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EMODnet Chemistry Spatial Data Infrastructure for marine observations and related information

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ABSTRACT

Scientific research as well as management of the marine environment, and sustainable blue growth are based on the availability of quality-assured observations, reliable data and solid scientific-based information. These represent three consecutive steps of Data-Information-Knowledge-Wisdom paradigm on the pyramid of wisdom, providing different layers of information. EMODnet (European Marine Observation and Data network) is one of the key infrastructures engaged in collecting, facilitating access and promoting use and re-use of marine observation and data products for both scientific research and marine environmental management. Its Spatial Data Infrastructure (SDI) represents a powerful mechanism to support the implementation of the Marine Strategy Framework Directive Article 19.3 in accordance with the INSPIRE Directive standards and implementing rules. Standardized, harmonized and validated chemical data collections are made available for water quality evaluation at a regional scale, establishing interoperability between the data sets from the many different providers (more than 60 in EMODnet Chemistry). Concentration maps of nutrients, chlorophyll-a and dissolved oxygen are computed on a standard grid, providing information at a regular time interval, per season and over several vertical layers, including the deepest one. Dedicated Open Geospatial Consortium standard services for browsing, viewing and downloading chemistry observation data and data products for the European waters have been developed, and are actively maintained and monitored. These results can provide knowledge layers and can also answer the needs of the directive on Maritime Spatial Planning (EU, 2014), which requires the integration of multidisciplinary data and information on the state of the marine environment with maritime and human activities.

1. Introduction

The Marine Strategy Framework Directive (MSFD) 2008/56/EC (EU, 2008) aims to protect the marine environment across Europe aiming to reach and maintain a Good Environmental Status (GES) of the EU's marine waters by 2020. The MSFD provides formal reporting requirements on the assessment of the marine waters (art. 8), determination of GES (art. 9), development of environmental targets and indicators (art. 10), development of monitoring programmes (art. 11), and Programme of Measures (PoM) (art. 13) that should be applied to marine (sub)-regions. European Member States (MS) have to report on each topics every six years respecting deadlines defined for each article in the implementation process.

MSFD Article 19.3 is particularly important in this context, stating that the data and information resulting from the initial assessment and from the monitoring programmes should be available, in accordance with the INSPIRE Directive standards and rules, to the European Environment Agency (EEA) and European Commission:

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[…] In accordance with Directive 2007/2/EC, Member States shall provide the Commission, for the performance of its tasks in relation to this Directive,[…] with access and use rights in respect of data and information resulting from the initial assessments made pursuant to Article 8 and from the monitoring programmes established pursuant to Article 11. […] such information and data shall also be made available to the European Environment Agency, for the performance of its tasks.

Directive 2007/2/EC (EU, 2007) lays down general rules setting up an Infrastructure for Spatial Information in Europe (INSPIRE) for the purposes of EU environmental policies and for policies or activities which may have an impact on the environment. Common Implementing Rules (IR) were adopted in a number of specific areas, specifically Metadata, Data Specifications, Network Services, Data and Service Sharing, Spatial Data Services, Monitoring and Reporting. Non legally-binding Technical Guidance documents describe detailed implementation aspects and relations with existing standards, technologies, and practices. All data should be described, managed and shared using INSPIRE Directive standards and rules as a common framework for sharing data in an open and interoperable way.

The long-term strategy for activities under Art 19.3, including how this might best be made operational using existing data flow mechanisms, was discussed since 2012 within the Marine Strategy Coordination Group (MSCG) and further within Working Group on Data, Information and Knowledge Exchange (WG DIKE) (WG DIKE, 2012, 2013) and presented to Marine Directors (November 2012). Making best use of existing mechanisms and platforms, including reporting under other EU Directives, the Data Collection Framework, EMODnet, GMES and Regional Sea Conventions.

In parallel, the EU Directorate-General Maritime Affairs and Fisheries (DG MARE) long-term strategy for marine and maritime sustainable growth provides funding and legislate for Marine Knowledge 2020 to unlock fragmented data from different sources. The EU initiative European Marine Observation and Data network (EMODnet) is an infrastructure finalized to sponsor, collect and simplify the data access, moreover it is dedicated to use and re-use of data for both scientific research and marine environmental management. The EMODnet aims are to improve the availability of fragmented datasets and to provide a set of tools to drive a sustainable development and implementing the EU policy Marine Knowledge 2020 (European Commission, 2012). Through a step-wise approach, the pilot components started in 2009 with few elements covering limited sea basins, in 2013 were extended to most European seas and it is now facing the high-resolution phase with the target to be fully deployed by 2020 (http://www.EMODnet.eu).

EMODnet, with its network of more than 110 organizations assembling marine data, metadata & data products within Europe in a uniform way, spans over seven discipline-based themes, namely bathymetry, geology, seabed habitats, chemistry, biology, physics, human activities, coastal mapping, and provides information to several indicators of the 11 GES descriptors (Fig. 1).

