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EMODnet Chemistry data Quality Control approach

Marina Lipizer - OGS

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EMODnet Chemistry data Quality Control approach

EMODnet Chemistry manages data related to:

- Eutrophication (nutrients such as nitrate, nitrite,ammonium, phosphate; chlorophyll, dissolved oxygen, and also silicate)
- Ocean acidity (pH, alkalinity, DIC,…)
- Contaminants (metals, hydrocarbons, pesticides,…)
- Marine litter (beach litter, seafloor litter, microlitter)

Measured in seawater, sediment, biota

Large number of substances, high heterogeneity

Standardized data management, **complete** metadata and data **Quality Control** are fundamental to guarantee data comparability.

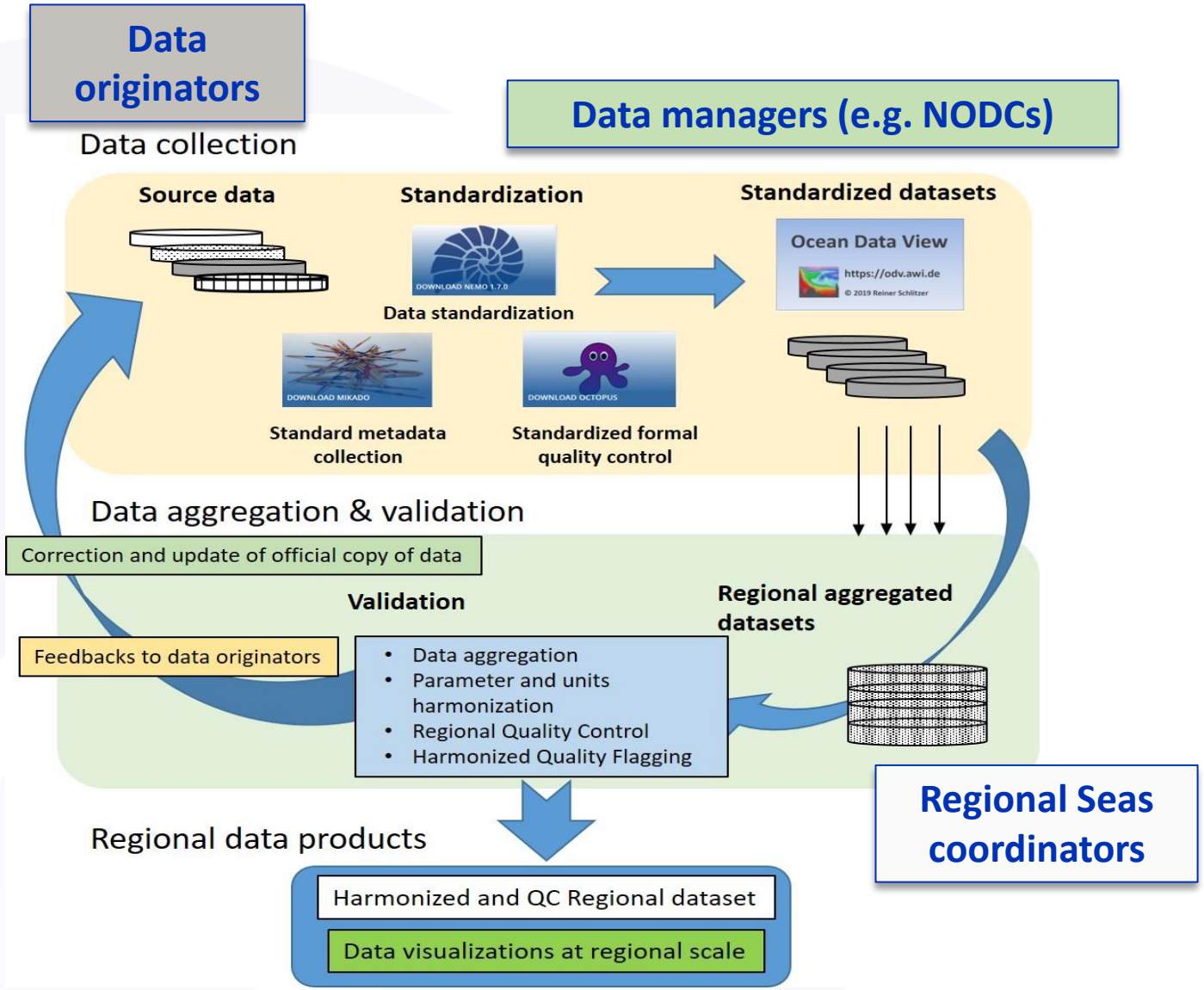
EMODnet Chemistry data Quality Control approach

- EMODnet Chemistry relies on **standards** (vocabularies, metadata and data formats, data QC procedures, data QC flagging scales,…), **tools** (softwares – Ocean Data View) and **services** (metadata access interface, data transfer protocols) implemented within **SeaDataNet**, the Pan European Infrastructure for Ocean & Marine Data Management (https://www.seadatanet.org/)
- Data validation follows a:

"Quality Control loop" involving data **originators**, data **managers** and **regional sea coordinators**

The results of the Quality Control Loop are: Regional Sea standardized, aggregated, harmonized, validated, datasets

- **Standardized:** common metadata, data dictionaries, data formats
- **Aggregated:** parameters related to the same chemical substance are "aggregated" using dedicated tools (based on ODV Software)
- **Harmonized:** conversion to standard units, based on major EU directives and agreed within the EMODnet Chemistry scientific community
- **Validated:** based on commonly agreed data Quality Control protocols



EMODnet Chemistry data Quality Control approach

Data originators

- **Quality Assurance information from data originators:** large efforts to collect updated, detailed and harmonized methodological and QA information from all data providers. Information available with the metadata (documents with **doi**)

Questionnaire regarding QA/QC procedures for seawater, biota, and sediment samples

A fundamental requirement of collaborative monitoring programmes on marine pollution is the inter-comparability of data obtained from participating laboratories irrespective of the country of origin. The production of 'true' data requires that all partners adopt good field and laboratory procedures to assure quality assurance/quality control (QA/QC) of data input to the EMODnet Chemistry portal. To achieve this, this new questionnaire regarding **ISO/IEC 17025:2017** has been provided to all partners and subcontractors to obtain more comprehensive information than in the previous questionnaire (ca. 2014) in order to uniform the quality and reliability of chemical data introduced into EMODnet Chemistry.

Partner or subcontractor (click on the cell and then hover over the right hand side to select from the dropdown list):
Full name: #N/D
EDMO number: #N/D
Country: #N/D
Date of compilation:

Please answer the following questions regarding the laboratory/laboratories that chemical data provided to EMODnet Chemistry originate from:

	Yes/no etc. (select from drop-down list)	Expand/other comments:
Are laboratory activities performed by properly qualified people?		
Is the laboratory accredited (ISO 17025)? If more than one laboartory is used, provide details on their individual accrediation in the comments.		
Are equipment properly maintained and calibrated prior to analysis?		
Is there a set of methods specified as acceptable for use in the laboratory?		
Are certified reference materials used?		
Are the accuracy, precision, and limit of detection/quantification of the methods determined?		
Are quality control samples run routinely and the results evaluated before data are released?		
Are control charts recorded to test bias and reproducibility?		
Are data controlled by a competent authority (apart from accreditation bodies)?		

Please complete the worksheets labelled 'Seawater', ' Biota', and 'Sediment' by providing comprehensive information for each chemical determinand measured as part of your marine monitoring, or that of the data originator if your institute is a data holding centre. In some cases, drop-down lists are available. For columns shaded in blue, green, or yelllow, the information is obligatory. For columns shaded in grey, do not insert any information. For unshaded columns, information is requested but not mandatory. If required, there is a column for additional notes at the end of each row.

Data managers (e.g. NODCs)

- **Use of SDN standards and tools**

SeaDataNet

National Oceanography Centre
British Oceanographic Data Centre BODC

NERC Vocabulary Server

Ocean Data View
https://odv.awi.de
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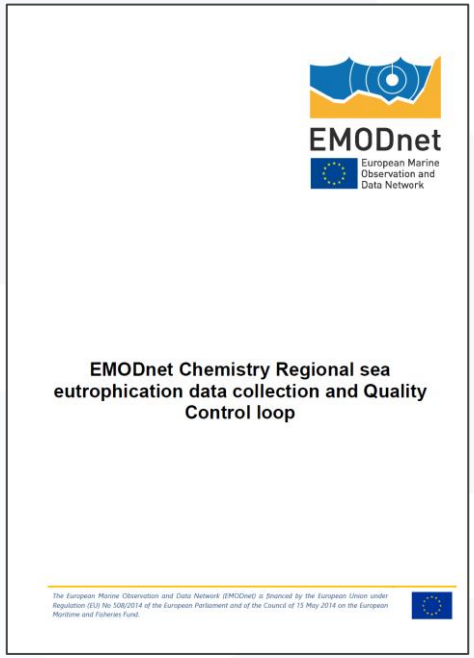
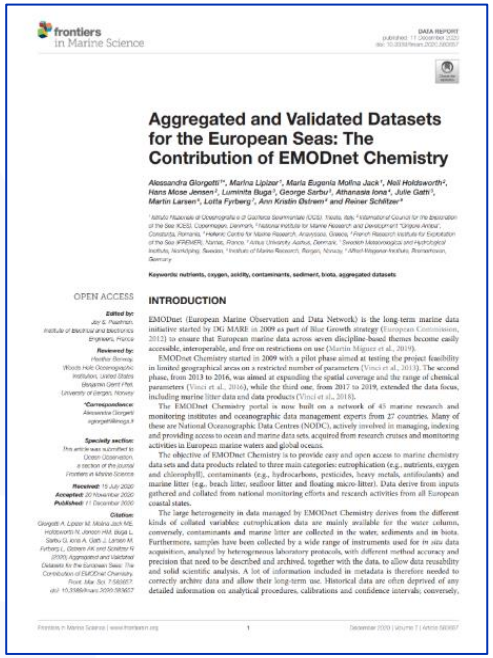
Regional Seas coordinators

