EMODnet Lot 3 – Chemistry

EXECUTIVE SUMMARY

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INDEX

INTRODUCTION

Setting up a European Marine Observation and Data NETwork

In the EU Green Paper on Future Maritime Policy for the European Union, the Commission proposed a new European Marine Observation and Data Network (EMODnet). Following an overwhelmingly positive response from stakeholders to its proposal, the European Commission, in its EU's Maritime Policy Blue Book, adopted in October 2007 and welcomed by the European Council in December 2007, undertook to take steps towards EMODnet in order to improve availability of high quality data. EMODnet will provide data on scales defined by the regions and sub-regions of the Marine Strategy Framework Directive. The parameters to be collated are chosen to fit in with the requirements of the Directive.

Five service contracts were launched for creating pilot components of the European Marine Observation and Data Network (EMODnet):

- Lot 1 – Hydrographic data
- Lot 2 – Marine geological data
- Lot 3 – Chemical data
- Lot 4 – Biological data
- Lot 5 – Physical data

One of the outcomes of these contracts will be a better understanding of the ability of the present monitoring network to meet the needs of the Directive.

EMODnet, as open data system, should be directly available for viewing through WISE-Marine. WISE-Marine is being developed along a timeline which is in parallel to this EMODNET preparatory action. The data collated and processed will feed into the European Atlas of the Seas.

EMODnet Chemistry project is undertaken by 25 partners representing the SeaDataNet network of Data Centres, selected on their geographical coverage and specific expertise. These Data Centres already manage a large volume of relevant data sets and can enlarge the available collections from data holders in their country. Moreover the SeaDataNet partnership includes ICES, which acts as data centre for monitoring data for OSPAR, HELCOM and EIONET ensuring consistency is maintained with existing data reporting routes.

The EMODnet tender for Chemical data asked for data sets from the Greater North Sea and the Black Sea region. However, we planned to expand the pilot regions with five spots from the Mediterranean (Balearic Sea, Gulf of Lion, North Adriatic Sea, Gulf of Athens and NE Levantine basin). It concerns the following geographical regions:
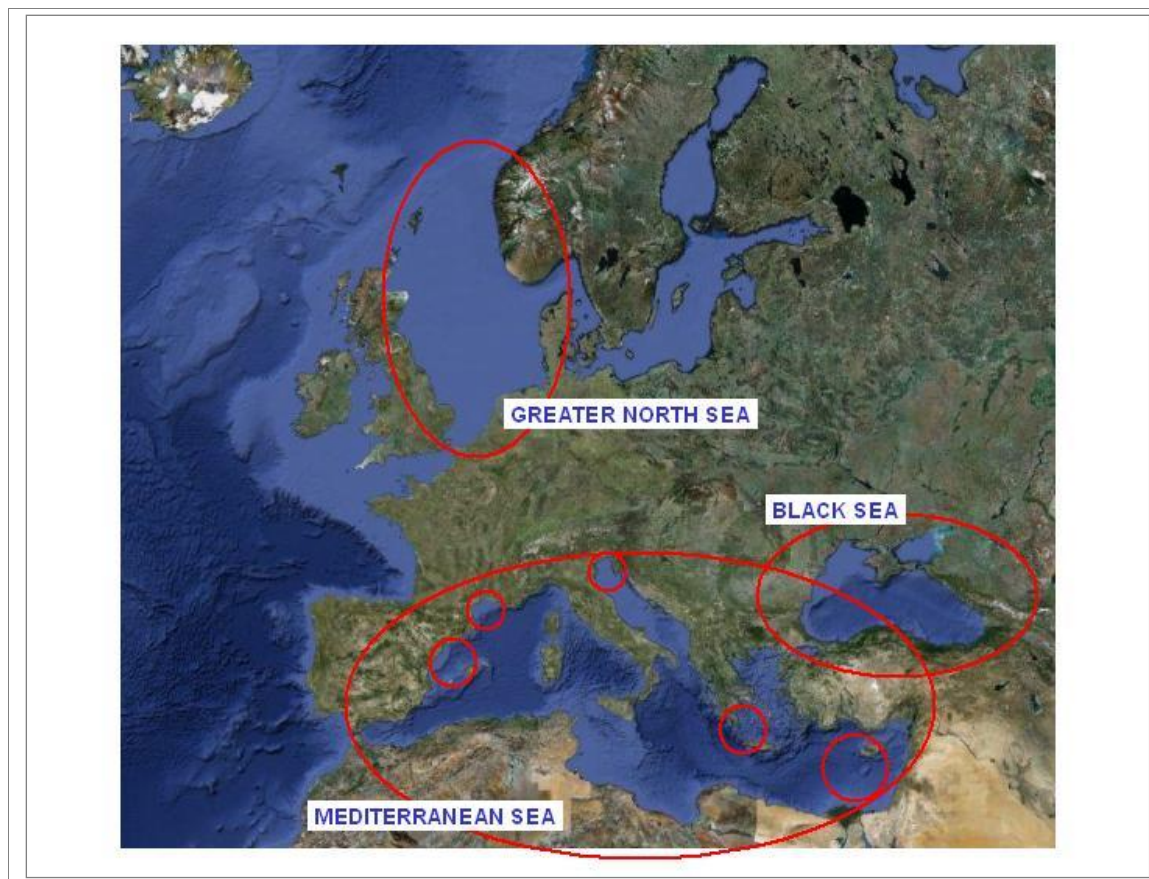
EMODnet Chemistry is focused on the groups of chemicals required for monitoring the Marine Strategy Framework Directive:

