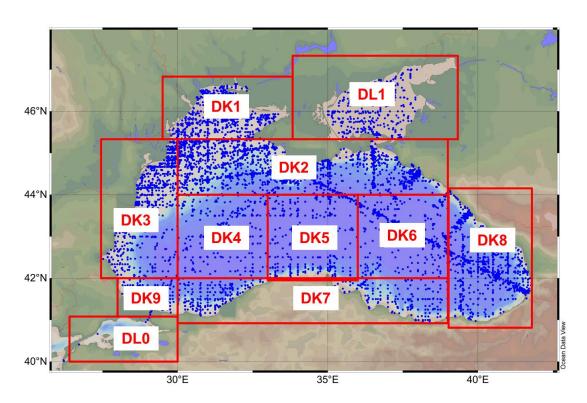
Code-Region Name	рН				
	0 - 200 m		201 m -	bottom	
DF1 - Algero-Provencal	7.5	8.5	7.5	8.5	
DF2 - Gulf of Lions	7.5	9.0	7.0	9.0	
DS1 - Alboran Sea	7.5	8.5	7.0	8.5	
DS2- Balearic Sea	7.5	8.5	7.5	8.5	
DS3 - Algerian Basin SW	7.5	8.5	7.5	8.5	
DS4 - Algerian Basin SE	7.5	8.5	7.5	8.5	

#### **Black Sea**

The broad-range check values in the Black Sea were defined within EU-MAST/MEDAR/MEDATLAS II project (Mediterranean Data Archeology and Rescue of temperature, salinity and bio-chemical parameters, 1998-2001) and during the EMODNET Chemistry Pilot Project (2009-2012) by MHI.

Figure 2: Regional sub-domains defined in the Mediterranean for the broad range check.

#### **MEDAR/MEDATLAS Sub-domains for Black Sea**



**Table 16:** Geographical limits of the Black Sea regions for broad range scale definition and the corresponding maximum depth.

Code	Region Name	Lat. min	Lat. max	Lon. min	Lon. max	Max depth
DK0	BLACK SEA AND SEA OF ASOV	40 12.00′	47 24.00'	27 18.00′	41 54.00′	2313
DK1	BLACK SEA NORTH WEST SHELF	45 20.00'	46 50.00'	29 30.00'	33 50.00′	1000
DK2	BLACK SEA NORTH SLOPE	44 00.00'	45 20.00'	30 00.00'	39 00.00′	1500
DK3	BLACK SEA WEST SLOPE	42 00.00'	45 20.00'	27 30.00′	30 00.00′	1500
DK4	BLACK SEA WEST ABYSSAL	42 00.00'	44 00.00'	30 00.00'	33 00.00′	2313
DK5	BLACK SEA CENTRAL ABYSSAL	42 00.00'	44 00.00'	33 00.00'	36 00.00'	2313
DK6	BLACK SEA EAST ABYSSAL	42 00.00'	44 00.00'	36 00.00'	39 00.00′	2313
DK7	BLACK SEA SOUTH SLOPE	40 55.00′	42 00.00'	30 00.00'	39 00.00′	1500
DK8	BLACK SEA SOUTH-EAST SLOPE	40 50.00′	44 10.00'	39 00.00′	41 40.00'	1500



DK9	BLACK SEA ADJACENT TO BOSPHORUS	41 05.00′	42 00.00′	28 00.00′	30 00.00′	1500
DL0	MARMARA SEA	40 12.00'	41 05.00′	26 50.00'	30 00.00′	1000
DL1	SEA OF AZOV	45 20.00'	47 20.00'	33 50.00'	39 20.00'	200

**Table 17:** Minimum and maximum control in the Black Sea regions as used for the broad-range check nutrients and physical parameter (T, S).

Code	Region Name		Oxygen (ml/l)		ygen nol/l)	Ammonium (μmol/l)	
DK0	BLACK SEA AND SEA OF ASOV	0	13.3	0	600	0	100
DK1	BLACK SEA NORTH WEST SHELF	0	13.3	0	600	0	15
DK2	BLACK SEA NORTH SLOPE	0	12.7	0	570	0	70
DK3	BLACK SEA WEST SLOPE	0	12.8	0	580	0	96
DK4	BLACK SEA WEST ABYSSAL	0	10	0	450	0	98
DK5	BLACK SEA CENTRAL ABYSSAL	0	8.4	0	380	0	100
DK6	BLACK SEA EAST ABYSSAL	0	10.6	0	480	0	105
DK7	BLACK SEA SOUTH SLOPE	0	0 8.8		400	0	94
DK8	BLACK SEA SOUTH-EAST SLOPE	0	0 11.5		520	0	100

Code	Region Name	Nitrat	te	Nitrite	?	Phosphate	
		(μmol/l)		(μmol/l)		(µmol/l)	
DK0	BLACK SEA AND SEA OF ASOV	0	33	0	15	0	13
DK1	BLACK SEA NORTH WEST SHELF	0	33	0	6	0	6
DK2	BLACK SEA NORTH SLOPE	0	24	0	3	0	10
DK3	BLACK SEA WEST SLOPE	0	20	0	1.5	0	10
DK4	BLACK SEA WEST ABYSSAL	0	15	0	0.8	0	10
DK5	BLACK SEA CENTRAL ABYSSAL	0	13	0	0.8	0	11
DK6	BLACK SEA EAST ABYSSAL	0	13	0	1	0	12
DK7	BLACK SEA SOUTH SLOPE	0 10		0	0.5	0	10
DK8	BLACK SEA SOUTH-EAST SLOPE	0 21		0	15	0	13

Code	Region Name	Silica	te		ρΗ	Alkalin	ity
		(µто	(μmol/l)			(µmol/	<i>)</i>
DK0	BLACK SEA AND SEA OF ASOV	0	330	7	9.1	1000	4600
DK1	BLACK SEA NORTH WEST SHELF	0	160	7.4	9.1	1200	4300
DK2	BLACK SEA NORTH SLOPE	0	200	7.2	8.9	1400	4500
DK3	BLACK SEA WEST SLOPE	0	310	7.5	8.9	2800	4200
DK4	BLACK SEA WEST ABYSSAL	0	330	7.4	8.9	2900	4500
DK5	BLACK SEA CENTRAL ABYSSAL	0	330	7.5	9	2800	4500
DK6	BLACK SEA EAST ABYSSAL	0	320	7.5	8.7	2700	4600
DK7	BLACK SEA SOUTH SLOPE	0 310		7.6	8.7	2700	4200
DK8	BLACK SEA SOUTH-EAST SLOPE	0 310		7.5	8.9	1900	4500