Each of the EMODnet themes have created a data portal providing access to data archives managed by local, national, regional and international organizations. Through these thematic portals, users have access to standardized observations, data quality indicators and data products. These results should be free to access and use, following the FAIR (Findable, Accessible, Interoperable, Re-usable) guiding principles for scientific data management and stewardship (Wilkinson et al., 2016).

EMODnet Chemistry focuses on eutrophication, marine contaminants and, in the last phase, on marine litter. In Table 1 examples of parameters managed by EMODnet Chemistry.

EMODnet Chemistry consortium represents a network of 46 interconnected National Oceanographic Data Centres (NODCs), marine information services and monitoring agencies, from 27 coastal states bordering the European seas, further developing SeaDataNet standards (https://www.seadatanet.org), following INSPIRE rules and Open Geospatial Consortium (OGC) protocols. In detail, the basis adopted are the same used in SeaDataNet, which implies a distributed infrastructure for data management. Nowadays, SeaDataNet is the *de facto* European infrastructure for data management and sharing and involves more than 100 NODCs from 35 countries. Moreover, SeaDataNet is actively concerned with adoption of INSPIRE standards that ensure the interoperability.

Interoperability is guaranteed by using of common formats for data and metadata; furthermore, the adoption of common vocabularies assures a homogeneous syntax and semantics (following INSPIRE rules).

In order to facilitate a harmonized approach to environmental status assessment in European sea basins, EMODnet Chemistry has focused on the collection, harmonization and Quality Control of data gathered from national monitoring efforts and from research activities at regional scale for five EU sea regions (Baltic Sea, North Sea, Eastern Atlantic Sea, Black Sea and Mediterranean Sea). These marine observations are exposed with Common Data Index (CDI) Metadata profiles, based upon ISO 19115–19139 standards and supported by SeaDataNet Common Vocabularies, and are downloadable in SeaDataNet ODV and NetCDF standard formats on the web portal and through OGC Web Map Service (WMS), Web Feature Service (WFS) and Catalog Service for the Web (CSW). EMODnet Chemistry provides standardized, aggregated and validated datasets on chemical substances relevant for the assessment of Good Environmental Status (GES) according to the MSFD Descriptors 5 (Eutrophication), Descriptors 8 (Contaminants), Descriptors 9 (Contaminants in seafood) and, starting from 2018, Descriptor 10 (Marine Litter) in the five major EU sea regions.

Furthermore, as a useful tool for a common environmental status assessment throughout European sea basins, 4D concentration maps for nutrients, chlorophyll and dissolved oxygen are computed at regional scale. Dedicated OGC WMS standard services for browsing, viewing and downloading chemistry source data sets and data products for the European waters are developed, maintained and monitored. In detail, the use of viewing services for data products (WMS, WFS and CSW) guarantees the compliance with OGC standards that are a means of interoperability.

EMODnet Chemistry outcomes attracted the interest of UNEP/MAP in view of the preparation of the Quality Status Report 2017 (QSR2017) and of the Black Sea Commission (BSC). Both requested access to the regional standardized, aggregated and validated datasets.

2. From marine observations to data to information

The meaning of the term ***marine data*** may change depending on the context. Scientists and oceanographers refer to measurements at sea as coming from in situ or remote observations. Model results, reflecting simulation of future conditions, are considered as marine data. Decision makers identify environmental data as a synthesis of knowledge extracted from observations. All are correct. Nevertheless, these differences must be considered in light of EU policies to avoid ambiguities in the application of European directives. Moving to a higher level in Data-Information-Knowledge-Wisdom pyramid, data products are the result of a process including computation or, more generally, elaboration of data. To obtain a data product, additional elements may be provided like national, regional or EU determined thresholds to compare data with and get information from data.

Looking in more detail at the articles of the MSFD that make mandatory for the Member States to report to the EC, it is relevant to separate and distinguish between ***information*** and ***data*** in order to analyse possible improvements in the data management process.

The International Oceanographic Data and Information Exchange (IODE) of the Intergovernmental Oceanographic Commission (IOC) of UNESCO (https://www.iode.org/index.php?option=com_content&view=article&id=3&Itemid=33) gives the following definitions:

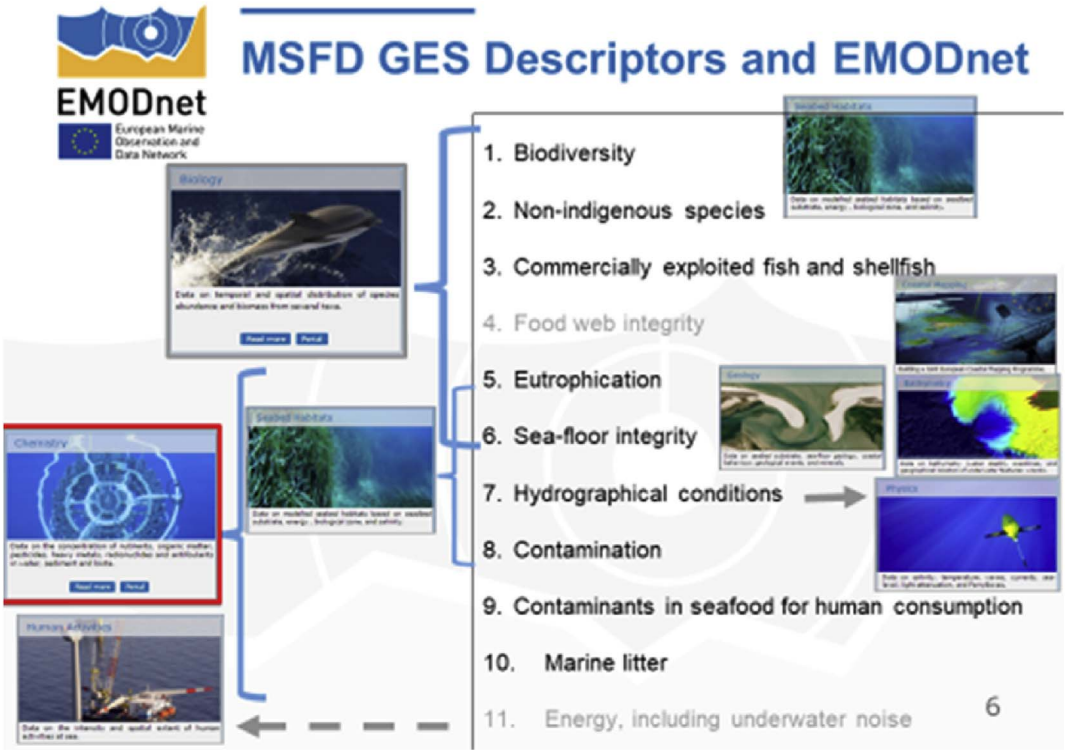

Fig. 1. EMODnet thematic portals in relationship with MSFD environmental descriptors.

Table 1
List of parameters covered by EMODnet Chemistry.

Eutrophication and acidification	Examples
Nutrients	NO_3, PO_4, SiO_4, NO_x, NH_4, Total N, Total P, Si
Dissolved gasses	Oxy
Acidity	pH, pCO_2
Chlorophyll	Chl-a
Contaminants	
Antifoulants	Organometallic and organometalloid
(Heavy) metals	Cd, Cu, Pb, Hg, Zn, …
Hydrocarbons	Polycyclic aromatic (PAHs) and aliphatic
Pesticides and biocides	DDT, DDD, DDE, …
Polychlorinated biphenyls	PCBs
Radionuclides	Radioactivity
Marine litter	Beach liter, sea floor litter, micro litter

d*ata* are observable, raw *values* that result from research or monitoring activities; these values can be numerical (as in temperature or salinity measurements) or nominal (as in species lists for a particular region). A step over would be to identify observations and data. The latter being the result of harmonization, standardization and validation process, applied when merging observations from different sources, sensors and purposes. The term *information* is commonly used to mean data that have already been processed and/or interpreted results. In that sense, so-called *metadata*, i.e. data about data (e.g. by whom, at what time, where and how the results were collected) can be considered a special kind of *information*.

In the current phase of MSFD implementation, MS have reported in most cases information (text report, metadata about monitoring programmes, etc.) and in very few cases data. This difference is underlined in the minutes of the 13th Meeting of Working Group on Data, Information, and Knowledge Exchange (WG DIKE, 2016).

Observations and data follow a data policy that specify the usage licence, is defined by data originators at dataset level and is affected by the sensitivity of measurements. EMODnet Chemistry technical infrastructure enables the data owner to apply a defined data policy including usage license to their data sets, thus retaining full control over access to the resource. It also allows a form of negotiation to take place – where the data owner is able to evaluate each request of their data and give rights based on specific uses. In parallel, data information (metadata) and data products, have, following EU recommendations, free access policy, with proper acknowledgment of originators.

The increasing use of the Digital Object Identifier (DOI) to provide a persistent identifier to datasets and data products (or information), allows recognition and credit for the production of data to be duly acknowledged, and also tracks the use and impact of specific datasets.