- **Quality Control procedures:** QC steps carried out on all regional sea data collection of eutrophication (next page)





*Giorgetti A, Lipizer M, Molina Jack ME, Holdsworth N, Jensen HM, Buga L, Sarbu G, Iona A, Gatti J, Larsen M, Fyrberg L, Østrem AK and Schlitzer R (**2020**) Aggregated and Validated Datasets for the European Seas: The Contribution of EMODnet Chemistry. Front. Mar. Sci. 7:583657. doi: 10.3389/fmars.2020.583657*

EMODnet Chemistry data Quality Control approach

Regional dataset Quality Control procedures:

Regional sea data collection preparation:

- Import original ODV text files in ODV, and preparation of separate collections according to the primary variable (e.g.: time, depth, pressure): one for time series, other for profiles (if needed: one collection for ocean depth profiles and one for ocean pressure profiles);
- Correct format errors;
- **Run the P35 aggregation using the Best-Of ODV algorithm;**
- Merge the ocean pressure and the ocean depth collections into one depth profiles collection using Depth/Pressure conversion;

P35: SDN vocabulary (https://vocab.nerc.ac.uk/collection/P35/current/) used to aggregate variables described by P01 vocabulary which refer to the same chemical substance (e.g. Concentration of nitrate {NO3- CAS 14797-55-8}), measured with different methods or instruments or expressed with different units. The aggregated variable (e.g. Water body nitrate) is expressed with **harmonised units**, after proper conversion. Concentrations expressed "per unit mass" have been converted to "unit volume" using a constant density of: 1.025 kg/l.

Consider that:

Eutrophication is decribed by many substances: nitrite, nitrate, nitrite+nitrate, ammonium, DIN (nitrite+nitrate+ammonium), phosphate, total nitrogen, total phosphorus,…

EMODnet relies on BODC vocabulary P01 which codes the measurement substance **but also** keeps sampling and/or analytical information connected:

> e.g. Concentration of nitrate {NO3- CAS 14797-55-8} per unit volume of the water body [dissolved plus reactive particulate <GF/F phase] by filtration and colorimetric autoanalysis and correction for nitrite)

This implies that Nitrate is coded with different P01!

EMODnet Chemistry data Quality Control approach

Aggregation with a dedicate vocabulary (P35) is carried out to combain data related to the same substance, adopting conversion factors when needed*

P35 - Water body nitrate (standard unit: umol/l)

P01

Concentration of nitrate {NO3- CAS 14797-55-8} per unit volume of the water body [dissolved plus reactive particulate phase] by colorimetric autoanalysis and correction for nitrite

Concentration of nitrate {NO3- CAS 14797-55-8} **per unit mass of the water body** [unknown phase]

Concentration of nitrate {NO3- CAS 14797-55-8} per unit volume of the water body [dissolved plus reactive particulate <unknown phase] by filtration and ion chromatography

Concentration of nitrate {NO3- CAS 14797-55-8} per unit volume of the water body [dissolved plus reactive particulate <0.4/0.45um phase] by filtration and colorimetric autoanalysis and correction for nitrite

Concentration of nitrate {NO3- CAS 14797-55-8} per unit volume of the water body [dissolved plus reactive particulate <GF/F phase] by filtration and colorimetric autoanalysis and correction for nitrite

Concentration of nitrate {NO3- CAS 14797-55-8} per unit volume of the water body [dissolved plus reactive particulate <unknown phase] by filtration and manual colorimetric analysis and correction for nitrite

Concentration of nitrate {NO3- CAS 14797-55-8} per unit volume of the water body [dissolved plus reactive particulate phase]

Concentration of nitrate {NO3- CAS 14797-55-8} per **unit volume of the water body** [unknown phase]

….

*Concentrations expressed “per unit mass” have been converted to “unit volume” using a constant density of: 1.025 kg/l.

EMODnet Chemistry data Quality Control approach

Quality Control loop:

- **Use of common data Quality Flagging scale** (erroneous data **NOT** eliminated but flagged according to common rules)

Code	Description
0	no quality control
1	good value
2	probably good value
3	probably bad value
4	bad value
5	changed value
6	value below detection
7	value in excess
8	interpolated value
9	missing value
A	value phenomenon uncertain
B	nominal value
Q	value below limit of quantification

This is important as QF can be modified by scientists, if needed, and even «Bad data» mayn provide useful information.