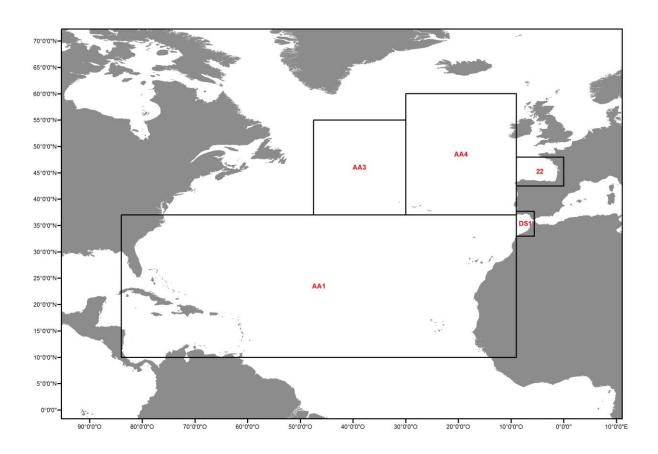
Code	Region Name	Salinity	(psu)	Tempero	ture (°C)
DK0	BLACK SEA AND SEA OF ASOV	0	24	-1	29
DK1	BLACK SEA NORTH WEST SHELF	0	21	-1	28
DK2	BLACK SEA NORTH SLOPE	4	23	2	28
DK3	BLACK SEA WEST SLOPE	7	23	3	27
DK4	BLACK SEA WEST ABYSSAL	12	24	5	27
DK5	BLACK SEA CENTRAL ABYSSAL	16	23	5	27
DK6	BLACK SEA EAST ABYSSAL	15	23	6	28
DK7	BLACK SEA SOUTH SLOPE	13	24	6	28
DK8	BLACK SEA SOUTH-EAST SLOPE	4	23	6	29

DK9	BLACK SEA ADJACENT TO BOSPHORUS	No Regional Limits defined for the parameters.
DL0	MARMARA SEA	Global limits (DKO - BLACK SEA AND SEA OF
DL1	SEA OF AZOV	AZOV) are taken for QC of the parameters.

### Atlantic area

The broad-range check values in the Atlantic area are defined within our internal QA/QC control software.

Figure 3: Regional sub-domains defined in the Atlantic area for the broad range check.



**Table 18:** Geographical limits of the Atlantic regions for broad range scale definition and the corresponding maximum depth.

Code	Region name	Lat. min	Lat. max	Lon min.	Lon max.	Max depth
AA1	NORTH ATLANTIC 1	10 00.00′	37 00.00′	-84 00.00'	-09 00.00'	6000
AA3	NORTH ATLANTIC 3	37 00.00'	55 00.00'	-47 30.00′	-30 00.00′	6000
AA4	NORTH ATLANTIC 4	37 00.00'	60 00.00′	-30 00.00′	-09 00.00′	6000
DS1	GIBRALTAR STRAIT	33 00.00'	37 42.00′	-09 00.00′	-05 36.00'	3000
22	Bay of Biscay	42 30.00'	48 00.00'	-09 00.00′	00 00.00′	5000



**Table 19:** Minimum and maximum control values in the Atlantic regions as used for the broad-range check of hydrological core parameters.

Code-Region Name	Oxygen (ml/l)		Nitrate (μmol/l)		Phosphate (μmol/l)		Silicate (μmol/l)		рН	
AA1 - NORTH ATLANTIC 1	0	7	0	48	0	3.6	0	150	7.5	8.4
AA3 - NORTH ATLANTIC 3	ND	ND	0	48	0	3.6	0	150	ND	ND
AA4 - NORTH ATLANTIC 4	ND	ND	0	48	0	3.6	0	150	ND	ND
DS1 - GIBRALTAR STRAIT	0	7	ND	ND	ND	ND	ND	ND	ND	ND
22 - Bay of Biscay	0	7	0	48	0	3.6	0	150	ND	ND
Global	0	10	0	56	0	4	0	200	7.4	8.4

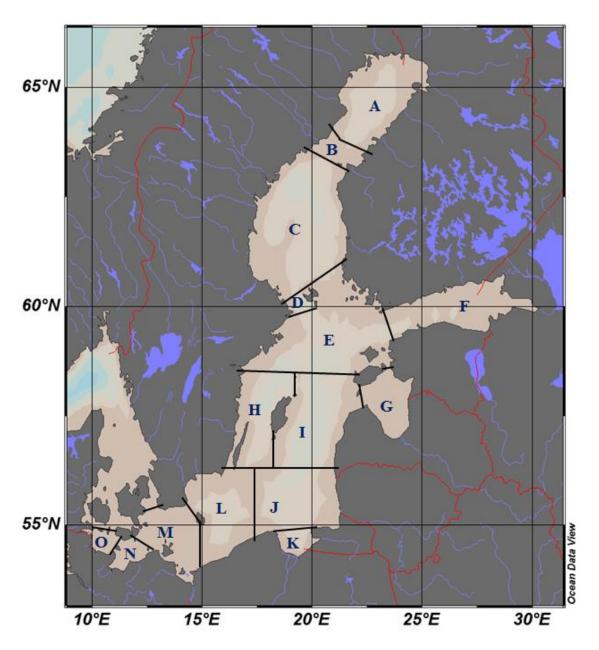
REGION	Alkalin (μmol/	•	Ammol/		Chlorop (μg/l)	hyll-a	Nitrite	(μmol/l)	Total N (μmol/	_	Total pho (μmol/l)	sphorus
Global	1500	2500	0	10	0	99	0	10	0	90	0	10

ND: No Data

### **Baltic Sea**

The broad-range check values in the Baltic Sea are defined on the basis of the available data.

Figure 4: Regional sub-domains defined in the Baltic Sea for the broad range check.



- A. Bothnian Bay
- B. The Quark
- C. Bothnian Sea
- D. Åland Sea
- E. Northern Baltic Sea Proper
- F. Gulf of Finland



- G. Gulf of Riga
- H. Western Gotland Basin
- I. Eastern Gotland Basin
- J. South Eastern Basin
- K. Gdansk Basin
- L. Bornholm Basin
- M. Arkona Basin
- N. Bay of Mecklenburg
- O. Bay of Kiel

**Table 20:** Geographical limits of the Baltic Sea regions for broad range scale definition and the definition of surface and deep water layers.