3. EMODnet chemistry results (observations, data and products)

EMODnet Chemistry Spatial Data Infrastructure establishes interoperability between data sets from different providers (> 60 in EMODnet Chemistry) and towards other types of data as physical oceanography, bathymetry, geology, etc. and these contribute to overcome the large heterogeneity of observations at the basis by regional validation and transformation to a common framework. Moreover, Quality Assurance and Quality Control (QA/QC) information collected from partners are included with monitoring data (i.e. use of Certified Reference Material, participation to inter-calibration network, accreditation, methodology used to assess Limit of Quantification/Detection and uncertainty). Data collected follow the principles of SeaDataNet: metadata are freely accessible on CDI (Common Data Index) data portal (http://seadatanet.maris2.nl/v_cdi_v3/search.asp) and observations are downloadable according to the originator data policy. Number of observations made available per parameter and per sea region is provided in Appendix A (information updated at November 2016) (Giorgetti et al., 2016). One CDI (Common Data Index) identifies a series of observations made at sea in the water column (vertical profile) or in time (time series), with granularity defined by data originator, sometimes in consultation with data managers. The increase in total number of CDIs is shown in Fig. 2.

According to the requirements of MSFD Article 19.3, Member States should provide public access to data and data products for the EEA and

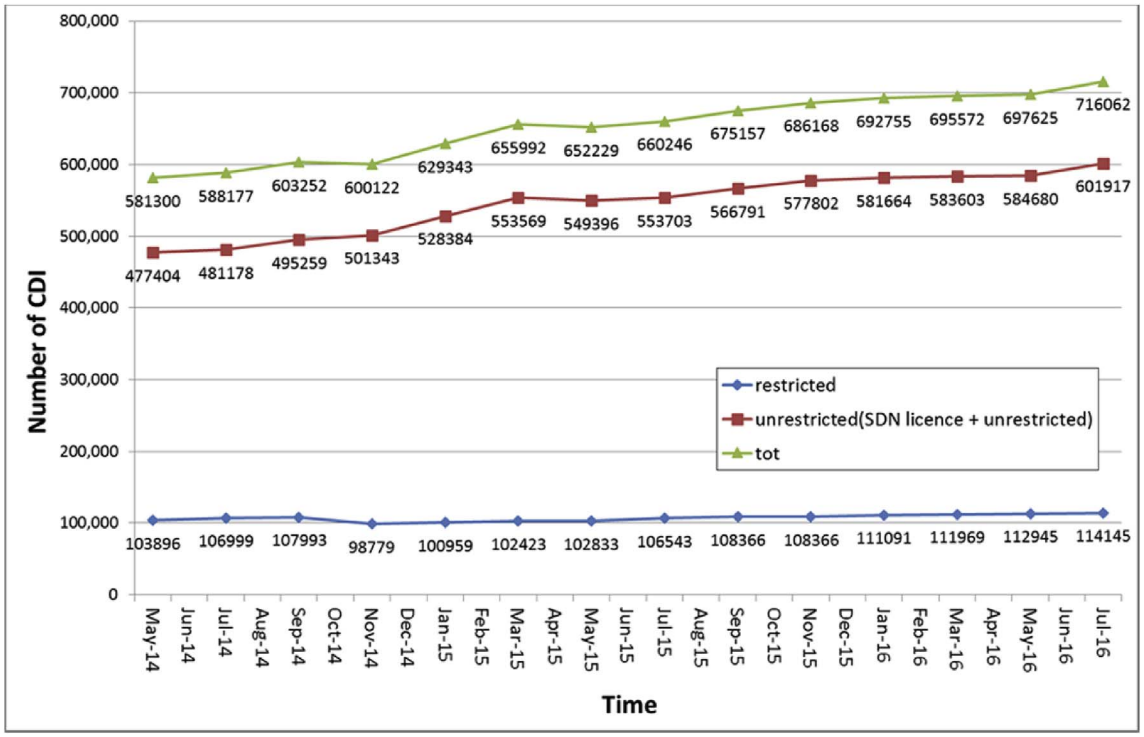

Fig. 2. Number of CDIs (dataset identifiers) in EMODnet Chemistry by access licence type from May 2014 to July 2016.

the EC using relevant INSPIRE standards. This should make best use of existing mechanisms, including reporting under other EU Directives, the Data Collection Framework, EMODnet, GMES and Regional Sea Convention mechanisms (WG DIKE, 2013). This should also contribute to the development of WISE-Marine (the web-based portal for sharing information to the marine community on the marine environment in relation to the MSFD).