EMODnet Chemistry data Quality Control approach

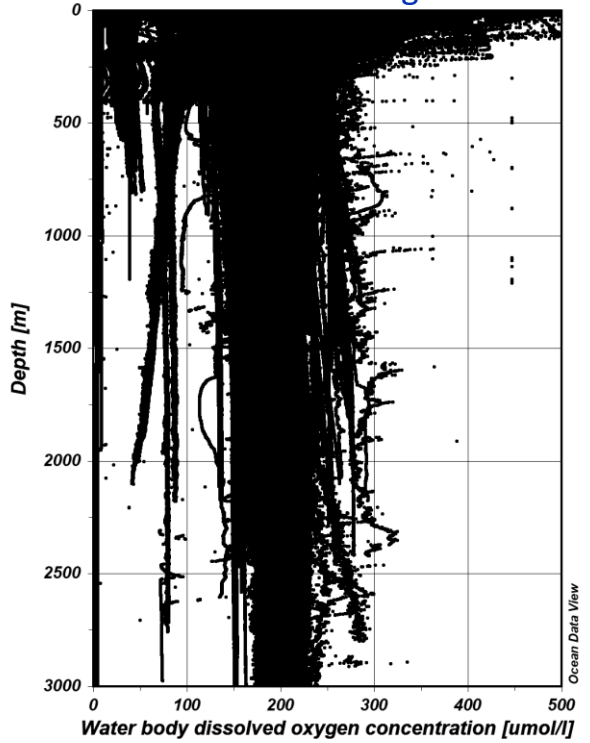
Quality Control loop:

Semi – automatic checks:

- Negative values → QF=4 (**Exceptions according to expert knowledge**: negative temperatures in the northern seas; dissolved oxygen in the Baltic flagged with QF=6, if not obviously wrong);
- For default values used for **missing** data, such as 9999 or 999.999, → QF=9;
- Stuck data (constant profile/constant values) → QF=4;
- Values equal to 0 → QF=6 (Exceptions according to expert knowledge: cases where 0 values are obviously wrong → QF=4);
- Spikes detection → QF=3 or QF=4;
- Regional “broad range” check: data are compared with expected ranges encountered in a particular region; however, concentration ranges have been proposed mostly for open sea areas and do not account for large variability in coastal areas;

Example: Mediterranean Sea

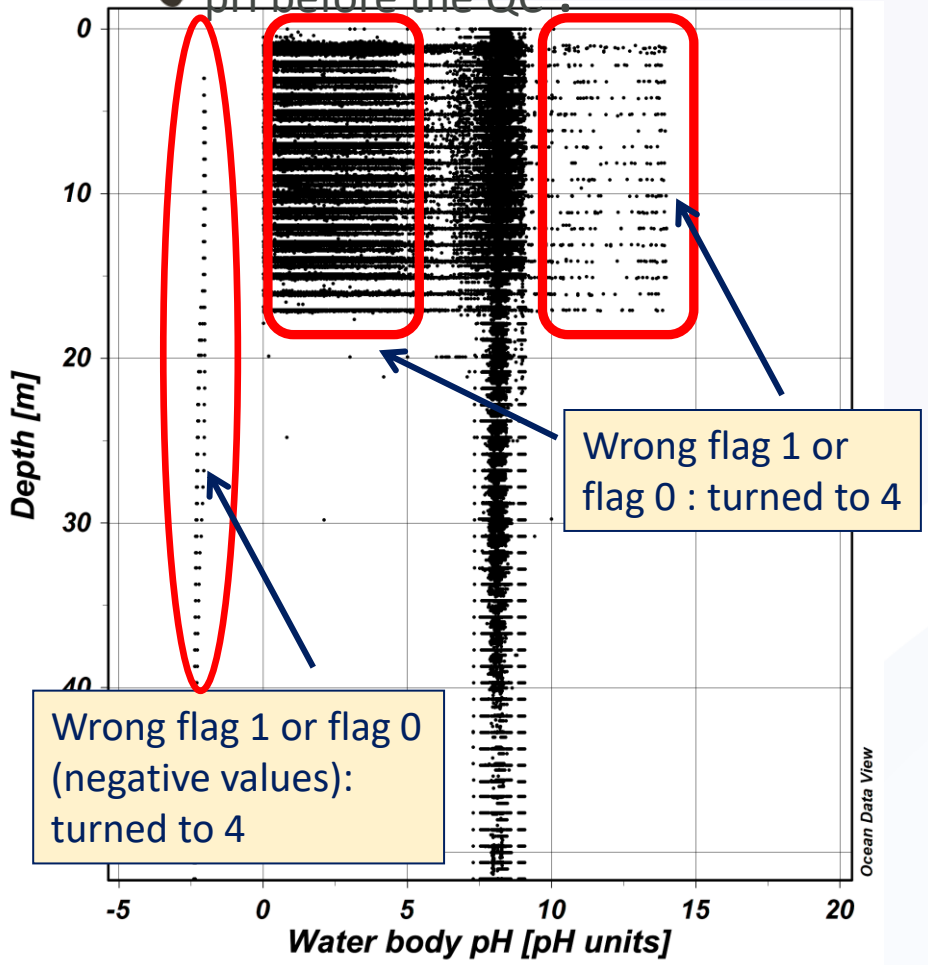
Stuck data
Values = 0
Outside broad ranges