Code	Region name	Lat.	Lat.max	Long.	Long.max	Max	Surface	Deep
		Min		Min		depth	water	water
Α	Bothnian Bay	63 30.00'	65 50.00'	20 40.00'	25 30.00′	146	0 - 50	50 - 140
В	The Quark	63 00.00'	64 00.00′	19 40.00'	21 40.00′	49	0 - 50	"_"
С	Bothnian Sea	60 20.00'	63 30.00′	17 00.00′	21 40.00′	293	0 - 50	50 - 250
D	Åland Sea	59 40.00'	60 20.00′	18 10.00′	21 00.00′	301	0 - 50	50 - 290
Ε	Northern Baltic Sea	58 30.00'	59 40.00′	16 50.00′	23 30.00′	459	0 - 60	60 - 450
	Proper							
F	Gulf of Finland	59 10.00'	60 50.00′	23 20.00′	30 20.00'	123	0 - 40	40 - 110
G	Gulf of Riga	57 00.00′	58 30.00′	21 50.00′	24 40.00′	51	0 - 25	25 - 50
Н	Western Gotland	56 20.00'	58 30.00′	16 20.00'	22 00.00′	205	0 - 50	50 - 200
	Basin							
1	Eastern Gotland Basin	56 20.00'	58 30.00′	18 20.00′	22 20.00′	249	0 - 60	60 - 240
J	South Eastern Basin	54 20.00'	56 20.00'	16 30.00'	20 10.00′	114	0 - 40	40 - 100
Κ	Gdansk Basin	54 20.00'	55 00.00'	18 40.00'	20 30.00′	114	0 - 70	70 - 110
L	Bornholm Basin	54 00.00'	56 20.00'	15 00.00'	16 30.00′	105	0 - 40	40 - 100
М	Arkona Basin	54 00.00'	55 30.00'	12 00.00′	15 00.00'	53	0 - 30	30 - 50
Ν	Bay of Mecklenburg	54 00.00'	54 40.00′	10 50.00′	12 30.00′	26	0 - 15	15 - 25
0	Kiel Bay	54 40.00'	55 00.00'	09 40.00′	11 30.00′	35	0 - 15	15 - 35

**Table 21:** Minimum and maximum control values in the surface and bottom layers for the Baltic Sea regions as used for the broad-range check of hydrological core parameters.

Code	Region name		Oxygen (	Chlorophyll-a (μg/l)			
		Surface min	max	Bottom min	max	Surface min	max
Α	Bothnian Bay	4	11	5	11	0	5
В	The Quark	5	11	"_"	"_"	1	3
С	Bothnian Sea	0	12	0	11	0	99
D	Åland Sea	5	12	4	10	0	9



Ε	Northern Baltic Sea Proper	-5	12	-5	11	0	23
F	Gulf of Finland	0	13	-1	11	0	
G	Gulf of Riga	1	13	7	9	1	7
Н	Western Gotland Basin	-0.5	10	-3	14	0	34
/	Eastern Gotland Basin	-0.2	12	-8	9	0	36
J	South Eastern Basin	2	21	-4	11	0	31
K	Gdansk Basin	1	10	-3.5	9	0	31
L	Bornholm Basin	1	13	-4	11	0	53
М	Arkona Basin	0	15	0	11	0	50
N	Bay of Mecklenburg	0	21	0	17	0	21
0	Kiel Bay	1	27	0	17	0	50

Code	Region name	Pi	hosphate	(μmol/l)		Tot	al phosph	orus (µmol,	<b>/</b> 1)
		Surface min	max	Bottom min	max	Surface min	max	Bottom min	max
Α	Bothnian Bay	0	0.9	0	3.5	0	1	0	8.4
В	The Quark	0	0.7	"_"	"_"	0	1.4	"_"	"_"
С	Bothnian Sea	0	13	0	4	0	13	0	8.1
D	Åland Sea	0	1.1	0	3	0	1.8	0	3.3
Ε	Northern Baltic Sea Proper	0	36	0	12	0	30	0	16
F	Gulf of Finland	0	6	0	11	0	4	0	11
G	Gulf of Riga	0	1	0	2	0	1.4	0	2
Н	Western Gotland Basin	0	36	0	20	0	40	0	20
1	Eastern Gotland Basin	0	3	0	10	0	4	0	12
J	South Eastern Basin	0	11	0	10	0	16	0	17
K	Gdansk Basin	0	11	1	10	0	16	1	10
L	Bornholm Basin	0	11	0	15	0	13	0	25
М	Arkona Basin	0	28	0	7	0	28	0	7.1
N	Bay of Mecklenburg	0	13	0	13	0	18	0	13
0	Kiel Bay	0	3.6	0	17	0	4	0	19



Code	Region name		Nitrite	(μmol/l)			Nitrate (μr	nol/l)	
		Surface	max	Bottom	max	Surface	max	Bottom	max
		min		min		min		min	
Α	Bothnian Bay	0	0.9	0	0.8	3	11	0	10
В	The Quark	0	0.6	"_"	"_"	0	15	"_"	"_"
С	Bothnian Sea	0	2.2	0	1.5	0	14	0	12
D	Åland Sea	0	0.5	0	0.5	0	7	0	8
Ε	Northern Baltic Sea Proper	0	4.2	0	3.4	0	71	0	15
F	Gulf of Finland	0	3.4	0	1.1	0	195	0	11
G	Gulf of Riga	0	1.2	0	0.7	NED			
Н	Western Gotland Basin	0	10	0	2.7	0	99	0	34
1	Eastern Gotland Basin	0	1.1	0	4.4	0	11	0	17
J	South Eastern Basin	0	2	0	2.3	0	12	0	15
K	Gdansk Basin	0	3.3	0	2.4	0	215	0	17
L	Bornholm Basin	0	1.7	0	3	0	48	0	19
М	Arkona Basin	0	5.2	0	1.9	0	340	0	40
N	Bay of Mecklenburg	0	2.1	0	1.9	0	13	0	13
0	Kiel Bay	0	1.9	0	1.3	0	15	0	14

ND=No Data; NED= Not Enough Data

Code	Region name	Α	mmoniu	m (μmol/l)		Total nitrogen (μmol/l)			
		Surface	max	Bottom	max	Surface	max	Bottom	max
		min		min		min		min	
Α	Bothnian Bay	0	23	0	7	10	56	10	44
В	The Quark	0	25	"_"	"_"	10	24	"_"	"-"
С	Bothnian Sea	0	99	0	9	6	33	8	34
D	Åland Sea	0	3	0	7	9	29	9	35
Ε	Northern	0	85	0	34	8	39	4	54
	Baltic Sea								
	Proper								
F	Gulf of Finland	0	25	0	31	0	380	3	43
G	Gulf of Riga	0	2	0	3	22	44	24	40
Н	Western	0	98	0	25	10	25	10	70
	Gotland Basin								
1	Eastern	0	3	0	73	0	40	0	73
	Gotland Basin								



J	South Eastern	0	43	0	29	0	67	0	70
	Basin								
K	Gdansk Basin	0	43	0	30	2	226	2	63
L	Bornholm	0	32	0	30	0	80	2	63
	Basin								
M	Arkona Basin	0	63	0	17	0	610	0	209
Ν	Bay of	0	24	0	28	0	465	0	63
	Mecklenburg								
0	Kiel Bay	0	12	0	54	3	390	3	72