1. synthetic compounds (i.e. pesticides, antifoulants, pharmaceuticals),

2. heavy metals,

3. radionuclides;

4. fertilisers and other nitrogen- and phosphorus-rich substances;

5. organic matter (e.g. from sewers or mariculture);

6. hydrocarbons including oil pollution.

Based on SeaDataNet (SDN) experience, the following strategy was proposed as approach for the EMODnet pilots:

- Develop a high-end dedicated portal, outfitted with a powerful spatial database, that is complemented with WMS, WFS and WCS services (OGC) to serve users and to provide layers for the wider community (e.g. the other EMODnet portals, the prototype European Atlas of the Seas, and the broad-scale European Marine Habitats map);

- Provide data sets for producing interpolated maps with specific resolution for each geographical region, that are loaded and integrated afterwards into the portals' spatial database;

- Include a metadata discovery service in the portal, by adopting the SeaDataNet Common Data Index (CDI) metadata standard, that *inter alia* gives clear information

about the background data, the access restrictions and distributors; this also maintains the relationship of the EMODnet portals with the SeaDataNet distributed infrastructure.

So far, the technical set-up is based on SeaDataNet V1 infrastructure, using the principle of 'adopted and adapted'. In fact, EMODnet Chemistry adopts and adapts:

- SDN Standards for background data, metadata and product. This in particular includes CDI (xml ISO 19115) metadata, ODV data format for background data exchange, SDN standard vocabularies (like P021 for CDI generation, P061 for units, P011 for ODV generation),

- CDI mechanism to access data with data policy management,

- SDN Security Services for user registrations,

- SDN Delivery Services for data access and downloading,

- SDN Products metadata catalogue

- SDN Products viewing services for discovery, visualization and downloading of data products.

- SDN software tools (MIKADO metadata mapping and xml generator, NEMO formatting tool, DIVA software tool to produce gridded data products and error maps as NetCDF files, ODV software for "time series" products generation and QC check).

In particular, during the first year of project activities, the need was identified for specific methods to visualise parameters showing a not homogeneous spatio-temporal distribution which the EMODnet chemical lot considers. A specific workshop was organised to solve the issue and a new set of products were released, at first as a prototype. As a consequence, ODV/DIVA softwares were upgraded to produce maps, plots and related metadata (DIVAdoXML) and the Ocean Browser Products Viewing Service functionalities upgraded to visualize station maps with links to time series plots.

THE CHEMICAL DATA

EMODnet Chemistry aims to assemble fragmented and inaccessible marine data into interoperable, continuous and publicly available data streams for complete maritime basins.

Each EMODnet partner had collected data and compiled metadata of the dataset under the supervision of the three regional leaders:

-NERI-MAR for the Greater North Sea;

-HCMR for the Mediterranean;

-MHI for the Black Sea.

The data and metadata follow the SeaDataNet infrastructure:

- common vocabularies;
- ISO 19115 metadata standard for all metadata directories;
- XML Validation Services to quality control the XML metadata maintenance;
- Data Transport Formats for data sets delivery;
- quality control protocols and flag scale:
- standard software tools;

The Common Data Index (CDI) is the central data discovery service for EMODnet enabling users to have a detailed insight of the availability and geographical extent of data, archived at the connected data centres. It gives the description of individual data sets and measurements with key fields (what, where, when, how, who etc.). The data can be downloaded and accessed following SeaDataNet Data policy and User licence:

http://EMODnet-chemistry.maris2.nl/v_cdi_v2/search.asp.