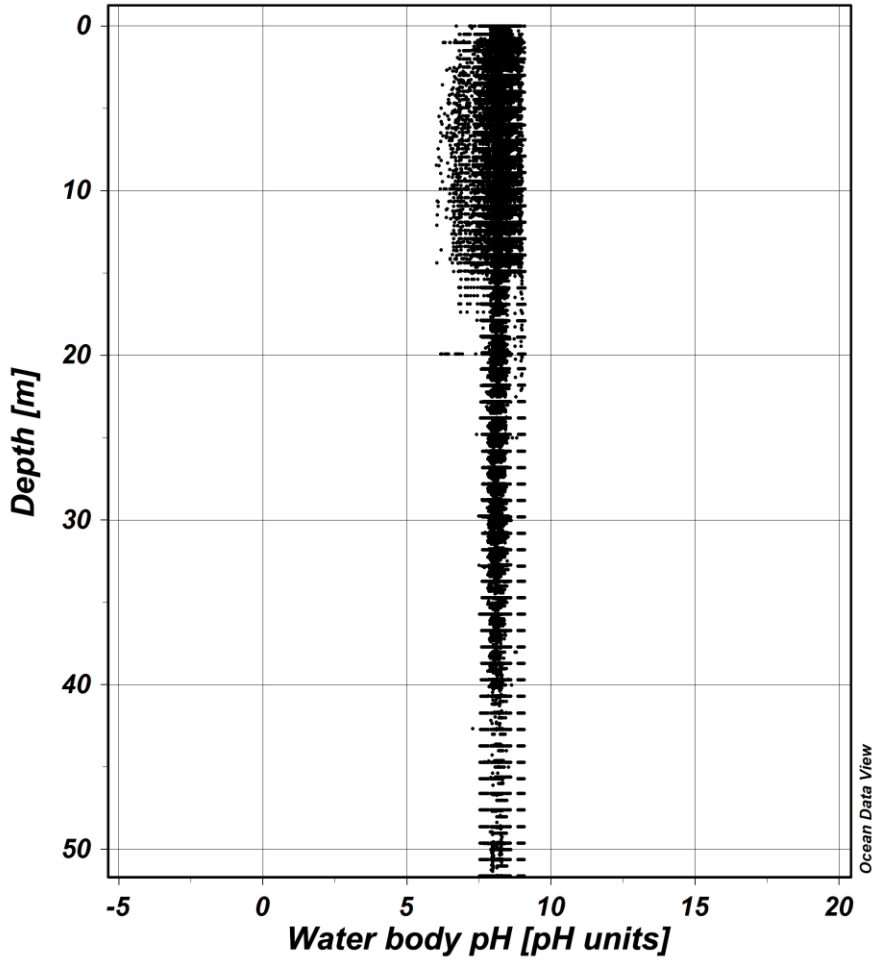
QC pH - not flagged/flagged

MEDITERRANEAN

- pH before the QC :