Code	Region name		Silicate (μn	nol/l)	
		Surface min	max	Bottom min	max
Α	Bothnian Bay	4	225	2	51
В	The Quark	0	230	"_"	"_"
С	Bothnian Sea	0	230	0	91
D	Åland Sea	0	92	0	62
Ε	Northern Baltic Sea Proper	0	140	0	113
F	Gulf of Finland	0	141	0	84
G	Gulf of Riga	0	30	0	51
Н	Western Gotland Basin	0	115	0	226
1	Eastern Gotland Basin	0	74	0	200
J	South Eastern Basin	0	115	0	120
K	Gdansk Basin	0	246	0	85
L	Bornholm Basin	0	220	0	115
М	Arkona Basin	0	300	0	80
N	Bay of Mecklenburg	0	195	0	101
0	Kiel Bay	0	180	0	155

Code	Region name		рН				Alkalinity (μmol/l)			
		Surface	max	Bottom	max	Surface	max	Bottom	max	
		min		min		min		min		
Α	Bothnian Bay	6.5	8.8	7.3	8.2	500	1100	600	1200	
В	The Quark	6	8.8	"_"	"_"	ND				
С	Bothnian Sea	6	9	6.7	8.4	800	1800	1000	1800	
D	Åland Sea	7.5	8.7	7.4	8.5	ND				
Ε	Northern	6.5	9.4	6.5	8.4	ND				
	Baltic Sea									
	Proper									
F	Gulf of Finland	6.2	9	6.8	8.7	700	1200	1200	1700	
G	Gulf of Riga	7.3	9.4	7.3	8.8	ND				



Н	Western	6.5	9.5	6.7	10	NED			
	Gotland Basin								
1	Eastern	6.8	9	6.5	8.3	1400	1700	1500	2100
	Gotland Basin								
J	South Eastern	6.5	9	6.7	9	NED			
	Basin								
K	Gdansk Basin	7.3	8.3	7.2	8.1	ND			
L	Bornholm	6.6	9	6.6	8.5	NED			
	Basin								
М	Arkona Basin	7	9.5	7	8.7	NED			
N	Bay of	7.2	10	7	8.3	ND			
	Mecklenburg								
0	Kiel Bay	5.6	9	6.9	8.3	ND			

NED=Not Enough Data; ND: No Data

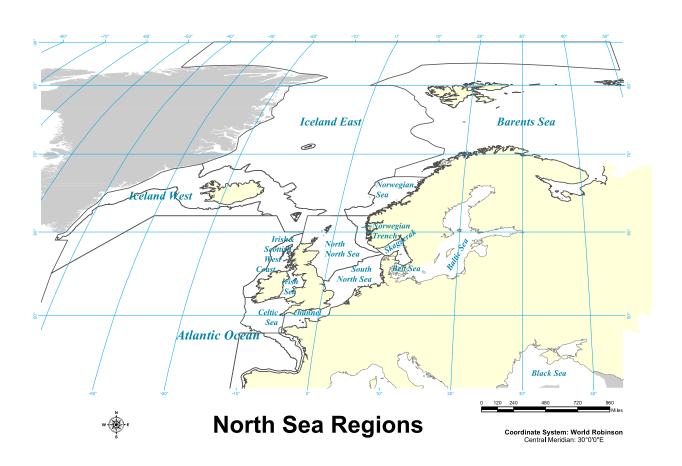


#### North Sea

The broad-range check values in the North Sea are defined on the basis of the available data. The Areas are checked in boxes shown in table 9, but mainly for the divisions used by OSPAR, e.g. North sea/Norwegian Trench. No data were available for Iceland West, and only the eastern part of Iceland East.

Top-bottom levels are set after typical depth profiles and chlorophyll profiles, and bottom depth is the deepest measurement in the areas. Nitrite, Alkalinity and pH was only available in Skaggerak and the Sound/Belt Sea.

Figure 5: Regional sub-domains defined in the North Sea for the broad range check





**Table 22:** Geographical limits of the North Sea regions for broad range scale definition and the corresponding maximum depth.

Code	Region name	Lat. Min	Lat.max	Long.	Long.	Max	Surface	Deep
				Min	max	depth	water	water
SBS	Sound-Belt Sea	54 50.00'	56 50.00'	9 30.00'	13 20.00'	65	0-5	5-65
Sk	Skaggerak	55 90.00'	60 00.00'	8 00.00'	13 00.00'	700	0-50	50-700
NT	Norwegian Trench	57 50.00°	62 00.00'	1 30.00'	8 00.00'	300	0-50	50-300
Ch	Channel	48 00.00'	51 30.00'	<i>-5 00.00′</i>	1 80.00'	110	0-20	20-110
NNS	North North Sea	54 00.00'	62 00.00′	-5 00.00°	8 50.00'	100	0-50	50-100
SNS	South North Sea	52 00.00'	<i>57 15.00′</i>	-0 85.00'	9 20.00'	50	0-10	10-50
CS	Celtic Sea	48 00.00'	52 17.00′	-11 50.00′	-1 00.00′	110	0-20	20-110
IS	Irish Sea	52 00.00'	56 00.00'	-8 00.00'	-2 50.00′	140	0-20	20-140
WC	Irish and Scottish	52 20.00'	60 00.00′	-12 00.00′	-5 00.00′	110	0-20	20-110
	West Coast							
IW	Iceland West	ND	ND	ND	ND	ND	ND	ND
ΙE	Iceland East	62 00.00'	73 26.00′	-5 00.00°	16 00.00'	3250	0-100	100-3000
NS	Norwegian Sea	62 00.00'	67 00.00′	5 00.00′	15 00.00'	900	0-100	100-800
BS	Barents Sea	67 00.00′	73 26.00′	7 70.00′	21 80.00′	1100	0-100	100-1100

ND=No Data

**Table 23:** Minimum and maximum control values in the surface and bottom layers for the North Sea regions as used for the broad-range check of hydrological core parameters

Code	Region name		Oxygen	(μmol/l)		Chlorophy	/II-a (μg/I)
		Surface		Bottom		Surface min	
		min	max	min	max		Max
SBS	Sound-Belt Sea	0	1000	0	925	0	700
Sk	Skaggerak	<0	725	<0	375	0	100
NT	Norwegian	45	425	130	335	0	13
	Trench						
Ch	Channel	220	320	210	325	0	80
NNS	North N. Sea	45	600	17	350	0	15
SNS	South N. Sea	40	850	110	750	0	300
CS	Celtic Sea	175	325	140	350	0	10
IS	Irish Sea	40	730	110	360\$	0	80
WC	I/S West Coast	210	335	180	420	0	30
ΙE	Iceland east	200	400	250	350	0	3,5
NS	Norwegian Sea	10	350	150	300	0	13
BS	Barents Sea	175	350	50	330	0	10