The CDI data discovery including its services for authentication accessing, and downloading is driven by the underlying central SeaDataNet database and infrastructure of connected data centres. Users can freely search and browse the CDI discovery services and identify relevant data sets.

The metadata and aggregated data products (GIS layers) in the EMODNET pilot are public domain and freely available for all users. However for data access (= downloading) the EMODNET pilot must respect the data copyrights of owners (see SeaDataNet Data policy and User licence), in particular for the background. For the chemical data the standard ODV ASCII data format is adopted.

The chemical parameters were grouped in the 3 matrices (water column, sediment, biota) to make a set of 17 selected parameters for product generation in the three regions.

All partners produced ODV files and sent them to the regional task leaders (NERI, MHI, HCMR). Besides, all partners produced the CDI entries and sent them to MARIS, to link the collected data to EMODnet CDI User interface.

The following table gives the total number of stations made available in the three regions as number of CDIs.

MSFD categories	entryterm_p021	Total CDI numbers		
		North Sea	Black Sea	Med Sea
Antifoulants	Concentration of other organic contaminants in biota	24		
	Concentration of other organic contaminants in sediment samples	1898	177	
	Concentration of other organic contaminants in suspended particulate material	636		
	Concentration of other organic contaminants in the water column	1560	2142	1
	Organometallic species conomentration parameters in biota	129		
	Organometallic species concentration parameters in sediments	583		
Fertilisers/Nitrogen	Ammonium concentration parameters in the water column	86575	5450	10166
	Dissolved inorganic nitrogen concentration in the water column	1448	65	1415
	Dissolved total and organic nitrogen concentrations in the water column		1770	
	Dissolved total or organic phosphorus concentration in the water column		1141	
	Nitrate concentration parameters in the water column	101316	10589	18278
	Nitrite concentration parameters in the water column	43223	10286	16380
	Nutrient concentrations in sediment pore waters			16
	Phosphate concentration parameters in the water column	108996	22059	19512
Heavy metals	Dissolved metal concentrations in the water column	3399	412	1
	Inorganic chemical composition of sediment or rocks	1198	663	88
	Metal concentrations in biota	2577		33
	Particulate metal concentrations in the water column	961		
	Total metal concentrations in water bodies	609	514	
Hydrocarbons	Concentration of other hydrocarbons in the water column	205	1677	
	Concentration of polycyclic aromatic hydrocarbons (PAHs) in biota	536		33
	Concentration of polycyclic aromatic hydrocarbons (PAHs) in sediment samples	3422		
	Concentration of polycyclic aromatic hydrocarbons (PAHs) in suspended particulate material	1051		
	Concentration of polycyclic aromatic hydrocarbons (PAHs) in the water column	323		
Organic matter	Carbon concentrations in sediment	2106		22
	Carbon concentrations in suspended particulate material	3159		
	Concentration of organic matter in sediments	29		6
	Dissolved organic carbon concentration in the water column		236	
	Dissolved organic carbon concentrations in sediment pore waters			16
	Nitrogen concentrations in sediment	401		16
	Nitrogen concentrations in suspended particulate material	3752		
	Particulate total and organic carbon concentrations in the water column	9163	20	2003
	Particulate total and organic nitrogen concentrations in the water column	65424	1956	3030
	Particulate total and organic phosphorus concentrations in the water column	61477	2034	1115
Others	Alkalinity, acidity and pH of the water column	12686	4968	27712
	Concentration of suspended particulate material in the water column	9026	984	6987
	Dissolved oxygen parameters in the water column	168279	33680	72087
	Raw oxygen sensor output	5151		
	Suspended particulate material grain size parameters			72
	Total dissolved inorganic carbon (TCO2) concentration in the water column		25	19
Pesticides	Concentration of polychlorobiphenyls (PCBs) in biota			33
	Concentration of polychlorobiphenyls (PCBs) in sediment samples	1325		
	Concentration of polychlorobiphenyls (PCBs) in suspended particulate material	163		
	Concentration of polychlorobiphenyls (PCBs) in the water column	323	384	
	Pesticide concentrations in biota	709		33
	Pesticide concentrations in sediment	1037	233	
	Pesticide concentrations in water bodies	213	904	
Radionucleides	Radioactivity in the water column	773	1195	48

Overview of CDI records for EMODNET chemistry categories in the regions - May 2012

CHEMICAL PRODUCTS AND QC

Since the beginning of the activities of EMODnet Chemistry the challenge was represented by:

- The complexity of the measurements covering 8 groups of parameters collected on 3 matrices (sediment, water column and biota)
- The heterogeneity related to:
    - the data distribution (coastal points time series Vs homogeneous sampling at basin level)
   - the measurement methods (instrument, method, target species, target basis, grain sizes).