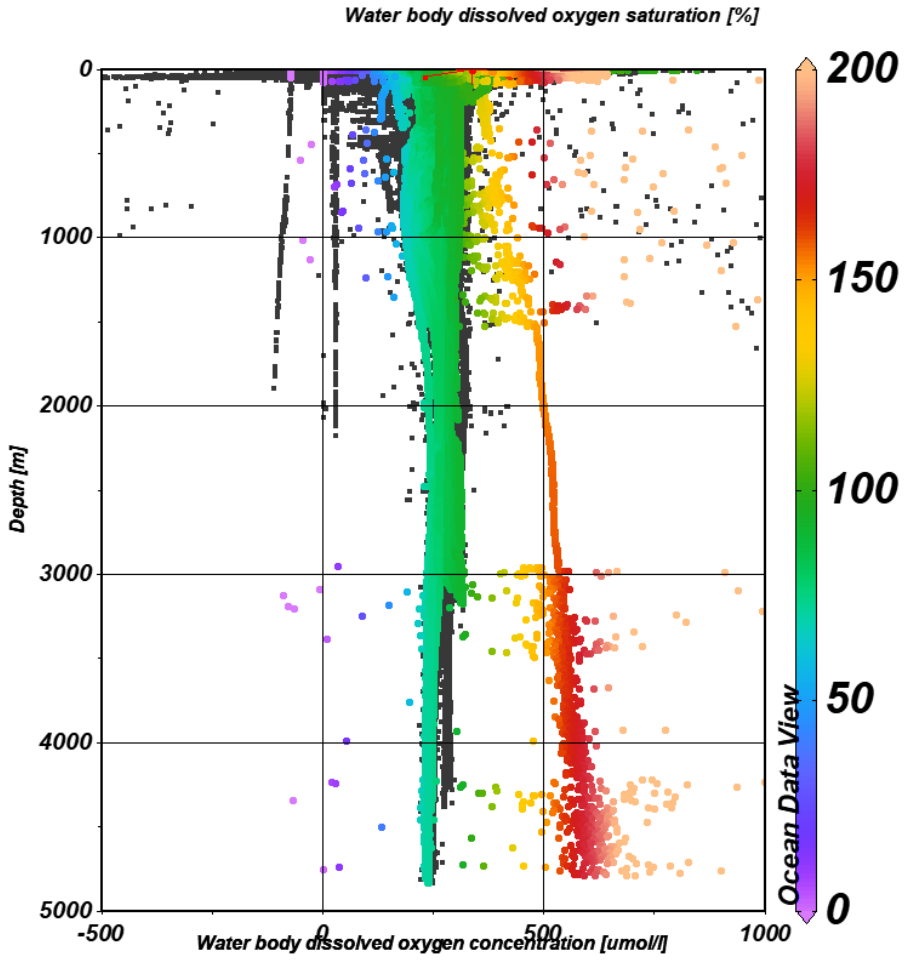


pH after the QC :



EMODnet Chemistry data Quality Control examples

Dissolved oxygen and %saturation (coloured data) in the North Sea and North Atlantic



- < 0 values can be wrong data (QF=4)

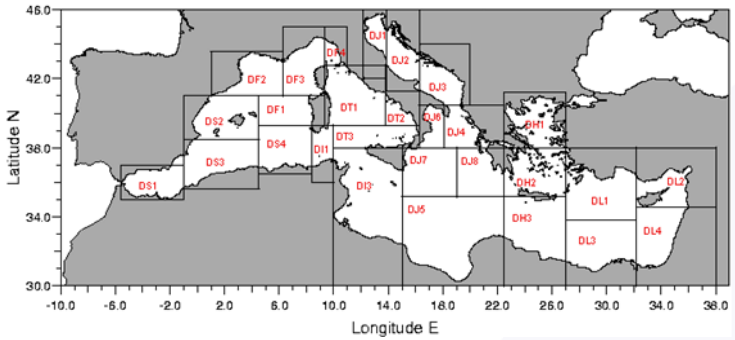
BUT: in some particular areas data can be good:

- < 0 values indicate hydrogen sulfide concentration in the water column
- zero concentration (anoxic conditions)
- < 50 % saturation (hypoxic conditions? wrong oxygen units?)
- > 150% in deep waters: wrong data (QF=4)

Need of expertiese on the specific parameters and on the specific areas, automatic check is not sufficient (and reliable!)

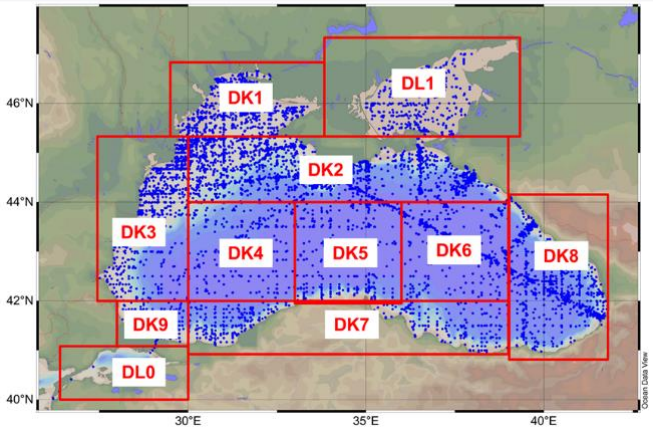
EMODnet Chemistry data Quality Control approach