Code	Region name		Phosphat	te (µmol/l)		To	tal phosph	orus (μmol,	/I)
		Surface		Bottom		Surface		Bottom	
		min	max	min	max	min	Max	min	max
SBS	Sound-Belt Sea	0	110	0	50	0	160	0	85
Sk	Skaggerak	0	30	0	10	0	1100	0	5
NT	Norw. Trench	0	4	0.2	3	NED	NED	NED	NED
Ch	Channel	0	16	0	2	NED	NED	NED	NED
NNS	North N. Sea	0	4.5	0.15	3.2	0.06	4	0.4	1
SNS	South N. Sea	0	25	0	6.5	0	22	0	13
CS	Celtic Sea	0	0.7	0	1	NED	NED	NED	NED
IS	Irish Sea	0	6	0	2	NED	NED	NED	NED
WC	I/S West Coast	0	4	0	1	NED	NED	NED	NED
ΙE	Iceland east	0	90	0.2	60	NED	NED	NED	NED
NS	Norwegian Sea	0	14	0	2	NED	NED	NED	NED
BS	Barents Sea	0	4	0.1	1.5	ND	ND	ND	ND

NED=Not Enough Data; ND: No Data

Code	Region name		Nitrate	(μmol/l)		^	Nitrite+Nitrate (μmol/l)				
		Surface		Bottom		Surface		Bottom			
		min	max	min	max	min	Max	min	max		
SBS	Sound-Belt Sea	0	110	0	55	0	1250	0	250		
Sk	Skaggerak	0	95	0	23	0	310	0	20		
NT	Norw. Trench	0	23	0	23	ND	ND	ND	ND		
Ch	Channel	0	80	0	22	0	400	0	23		
NNS	North N. Sea	0	13	1.2	15	0.5	15	1.3	13		
SNS	South N. Sea	0	550	0	100	0	310	0	85		
CS	Celtic Sea	0	10	0	11	0	10	0.7	10		
IS	Irish Sea	0	220	0	23	0	220	0	25		
WC	I/S West Coast	0	85	1	11	0	125	1	11		
ΙE	Iceland east	0	15	0.05	22	ND	ND	ND	ND		
NS	Norwegian Sea	0	23	1.5	16	ND	ND	ND	ND		
BS	Barents Sea	0	15	2	20	ND	ND	ND	ND		

ND=No Data;



Code	Region name		Ammoni	a (μmol/l)		Total-Nitrogen (μmol/l)				
		Surface		Bottom		Surface		Bottom		
		min	max	min	max	min	Max	min	max	
SBS	Sound-Belt Sea	0	900	0	300	0	1650	0	500	
Sk	Skaggerak	0	100	0	20	0	350	0	100	
NT	Norw. Trench	ND	ND	ND	ND	NED	NED	NED	NED	
Ch	Channel	0	11	0	6	2	17	6	15	
NNS	North N. Sea	0	5	0	6	4	60	7,5	35	
SNS	South N. Sea	0	100	0	55	0	850	0	180	
CS	Celtic Sea	0	5.5	0	7	NED	NED	NED	NED	
IS	Irish Sea	0	85	0	7	NED	NED	NED	NED	
WC	I/S West Coast	0	15	0	5	NED	NED	NED	NED	
ΙE	Iceland east	ND	ND	ND	NED	NED	NED	NED	NED	
NS	Norwegian Sea	ND	ND	ND	NED	NED	NED	NED	NED	
BS	Barents Sea	ND	ND	ND	ND	ND	ND	ND	ND	

ND=No Data; NED= Not Enough Data

Code	Region name		Nitrite	(μmol/l)		Silicate (µmol/l)				
		Surface	Surface	Surface	Surface	Surface		Bottom		
		min	min	min	min	min	Max	min	max	
SBS	Sound-Belt Sea	0	5	0	13	0	400	0	185	
Sk	Skaggerak	0	3.5	0	4	0	250	0	200	
NT	Norw. Trench	0	2.5	0	1	0	50	0.6	26	
Ch	Channel	0	2	0	1.5	0	36	0	20	
NNS	North N. Sea	0		0		0	8	0.7	9	
SNS	South N. Sea	0	7	0	6	0	250	0	50	
CS	Celtic Sea	0	1.4	0	1.6	0	5.5	0	7.5	
IS	Irish Sea	0	5	0	1	0	175	0	12	
WC	I/S West Coast	0	1	0	0.5	2	8	2	7	
ΙE	Iceland east	0	0.7	0	0.9	0	15	0.6	11	
NS	Norwegian Sea	0	2	0	0.5	0	50	0.5	26	
BS	Barents Sea	0	2	0	0.3	0	22	1	15	

ND=No Data; NED= Not Enough Data



Code	Region name	рН				Alkalinity (μmol/l)			
		Surface		Bottom		Surface		Bottom	
		min	max	min	max	min	Max	min	max
SBS	Sound-Belt Sea	8.11	8.20	8.14	8.21	ND	ND	ND	ND
Sk	Skaggerak	7.81	8.37	7.71	8.26	1885	2015	2280	2400
NT	Norw. Trench	NED	NED	NED	NED	ND	ND	ND	ND
Ch	Channel	ND	ND	ND	ND	ND	ND	ND	ND
NNS	North N. Sea	ND	ND	ND	ND	ND	ND	ND	ND
SNS	South N. Sea	ND	ND	ND	ND	ND	ND	ND	ND
CS	Celtic Sea	ND	ND	ND	ND	ND	ND	ND	ND
IS	Irish Sea	ND	ND	ND	ND	ND	ND	ND	ND
WC	I/S West Coast	ND	ND	ND	ND	ND	ND	ND	ND
ΙE	Iceland east	ND	ND	ND	ND	ND	ND	ND	ND
NS	Norwegian Sea	ND	ND	ND	ND	ND	ND	ND	ND
BS	Barents Sea	ND	ND	ND	ND	ND	ND	ND	ND

ND=No Data; NED= Not Enough Data



### 2. Common rules for products generation

Data products as interpolated regional maps for specific parameters will be generated by regional coordinators using the Diva software.

Diva interpolated maps will be generated for combinations of time periods, seasons, vertical layers, and parameters. The following specifications have been adopted:

- Time period: 10-year periods with yearly step from 1960 to 2014 (so 46 periods of 10 year), by seasons
- Seasons: defined per region
- Vertical layers: defined per region
- Parameters: NO3, NOx, Total Nitrogen, PO4, Total Phosphorus, SiO4, NH4.

Seasons as adopted in the **Mediterranean and Atlantic**: winter (January to March), spring (April to June), summer (July to September) and autumn (October to December).