Specific efforts have been dedicated to produce harmonized, aggregated and validated regional data set collections for the 5 major European sea regions and to prepare data products specifically relevant for Marine Strategy Framework Directive Descriptors 5 (eutrophication), 8 (chemical pollution) and 9 (contaminants in seafood), based on the guidance of the MSFD Common Implementation Strategy. The activity started with centralised data harvesting, followed by regional data aggregation, including parameter harmonization, and the implementation of the Data Validation Loop. The latter takes care that all identified errors and inconsistencies are documented by the regional coordinators and reported back to the originating data centres for local corrections and updating in their local databases and consequently in the Data Access Service (Vinci et al., 2017). The QA/QC procedures are specified in Barth et al. (2015). As last step, Data Interpolating Variational Analysis (DIVA) software has been applied to generate spatial interpolated concentration maps (Troupin et al., 2010), albeit only for those parameters that have sufficient spatial and temporal coverage at basin scales such as nutrients, dissolved oxygen and chlorophyll-a. Interpolated maps have been generated with a 10-year overlapping moving window (every map is representing the year of the middle 10-year period) in order to find a balance between the duration of the environmental evaluation cycle for member states (to provide maps with a time frame near to the 6-year process of the member states' evaluation) and the number of years that guarantee a sufficient data coverage, and at different standard depths, depending on data availability (Fig. 3).

In the case of data related to Descriptor 8 (chemical pollution) and 9 (contaminants in seafood), the heterogeneity of data is particularly high as the parameters are measured in different matrices (water, sediment, biota), in different sediment size classes, in different phases (dissolved/particulate), in different marine species and target issues/organs, with different sampling, analytical and normalization protocols. This results in a situation of fragmented datasets, where homogeneous data are needed to generate data products, for contaminants some further work are therefore needed to make data products comparable to the eutrophication and acidity data products.

Among the large list of contaminants managed by EMODnet, priority has been given to the following parameters:

- for Pesticides, we focused on p,p'-DDTs (including in this group p,p'-DDE, p,p'-DDT and p,p'-DDD) and HCB;
- for Antifoulants, we focused on TBT and TPT;
- for Heavy metals, we focused on mercury, cadmium, lead, plus copper and zinc. Regarding the water column, we prioritized on the dissolved phase;
- for Hydrocarbons, we focused on anthracene, benzo(*a*)pyrene, fluoranthene, naphthalene, phenanthrene;
- for Radionuclides, we focused on 137Cs;
- besides target groups indicated in the call, also polychlorinated biphenyl (PCBs) will be included and focus will be on: PCB118, PCB138, PCB153 and PCB180, plus PCB28, PCB52, PCB101 and PCB105.

For both subsets of data regarding eutrophication and contaminants, the basic idea is to:

- visualize the measurement density in a given time and space window,
- visualize a time evolution of a selected group of parameters,
- show concentration plots for a given time and space window and along the coast (Fig. 3).

Taking into account the large heterogeneity of data, in order to facilitate visualization, an aggregation procedure has been agreed within the EMODnet community. This aggregation is done with the use of a specific vocabulary with scientifically meaningful definitions driven by a community of experts.