To face this an Expert workshop was organized in September 2010. The results of this workshop highlighted that for the EMODnet Chemical lot, 2 main subsets of data are available depending upon the available data distribution:

- Data with an homogeneous distribution in time and space;
- Data with a not homogeneous distribution in time and space;

The common decision about the products generation was to generate:

- Standard Interpolated Maps, produced only for parameters with homogeneous distribution and suitable data coverage in time and space (measured on basin scale),
- "Time series plots", showing station maps with plots of measured time series for not homogeneous datasets as coastal points repeated in time and/or datasets with fragmented coverage.

To discriminate this a previous accurate data format Standardization and a Normalization analysis was performed by partners and the Regional leaders.
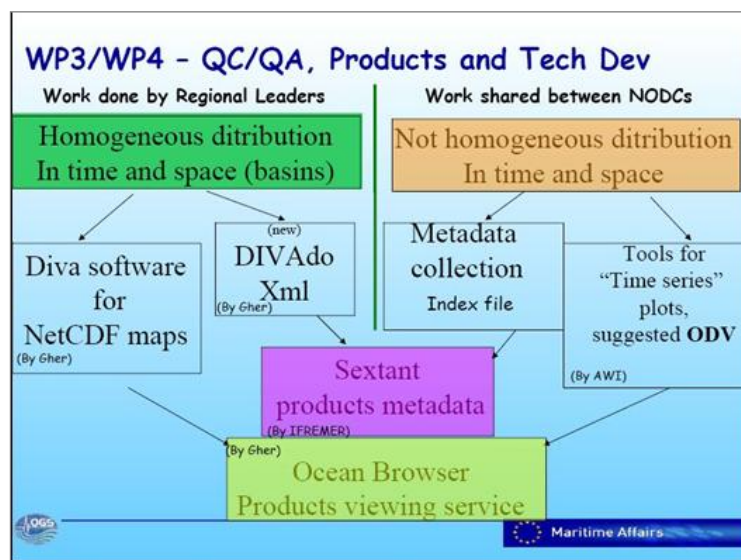
Overview of the workflow for the products generation after the Expert workshop

Besides, we had to decide which maps have to be produced and how to validate them before making them available, since strong gradients can appear for some of the parameters.

A first step for this was to examine the data availability and data distribution in space and time (gap analysis). Another possibility was to use the error field generated by DIVA to mask the interpolated fields in the areas where the error was above a fixed threshold.

In parallel, the opinion of experts was essential do determine whether a given map was meaningful or not. For this reason a work of critical revision of the generated products was done together with local experts and was followed by a Product Validation Meeting done in November 2011.

The total number of products available is given for DIVA interpolated maps and time series plots.

areas	temporal resolution	category
North Sea	Seasonal	nutrients
Black Sea	Annual	Nutrients , Metals, Radionuclides
	Monthly	Nutrients
	Seasonal	Nutrients
Mediterranean Sea – Adriatic	Annual	Nutrients
	Seasonal	Nutrients
Mediterranean Sea – Gulf of Athens	Annual	Nutrients
	Seasonal	Nutrients
Mediterranean Sea – Gulf of Lion	Monthly	Nutrients
Mediterranean Sea – Balearic Sea	Seasonal	Nutrients
Mediterranean Sea – Levantine Basin	Seasonal	Nutrients