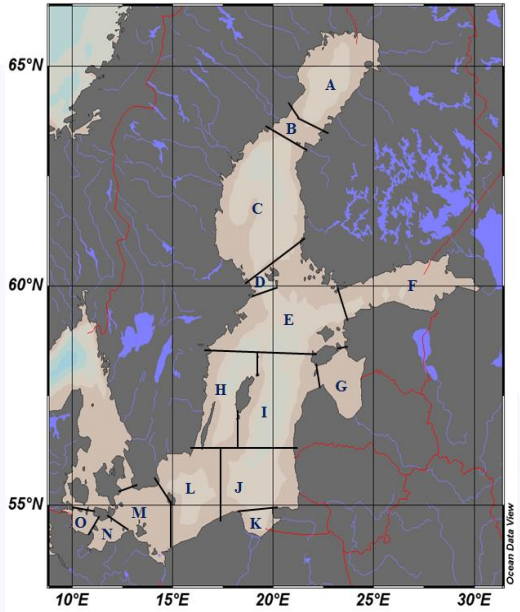
Broad ranges*



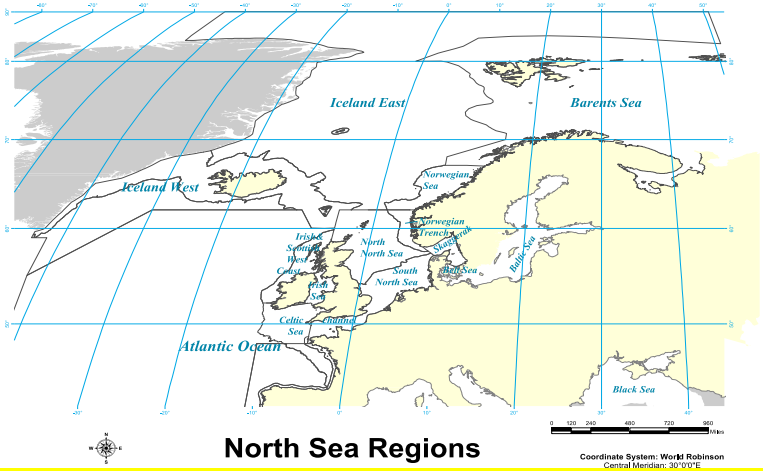
Code-Region Name	Oxygen (ml/l)				Nitrate (µmol/l)			
	0 - 200 m		201 m - bottom		0 - 200 m		201 m - bottom	
DJ1 - Adriatic North	3.0	10.0	/	/	.0	16.0	/	/
DJ2 - Adriatic Middle	3.0	9.0	2.0	9.0	.0	9.0	.0	9.0
DJ3 - Adriatic South	3.0	9.0	3.0	8.0	.0	9.0	.0	9.0
DJ4 - Ionian NE	3.0	8.0	3.0	6.0	.0	9.0	.0	9.0
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

MEDAR/MEDATLAS Sub-domains for Black Sea





Code	Region name	Nitrite (µmol/l)				Silicate (µmol/l)			
		Surface min	Surface min	Surface min	Surface min	Surface min	Max	Bottom 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
IE	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



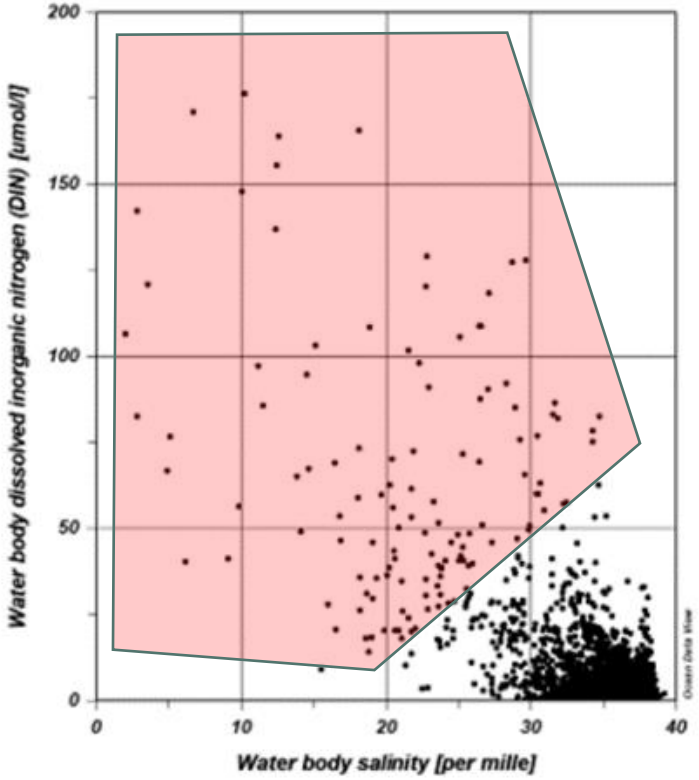
North Sea Regions

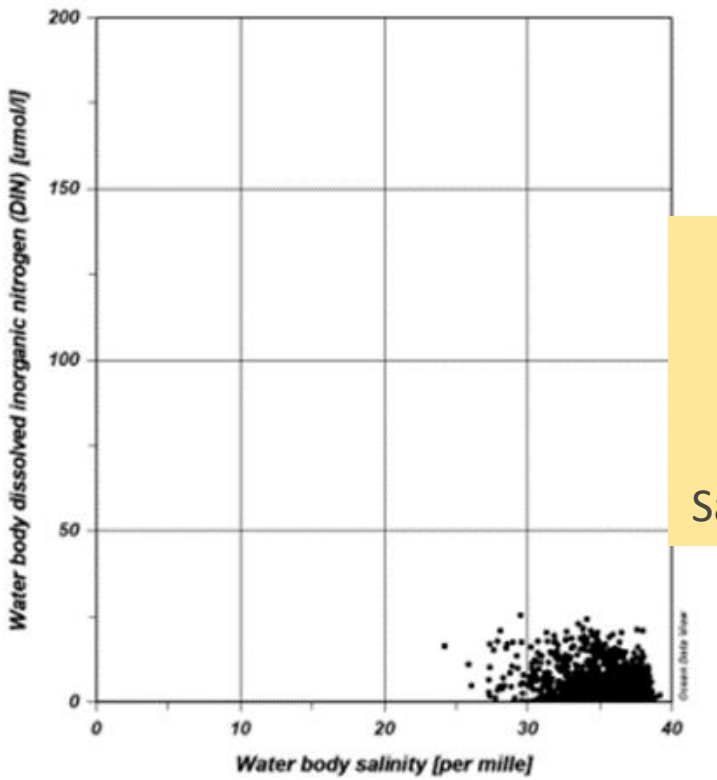
*possible exceptions in coastal areas upon data originator indications or expert judgement

*Ongoing work on updating open water ranges and on defining **coastal** ranges*

EMODnet Chemistry data Quality Control approach

Consequence of using open waters “broad ranges” to validate eutrophication data in coastal areas:





DIN well outside broad ranges

But also:

Salinity well outside broad ranges!