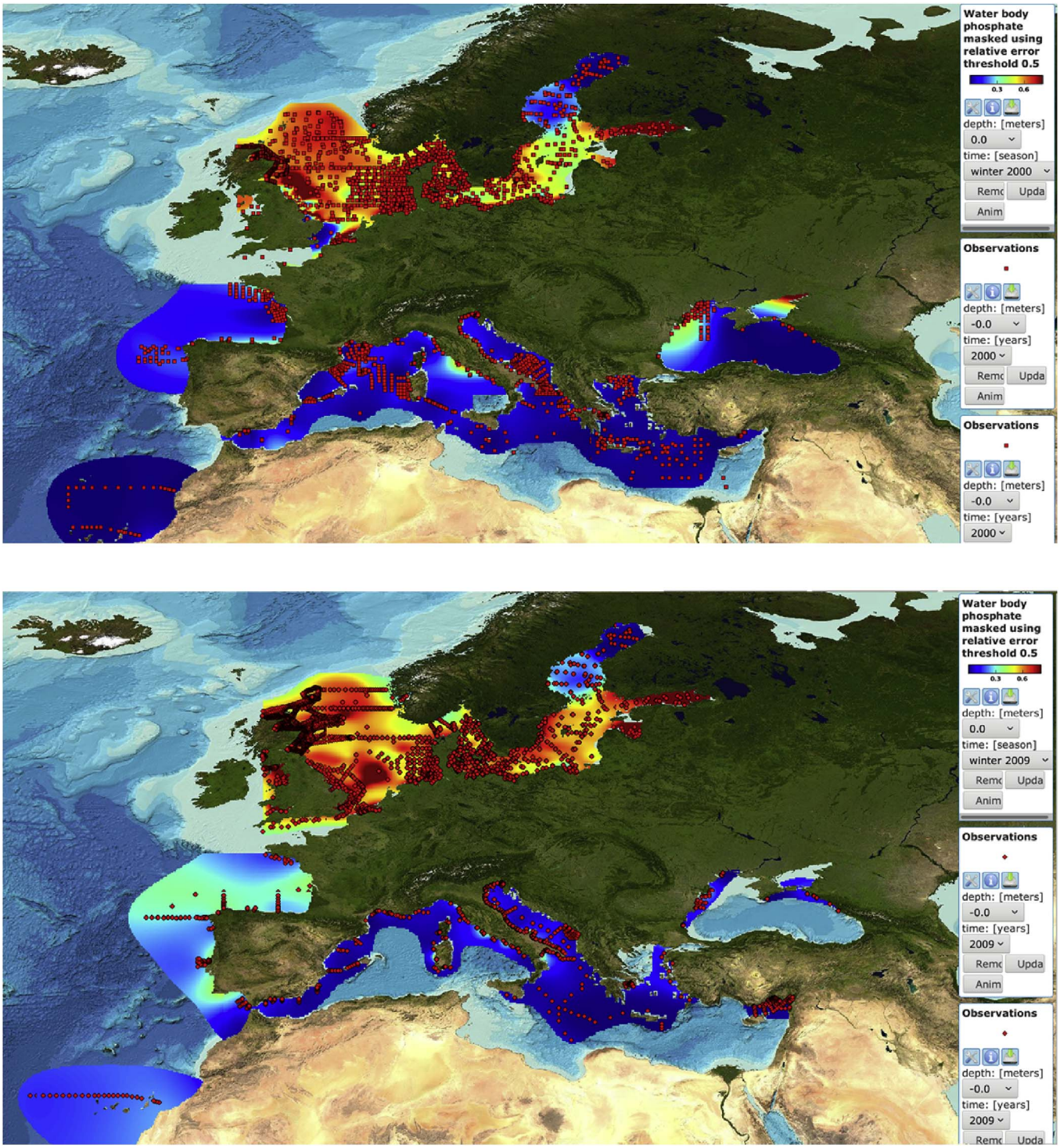

Fig. 3. 10 years average of water body phosphate concentration (μmol/l) in the surface layer for all EU sea basins for years 1995–2005 (centered in 2000) (upper image) and for years 2005–2015 (centered in 2009) (lower image); winter season.

All EMODnet Chemistry datasets and data products such as DIVA concentrations maps are described in the Sextant Products metadata catalogue, developed by IFREMER (Fig. 4). This facilitates searching for specific data products and the exchange and use of the Chemistry data products in other services, such as the Chemistry OceanBrowser (Barth et al., 2017), and other portals with OGC WMS support (http://sextant.ifremer.fr/en/web/EMODnet_chemistry/catalogue).

A dynamic visualization service has been implemented to produce plots of observation densities and of temporal evolution of selected observations The OceanBrowser Viewing service (http://ec.oceanbrowser.net/emodnet/) (Fig. 5), developed and maintained by University of Liege (Ulg), provides access to the DIVA interpolated maps. Output images are available as horizontal sections and vertical sections. The latter can be selected by drawing an appropriate transect. Ulg has included in the interface predefined coastal sections which allow a user to visualize as vertical sections.

The DIVA maps can not only be viewed but also downloaded as NetCDF (CF) data files. Ulg has also included support for the CDI Web Map Service (WMS) and Web Feature Service (WFS) services in the OceanBrowser Viewing service so that users can easily see which data