Overview of DIVA interpolated Maps in the regions - May 2012

MSFD categories	entryterm_p021	North Sea	Black Sea	Med Sea
Antifoulants	Organometallic species concentration parameters in sediments	5/5		
Fertilisers/Nitrogen	Ammonium concentration parameters in the water column	5/5	2/4	
	Nutrient concentrations in sediment pore waters			2/24
	Nitrate concentration parameters in the water column	8/11	1/2	
	Nitrite concentration parameters in the water column	2/3	1/2	
	Phosphate concentration parameters in the water column	8/17	1/2	
	Dissolved total and organic nitrogen concentrations in the water column	5/12		
	Dissolved total or organic phosphorus concentration in the water column	1/1	2/4	
Heavy metals	Metal concentrations in biota	2/23		11/62
	Dissolved metal concentrations in the water column	3/3	24/72	
	Particulate metal concentrations in the water column	2/4		
	Total metal concentrations in water bodies	2/2		
	Inorganic chemical composition of sediment or rocks	9/27		15/132
Hydrocarbons	Concentration of polycyclic aromatic hydrocarbons (PAHs) in sediment samples	7/10		
	Concentration of polycyclic aromatic hydrocarbons (PAHs) in biota			11/38
Organic matter	Carbon concentrations in sediment			2/6
	Dissolved organic carbon concentration in the water column	1/2		
	Nitrogen concentrations in sediment			2/6
	Dissolved organic carbon concentrations in sediment pore waters			2/6
	Particulate total and organic phosphorus concentrations in the water column	1/1		
Others	Alkalinity, acidity and pH of the water column		2/8	
	Dissolved oxygen parameters in the water column	1/1	2/4	
	Salinity of the water column		2/4	
	Silicate concentration parameters in the water column	2/2	2/4	
	Temperature of the water column	1/1	2/4	
	Concentration of suspended particulate material in the water column	1/1		
Pesticide	Pesticide concentrations in biota	2/23		4/14
	Pesticide concentrations in sediment	4/6		
		72/160	41/110	49/288

Overview of TS Plots in the regions - May 2012
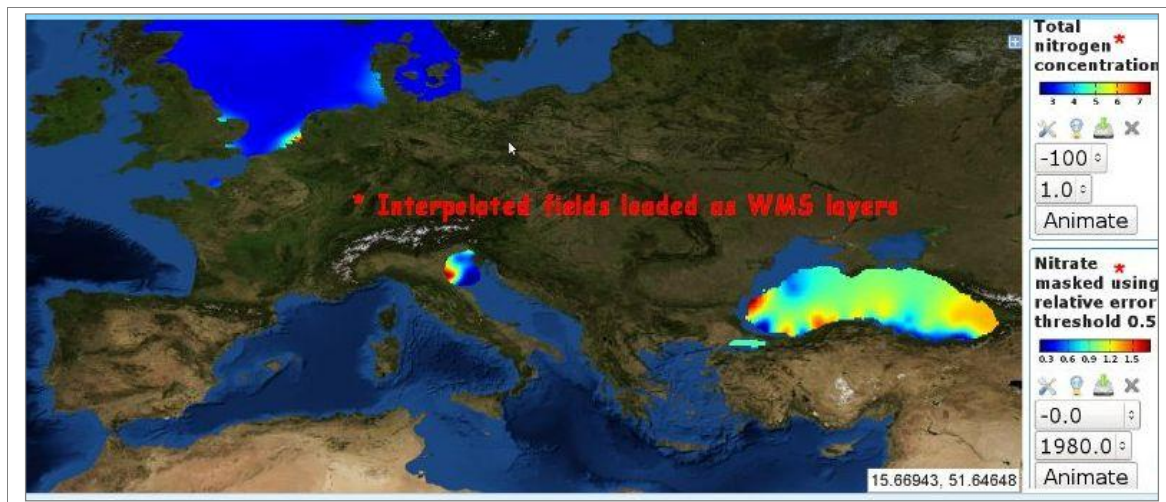
Screenshot with an example of DIVA interpolated maps in the three regions as visualized with the OceanBrowser
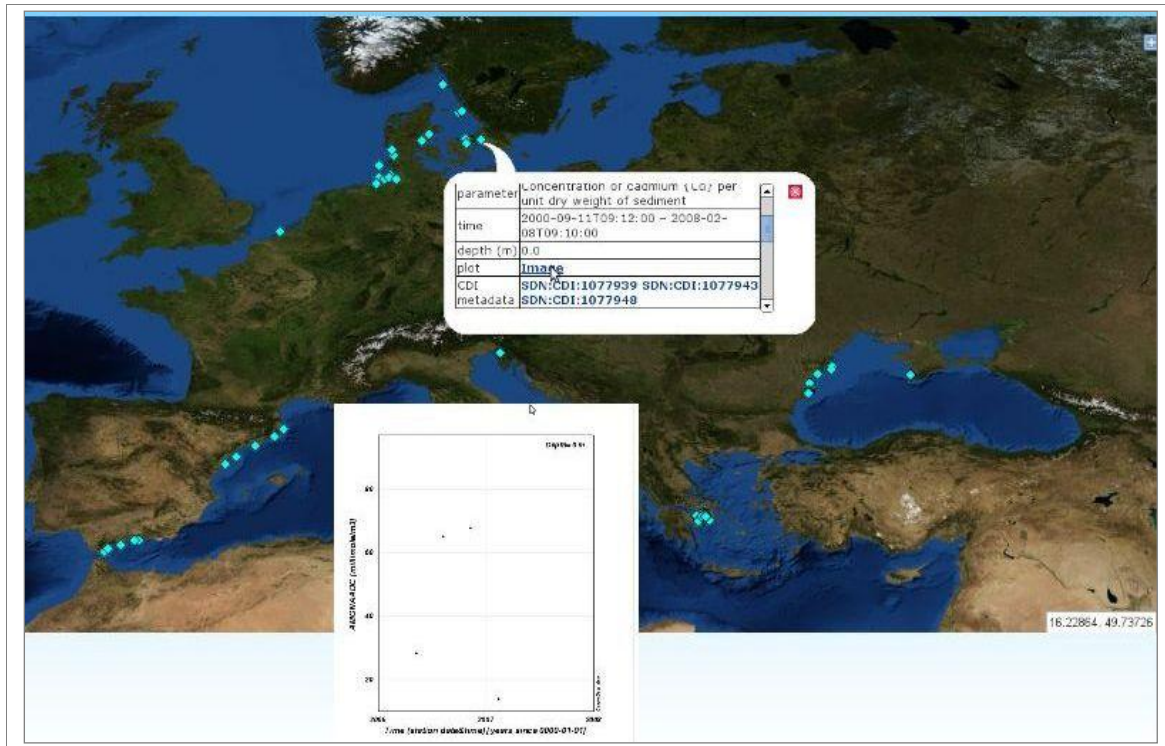
Screenshot with the total distribution of all available stations in the three regions, the selection list window with all plots available in one station, the Common Data Index (CDI) link and an example of Time series plot