Seasons in the **Baltic, North and Black Seas**: winter=Dec-Feb, spring=March-May, summer=June-Aug, autumn=Sept-Nov.

Vertical layers: defined per region

IODE standard levels as adopted in the **Mediterranean and Atlantic**: 0 (which includes data from 0-4 m depth), 5, 10, 20, 30, 40, 50, 75, 100, 125, 150, 200, 250, 300, 400, 500, 600, 700, 800, 900, 1000, 1100, 1200, 1300, 1400, 1500, 1750, 2000, 2500, 3000, 3500, 4000, 4500, 5000. All depths include data acquired within a layer  $\pm 3$  m of the standard depth.

IODE standard levels as adopted in the **Black Sea**: 0, 5, 10, 20, 30, 40, 50, 75, 100, 125, 150, 200, 250, 300, 400, 500, 600, 700, 800, 900, 1000, 1100, 1200, 1300, 1400, 1500, 1750, 2000, 2500.

Vertical layer in the **Baltic Sea**: 0, 5, 10, 15, 20, 30, 40, 50, 60, 70, 80, 90, 100, 125, 150, 175, 200, 225, 250, 275, 300.

Note: Kattegat is considered to be both HELCOM and OSPAR region. So the layers are "sea specific layers", defined as 0, 5, 10, 15, 20, 25, 30, 40, 50, 60, 70, 80, 90, 100.

Skagerrak: 0, 5, 10, 15, 20, 30, 40, 50, 75, 100, 125, 150, 200, 300, 400, 500, 600.

Diva parameters/settings for the actual product generation are defined in the following chapter.



Masking for Diva maps to error field to 0.3 and 0.5.

The input for the Diva process will consist of the regional metadata enriched SeaDataNet aggregated data collection files. From those collection files only the data with QF=1, 2, 6 should be used in the further Diva analyses as basis for the interpolated maps. Data with other qualifier flags should be ignored.

The output should be, according to the general rule agreed within EMODnet Chemistry community, 1 NetCDF file per season per parameter (including all years and all depths).

**Note**: "White spaces" issue should be solved in Diva but for the time being the Regional Leaders are invited to use "underscore" instead of "white spaces" in file naming to avoid problems with Diva



#### 3. General guidelines for DIVA settings

While performing a Diva analysis, the following steps have to be followed.

- 1. <u>Domain definition and topography</u>: Domain definition and topography: should be ok (check resolution not too fine nor too coarse). Masking by definition of regions should be left until the very end if any. Eliminate lowlands right from the start.
- 2. <u>Output resolution</u>: Decades with yearly step, by seasons. Regional definition of vertical levels and seasons. See Chapter 2. The general rule agreed within EMODnet Chemistry community is to create 1 NetCDF file per season per parameter (including all years and all depths).
- 3. <u>Data sets</u>: use the regional metadata enriched SeaDataNet aggregated data collection files as resulting from the Odv QA/QC activities (see Chapter 1) as input. Make sure data outside of your region are eliminated (via option in driver). QF selection: make sure that SeaDataNet QF scheme is used (Diva is not aware of QF schemes, it only selects data from a list of QF to be accepted). Filter for data sets with qualifier flags 1, 2, 6. The Diva products should be based upon these, while data with other qualifier flags must be ignored.
- 4. <u>Background fields</u>: make sure it has correct vertical coherence. Use climatological average (all data for a given season, with large L, low SN and possibly detrending).
- 5. <u>Statistical parameter</u>: SN and L: optimize but take with a 'grain of salt' and provide reasonable bounds. VERTICAL coherence (via option -30 in driver).

**Note**: EMODnet Chemistry group agreed on the use of fixed L and SN for all DIVA runs (for a parameter in a specific area). The parameters should be obtained by estimation from a good subsample (e.g. decade with a good data coverage).

- 6. <u>Outliers</u>: use the function outlier elimination ONLY if you are very confident or if you see a few bullseyes in the analysis (too many bullseyes indicate a too high SN) in statistical parameters and quality of your products (final fine-tuning). In all cases check if reasonable amount of data are flagged "outliers".
- 7. <u>Error fields</u>: always mask the results where relative error field exceeds 0.3 and 0.5 using the same approach as in SeaDataNet and EMODnet Pilot (zero means analysis is expected to be perfect, 1 means the analysis has an expected error as large as your first guess, the reference field).
- 8. <u>Advanced features</u>: use advection if you have info (provide velocity fields) or if you really have currents that are coastal (use second parameter in driver to create pseudo along-coast velocities). Detrending: if trends in years are expected. Change of variables: expecially for concentrations: apply log or logit.

Note: Use of Diva de-trending only for the calculation of reference field, not for the analysis



#### 9. Checking:

- Work on 4D netCDF file (the one which will be published and includes already masked fields).
- Check vertical coherence via vertical sections in the netCDF file
- Check presence of bullseye or other artifacts (too high SN or too small L, suspect data)
- Verify data coverage field to make sure you did not "loose" some data
- Look at Output/3Danalysis/Variablename.Metainfo.txt

Example of Diva settings: finetuning when more or less satisfied:

Data extraction: 0 = do nothing

boundary lines and coastlines generation: 0 = nothing cleaning data on mesh: 4 = 1 + outliers elimination

minimal number of data in a layer: 0

Parameters estimation and vertical filtering: -30 Minimal L (larger than output grid spacing): 0.25

Maximal L (domain length): 10

Minimal SN: 0.1 Maximal SN: 3

Analysis and reference field: 1

Note: SN= Signal to Noise ratio; L= correlation Length

Users should adapt the following lines for the NCDFinfo file. Note that the quote character should be a standard ASCII single quote (character number 39). Some UTF-8 characters look very similar but they cause problems during the creating of the NetCDF file.

- Title string for 3D NetCDF file: 'Diva 4D analysis'
- Reference time for data (ie: days since since 1900-01-01), if not climatological data: 'days since xxxx-01-01'
- Time value (that represents the data set), if not climatological data: 1200
- Cell methods string: 'time: mean within years time: mean over years'
- Institution name: where the dataset was produced: 'Hellenic Centre for Marine Research-Hellenic National Oceanographic Data Centre (HCMR-HNODC)'
- Production group and e-mail: 'Diva group. E-mails: a.barth@ulg.ac.be; swatelet@ulg.ac.be'
- Source (observation, radiosonde, database, model-generated data,...): 'observational data from SeaDataNet/EMODNet Chemistry Data Network'
- Comment, please adapt the season and month: 'Every year of the time dimension corresponds to a 10-year centred average for the winter season (December-March)'
- Author e-mail address (or contact person to report problems): 'Athanasia (Sissy) Iona <sissy@hnodc.hcmr.gr>'



# 4. Instructions for naming, metadata and upload of DIVA products

#### **Upload the DIVA analysis**

For analysis at seasonal scale, there should be 4 DIVA files. Every DIVA file includes the different years as a NetCDF time dimension.