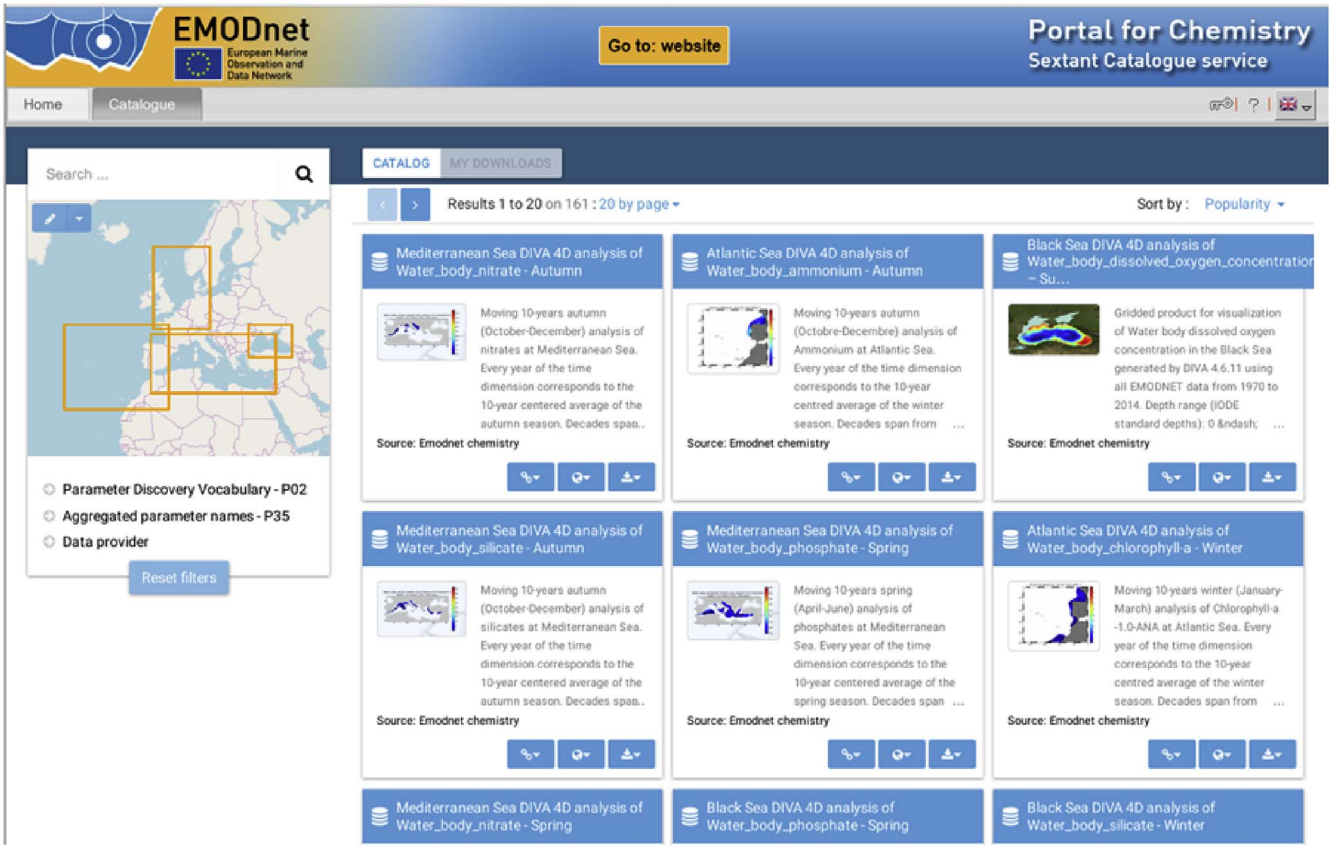

Fig. 4. Sextant Products metadata catalogue.

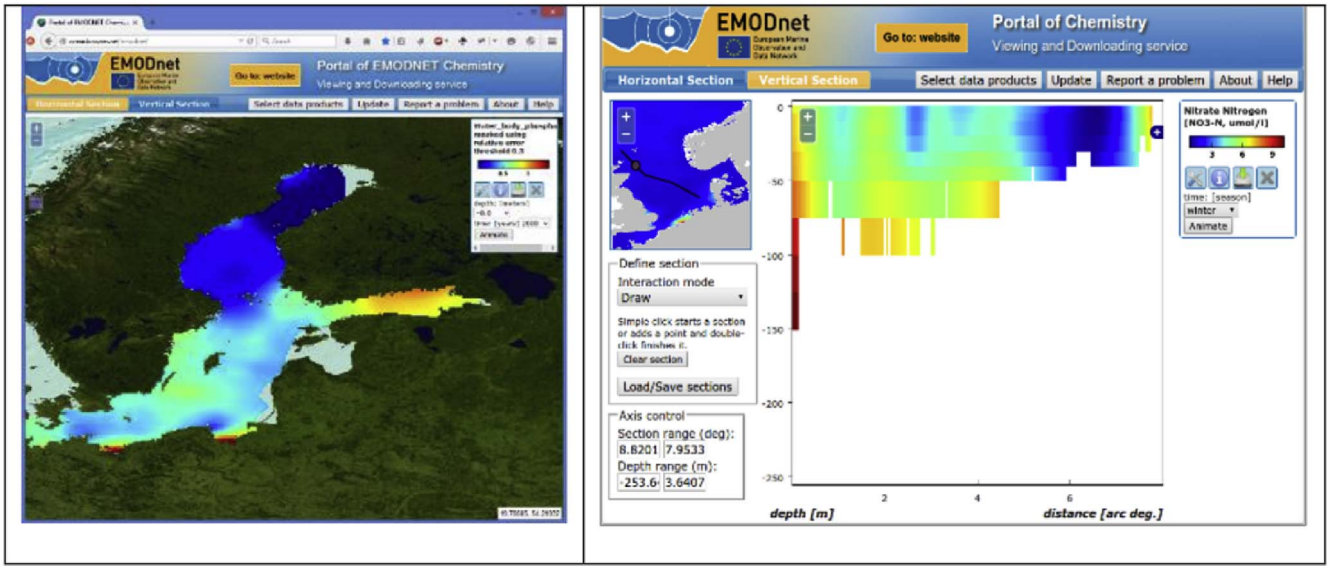

Fig. 5. OceanBrowser Viewing service.

sets overall are available in EMODnet Chemistry and their metadata for further information and possible shopping requests.