TECHNICAL DEVELOPMENT OF THE WEB PORTAL

The technical activities were dedicated to the development of the EMODnet Chemical portal (http://www.emodnet-chemistry.eu).

The EMODnet Chemical portal is made by the following sections:
- **Home**: giving information about the Chemical Lot Pilot project;
- **Overview**: giving general information about the European Marine Observation and Data Network and its on-going lots;
- **Metadata & Data**: giving access to the Common Data Index search masks;
- **Data Products**: giving access to the products generated during the activities thanks to the Ocean Browser service;
- **Partners**: a section giving information about involved institutes;
- **Extranet**: with restricted access for partners to share project documents;
- **Reports made to the EU**: for the official progress reports submitted to the EU;
- **Feedback**: with the links to the online survey to obtain suggestions from users to improve the service;
- **Meetings**: with the general information and the link to the presentations for the meetings of the three years of activities;
- **Work Area**: with the restricted access link to the project WIKI.

EMODNET Pilot portal for Chemistry available at http:// www.emodnet-chemistry.eu

THE CDI DATA DISCOVERY AND ACCESS SERVICE

The Data Discovery and Access service has been developed by MARIS as a dedicated version of the SeaDataNet Common Data Index (CDI) service. It provides the basis for giving overviews and access to identified chemical observation data sets that are managed at distributed data providers.
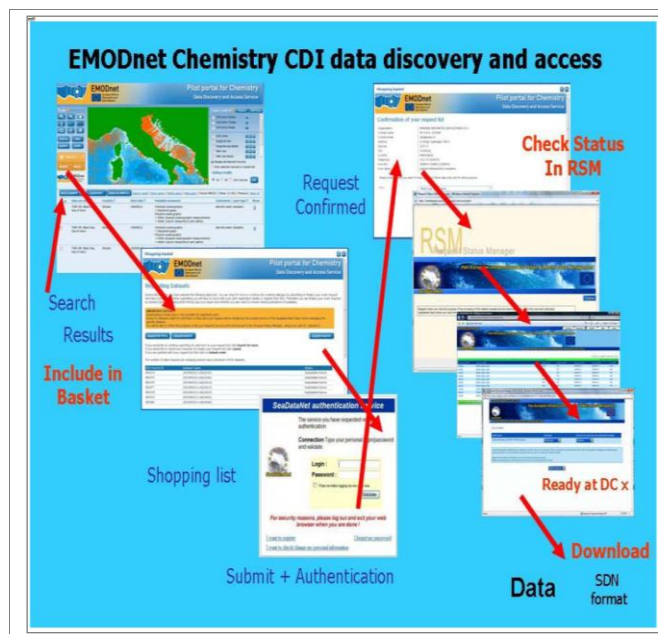
EMODnet Chemistry CDI discovery and data access mechanism