Before uploading a file, please:

- check visually the interpolated field (using for instance software as described here: http://modb.oce.ulg.ac.be/mediawiki/index.php/NetCDF\_format#Visualization\_of\_NetCDF\_files), and
- verify the required NetCDF attributes (in particular long\_name, unit, title, institution) are present and accurate. NetCDF attributes can be edited by using programs like matlab, octave, nco, ...

To upload a new file, you need the program sftp (not regular ftp). sftp is default on Linux. On Windows you will need a program like WinSCP, putty or FileZilla.

The user name is seadatanet, for the password ask us (a.barth@ulg.ac.be or swatelet@doct.ulg.ac.be).

The files should go into the following directory structure:

emodnet/<name of your domain>/<season name> (<start month>-<end month> - 10-years running averages)

For example:

emodnet/Baltic Sea/Winter (December-February) - 10-years running averages

You need to create the directories (unless they exist already).

The files with the DIVA analyses should not be renamed. The filenames should be kept as they are generated by DIVA.

The names of the domains currently used are:

- Baltic Sea
- Black Sea
- Mediterranean Sea
- North Sea

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For consistency, use for instance 'Black Sea' instead of 'BlackSea'.

Once the file are uploaded, the viewer is not updated automatically. Please sent us an email so that we can update the viewing service.

Before uploading the files, the XML files should be generated by divadoxml-gui.py (see below). The programme divadoxml-gui.py adds NetCDF attributes (like product\_id) to the DIVA NetCDF files which are necessary for the integration of OceanBrowser and Sextant.

#### How to complete DIVA XML Metadata for Sextant

**For every NetCDF file**, there should be **one generated XML file with additional metadata** for the Sextant catalogue. This XML file is generated by the divadoxml tool which requires the following information:

- Project: EMODNET Chemistry
- Title (default title is extracted from the NetCDF file)
- Date of first version: date of version 1.0
- Date of update: date of current revision
- Version: version number starting from 1.0 (first number: major updates, second number: minor updates)
- Abstract: Wikipedia-like syntax may be used for bold, italic underlined, bullets and hyperlinks. This should include:
- a brief description of the DIVA analysis
- which data was used
- special settings of DIVA (e.g. advection constraint, detrending,...)
- EDMO: the EDMO code number of your institution
- P35 code: the aggregated parameter code from

http://vocab.nerc.ac.uk/collection/P35/current/

- Path on OceanBrowser: the path where you will upload the analysis on the machine gher-diva (essentially the domain and possibly subdomain; see the folder structure on http://oceanbrowser.net/emodnet/). For the EMODNET DIVA products it should have the structure (as during the uploading step above, but without the leading emodnet/): <name of your domain>/<season name> (<start month>-<end month> 10-years running averages) for example: Baltic/Winter (December-February) 10-years running averages
- P02 keyword: discovery parameter from the list http://vocab.nerc.ac.uk/collection/P02/current/
- Area keywords: area keyword from the list http://vocab.nerc.ac.uk/collection/C19/current/

Note: Regional Leaders should use the last version of divadoxml, available on Gher wiki.



XML description generated by divadoxml should be submitted to Sextant following the instructions here: http://www.ifremer.fr/isi/sextant/emodnet-chemistry/EMODNET-CHEMISTRY-QUICKSTART-1.0.pdf. If you have any question about submitting the XML file, you can contact Ifremer at sextant@ifremer.fr.

#### How to upload the DIVA NetCDF to ULg

More information is available here:

http://modb.oce.ulg.ac.be/mediawiki/index.php/OceanBrowser Import Data

The source code of divadoxml.py is available at:

http://modb.oce.ulg.ac.be/mediawiki/upload/Alex/divadoxml-gui/?C=M;O=D

The INSTALL files contains the installation instructions are how to run this programme.



### 5. Metadata requested to assign DOIs to Emodnet Chemistry products

The general rule agreed within EMODnet Chemistry community is to create 1 NetCDF file per season per parameter (including all years and all depths). The same ratio should be followed for DOI assignment.

In the following list there are the **metadata** to assign DOIs to Emodnet Chemistry products:

- Creators:
  - o Creator (a permanent identifier for scientists as the ORCID could be used)
- Titles:
  - o Title:
- Publisher:
- PublicationYear:
- Subjects:
  - Subject: (can be multiple and P08 Disciplines vocabulary terms could be used like in R2R ODIP project case)
- Contributors:
  - o Contributor (a permanent identifier for scientists as the ORCID could be used)
- Dates: from.... to....
- Language:
- ResourceType:
- relatedIdentifier:
  - o relatedIdentifier (if needed one or more links to external sources can be added)
- Sizes:
- Formats:
- rightsList:
  - o rights:
- Descriptions:
- GeoLocations:
  - o geoLocationBox:
  - o geoLocationPlace:

The last DOI metadata kernel/schema V3.1 updated at October 2014 can be found at the following link:

http://schema.datacite.org/meta/kernel-3/example/datacite-example-full-v3.1.xml

Please find below an example that we filled with the help of Sissy a few months ago:



Creators: HCMR, Sissy IONA

Titles: Decadal Summer distribution of Nitrate at Adriatic Sea

Publisher: Emodnet Chemistry Project

PublicationYear: 2014 Subjects: Oceanography

Dates: decades from 19701979 to 20052014, observational data span from 1972-2012

Language: en

**ResourceType**: DIVA interpolated maps

Size: 60 Mb

**Formats**: NetCDF file (application/X-netcdf), zip file (application/zip)

**Descriptions**: Geostatistical data analysis by DIVA (Data-Interpolating Variational Analysis) tool. Moving 10 years windows were applied at nitrate data at each level and each month in order to calculate the decadal summer variability. As summer, months from July to Septembers are considered. Diva analysis is done at standards vertical levels of 0, 10, 20, 30, 50. 75 and 100 meters obtained by a weighted parabolic interpolation (Reiniger & Ross, 1968). A climatic seasonal field obtained by a semi-normed analysis was used as reference field taking data from all available years. Detrending was applied to the reference field to remove uneven spatial distributions in time.

#### **GeoLocations**:

geoLocationBox:Adriatic Sea geoLocationPlace:39.75 12 46 20



## 6. Guidelines to turn a set of SDN repeated stations into time series

**Note**: For EMODnet Chemistry data collections, it was convened not to create Generated Time series aggregated datasets from profiles because the viewing services developed by Gher and Deltares (WFS, WPS) are showing colored maps with the distribution of station and **density of measurements** for a given time and depth. Also, the service allows the user to create "on the fly" a profile plot or a time series plot. Therefore, the Regional Leaders provides only the two kind of aggregated datasets generated using ODV, namely ODV Profiles and ODV Time Series. Both sets of data should be used for Diva maps generation (see Sissy suggestions).