Very careful QC is required!

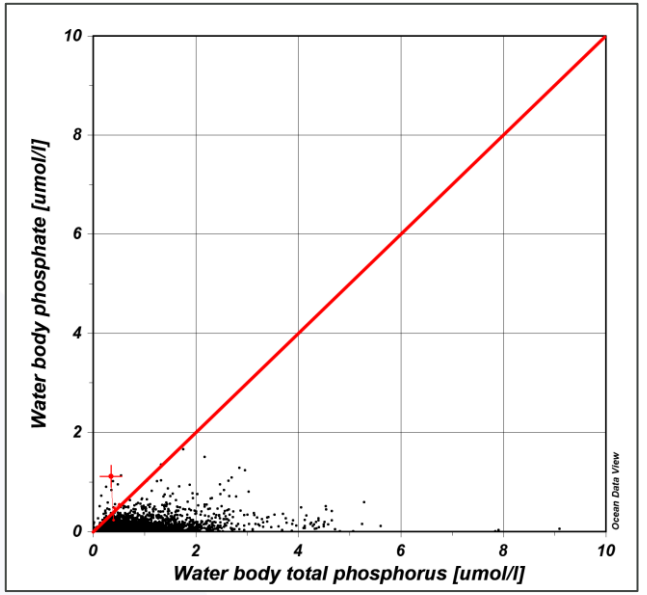
All data (left) and only QF 1, 2 (right): we lose river borne nutrients!

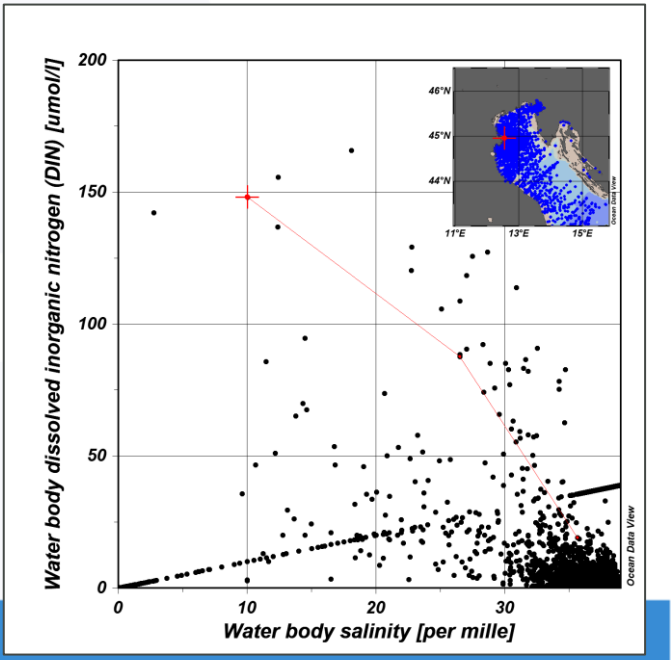
EMODnet Chemistry data Quality Control approach

Specific checks based on expert knowledge:

- ❑ Check cases where “NO3 plus NO2” is < NO3, inspect and assign proper QF
- ❑ Check ratios between inorganic nutrients (e.g. PO4, DIN, NO3+NO2) and total nitrogen and phosphorus (e.g. TP, TP): if ratios > 1, inspect and assign proper QF
- ❑ Check oxygen supersaturation in surface open waters: inspect and assign proper QF (the upper limit is capped at 115% saturation above 150 m, 130% above 100 m, and 150% above 10 m depth. Values above these upper limits are flagged as QF=4)
- ❑ Check salinity *versus* nutrient concentrations (low salinity = continental inputs → higher nutrients) and verify positions of anomalous data (eg. Close to rivers?)
- ❑ Check N/P ratios (relative proportion of Nitrogen to Phosphorus in open waters, far from continental inputs and in oxygenated waters, are fairly constant)

Not automatic checks – expert knowledge – area specific – time specific (global changes)





EMODnet Chemistry data Quality Control approach

Ongoing work:

- Update regional broad ranges (open waters) and propose ranges for coastal waters
- Update of «expert-based» QC checks (e.g. N/P ratios, pH,…)

EMODnet relies on an **«adaptive approach»,** «learning by doing» and improving additional QC steps, collecting users' feedbacks, to improve data quality

Thank you

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