Recent efforts, in EMODnet Chemistry, have been dedicated to the needs of the Directive on Maritime Spatial Planning (EU, 2014), which requires the integration of multidisciplinary data and information on maritime activities, on the state of the marine environment and on its vulnerability to human activities. Free and open access to information (over data and observations) is an important component of MSP process for environmental management, impact assessment, conservation and management of protected areas. These issues were addressed with a series of European marine and maritime data management initiatives (SeaDataNet, EMODnet and ODIP).

4. Conclusions

Lack of data, need of harmonization and coherence of data acquisition protocols among EU Member States have been identified as key issues limiting a common assessment of Good Environmental Status (GES) at regional and sub-regional scale and the promotion of a sustainable use of maritime space and of its resources. This paper describes

the results achieved by the EMODnet Chemistry (http://www.EMODnet-chemistry.eu) and the viewing services developed to download and share them. Observations, data and information are discussed, in relation to MSFD, WFD and MSP, which require the integration of multidisciplinary data and information on the state of the marine environment.

In the framework of EMODnet Chemistry, 160 thematic concentration maps were realized for five marine regions (Baltic Sea, North Sea, Eastern Atlantic Sea, Black Sea and Mediterranean Sea), covering 11 chemical parameters, 4 seasons and aggregated for 30 depth layers. These amounts of information are freely searchable and accessible. Besides the graphical maps, the underlying data products (i.e. DIVA interpolated maps) are freely available as NetCDF files. In addition, dedicated layers allowing access to row data used to compute the maps are freely accessible.

They could be a good starting point to examine and manage the environmental process, impact assessment, conservation of protected areas and data gaps analysis in the five sea basins.

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Appendix A. Overview of the available DIVA concentration maps

Number of controlled and validated data profiles and DIVA products (concentration maps) currently available for the five regional sea basins: Mediterranean Sea, Atlantic Sea, Baltic Sea, Black Sea and North Sea. DIVA analyses are made with 10-year moving average. Available depths are IODE standard depths within the interval given in the table.

	Parameter	Nr of profiles	Years	Depth interval
Atlantic Ocean	Ammonium	5001	1989-2010	0-3000
	Chlorophyll-a	13357	1990-2010	0-300
	Nitrate + nitrite	7472	1989-2010	0-3000
	Oxygen	21098	1968-2010	0-3000
	Phosphate	11319	1968-2010	0-3000
	Silicate	7110	1968-2010	0-3000
	Parameter	**Nr of profiles**	**Years**	**Depth interval**
Baltic Sea	Ammonium	29726	1960 - 2014	0 – 300
	Chlorophyll-a	18472	1980 - 2014	0 – 300
	Nitrate	19400	1960 - 2014	0 – 300
	Nitrate + nitrite	34760	1960 - 2014	0 – 300
	Oxygen	51359	1960 - 2014	0 – 300
	Phosphate	39036	1960 - 2014	0 – 300
	Silicate	30294	1960 - 2014	0 – 300
	Total nitrogen	31630	1960 - 2014	0 – 300
	Total phosphorus	33389	1960 - 2014	0 – 300
	Parameter	**Nr of profiles**	**Years**	**Depth interval**
Black Sea	Ammonium	6935	1980 - 2013	0 – 100
	Chlorophyll-a	1658	1995 - 2014	0 – 20
	Nitrate + nitrite	9354	1976 - 2013	0 – 150
	Nitrate	8274	1975 - 2013	0 – 150
	Oxygen	23102	1970 - 2014	0 – 250
	Phosphates	22728	1960 - 2013	0 – 300
	Silicate	19024	1960 - 2013	0 – 200
	Parameter	**Nr of profiles**	**Years**	**Depth interval**
Mediterranean Sea	Ammonium	14563	1977 - 2013	0 – 1000
	Chlorophyll-a	23105	1972 - 2015	0 – 2500
	Nitrate	21875	1960 - 2013	0 – 1500
	Nitrites	23101	1965 - 2013	0 – 1500
	Oxygen	74562	1971 - 2015	0 – 3000
	pH	30967	1959 - 2014	0 – 1500
	Phosphates	27894	1960 - 2013	0 – 1500
	Silicate	23102	1960 - 2013	0 – 1500
	Total nitrogen	5623	1990 - 2004	0 – 1000
	Total phosphorus	7628	1984 - 2007	0 – 1000
	Parameter	**Nr of profiles**	**Years**	**Depth interval**
North Sea	Ammonium	-	1960 - 2014	0 – 300
	Chlorophyll-a	-	1980 - 2014	0 – 30
	Nitrate	-	1960 - 2014	0 – 300
	Oxygen	-	1960 - 2014	0 – 300
	Phosphate	-	1960 - 2014	0 – 300
	Silicate	-	1960 - 2014	0 – 300
	Total nitrogen	-	1960 - 2014	0 – 300
	Total phosphorus	-	1960 - 2014	0 – 300

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