It is important to understand that the aggregated data must be provided in "ODV spreadsheet file" (e.g. txt ascii file) format and <u>not</u> in the "ODV collection" format.

The ODV spreadsheet files (e.g. txt files) must include the aggregated P35 variables.

The ODV spreadsheet files (e.g. txt files) will be either profiles or time series.

In case of time series, these txt files will be prepared in two ways:

- 1) ODV will create time series automatically
- 2) the regional leaders have to identify time series and construct them by following the instructions described below.

In case 1) the procedure is (this was also described in the QC report for the Mediterranean, with some small differences due to the fact that the aggregations were not provided then by ODV):

a) open ODV v4.6.3.3 (in windows only) and import the robot harvested data set with the metadata file data.csv: ODV then will create enriched collection based on the primary variable (pressure or depth profiles, and time series).

Exit ODV4.6.3.3

- b) In ODV 4.6.5 (windows or linux) or later versions, I open the above time series collection and immediately, without doing anything else, I export as aggregated SDN aggregated ODV collection (Export>Station data> SDN aggregated ODV collection)
- c) In ODV 4.6.5 or later versions, import SDN aggregated ODV collections of previous step, perform your QC, etc. When QC is complete, export your data as ODV spreadsheet files (e.g. txt files). These are the files we have to send to MARIS (and in DIVA analysis). The export can be either in one txt file that include all P35 variables in your area or separate txt files.

It is suggested to export in one unique file, unless MARIS prefers differently.

Note that the implementation of step c, depends on the content of robot harvested data in each area. For example, in the Mediterranean the exported SDN ODV collections include different P35 variables. HCMR creates one unique template collection, where the results of b are imported).

NOTE: steps a, b, c are common for vertical profiles also and not only for time series.



The steps 1 a, b, c, are the trivial work.

But, inside the harvested robot data sets, the regional leaders can identify more time series sets. These data have been documented as profiles in the CDIs, they concern mainly monitoring activities because they are repeated observations in fixed position. So, the regional leaders can follow the instructions for procedure 2) and construct additional time series and improve the time series products that are required by the MSFD.

In the case of the 2) procedure, in the following scheme we provide instructions on how to turn a set of SDN repeat stations into time series, one for every observed depth.

- 1. Use Import>SDN Formats and select all repeated stations\* and the corresponding metadata file (data.csv) to import the data and the metadata into the special version ODV v4.6.3.3
- 2. Define derived variable Time (station date&time).
- 3. Use Export>Station Data>ODV Spreadsheet File to export all stations into an ODV spreadsheet file. During export select all variables needed in the time series, including Time (station date&time). On the Spreadsheet File Properties dialog uncheck the Export history box, uncheck the Use compact output format, under Data filter choose Apply sample range and quality filters, then press OK. On the Sample Selection Criteria dialog click on Range, choose variable Depth and for the Acceptable Range enter in both fields the depth value for which the time series is desired (e.g., 30 for depth=30m).
- 4. Open the exported file in a text editor (or Excel) and make the following changes:
  - in the second and all following data lines remove the cruise and station labels, the date values in the yyyy-mm-ddThh:mm:ss.sss column. Do not remove the TABs between those columns. These changes are necessary so that ODV does not break the input into separate stations when labels, date change.
  - At the //<MetaVariable> block delete the lines starting with:

```
//<MetaVariable>label="LOCAL_CDI_ID" and 
//<MetaVariable>label="EDMO_code" and 
//<MetaVariable>label="CDI-record id"
```

 At the end of the //<DataVariable> block insert the following three lines: //<DataVariable>label="\_LOCAL\_CDI\_ID" value\_type="INDEXED\_TEXT" qf\_schema="SEADATANET" significant\_digits="0" comment=""</DataVariable> and

//<DataVariable>label="\_EDMO\_code" value\_type="INTEGER" qf\_schema="SEADATANET" significant\_digits="0" comment=""</DataVariable> and

//<DataVariable>label="\_CDI-record id" value\_type="INTEGER" qf\_schema="SEADATANET" significant digits="0" comment=""</DataVariable>

- rename the LOCAL\_CDI\_ID and EDMO\_code and CDI-record id entries in the column label line by prepending a "\_" character
- At the //<DataVariable> block, and at the line starting with: //<DataVariable>label="Depth [m]", rename is\_primary\_variable="T" to: is\_primary\_variable="F"



- At the //<DataVariable> block, and at the line starting with //<DataVariable>label="Time (station date&time) [years since 0000-01-01]", rename is\_primary\_variable="F" to:
   is primary variable="T
- change line 9 to: //<DataType>TimeSeries</DataType>.
- 5. If you use Excel to make the changes of step 4 and save the file as txt (Tab delimited) file, it might happen that Excel puts: a) quotes(") at the beginning, end of all Meta and Data Variables blocks lines and b) Tabs at the end of all comments rows. So, you have to remove manually a) and b) characters in order ODV to import the data correctly
- 6. Import the modified file by dropping onto ODV v4.6.4 or later versions. Press F9, then Enter to produce time-series plots.

Instead of making the depth selection in step 3, you can also export all depths and make the depth selection in step 6, thus avoiding repetition of 3-6 for all individual depths.

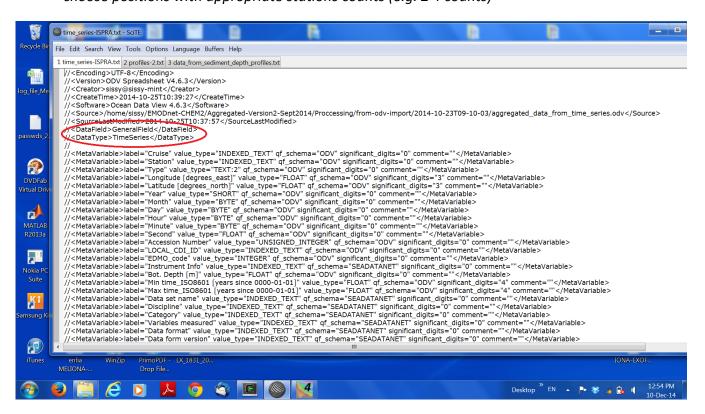
\*How to identify repeated stations:

#### Either

you already know in your data set which repeated stations are conducted within the framework
of a monitoring activity,

or

 using ODV data bins plots (right click on map, then Extras>Statistics>X/Y distribution) and choose positions with appropriate stations counts (e.g. ≥ 4 counts)





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