The CDI Data Discovery and Access service provides three search interfaces:

- Quick search: search mask without Geobox embedded;

- Extended search: search mask with Geobox embedded;

- Variables Vs Marine Regions: a Matrix with a CDI access point that gives an overview of variables and whether there are measurement data available for specific marine regions.

Here an example of a search sequence using the CDI Extended search:

Selection of an area thanks to the Geobox selection on the left upper side TOOLS box

Result of the Geobox selection

Obtaining information about a profile thanks to the "INFO" button on the the left upper side of TOOLS box. On the middle right side of the screen it's possible to use the buttons to obtain respectively: an XML file of the profile, order the CDI with the shopping basket, print the metadata of the selected CDI.
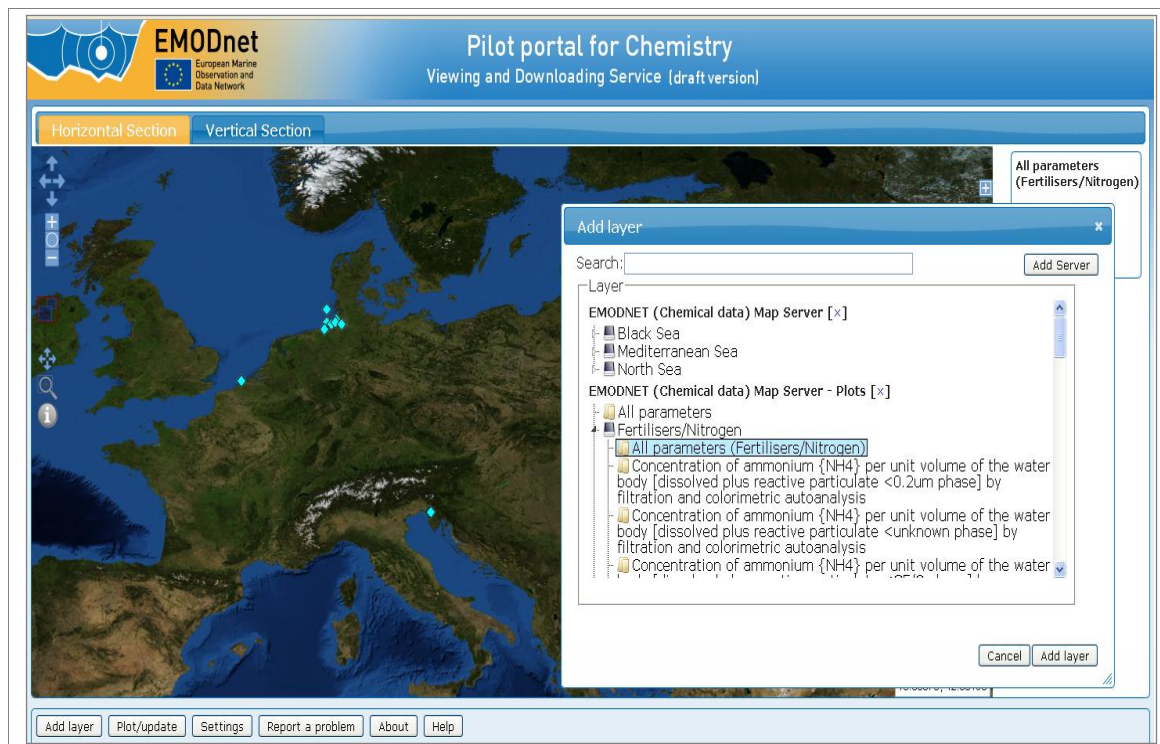
THE OCEANBROWSER

The Chemical Data Products Viewing and Downloading service gives access to integrated maps of selected parameters. The service is available in the DataProducts section of the portal and is based on OGC standards. This web based viewer of climatologies called OceanBrowser was developed by GHER group of Liege University.

The viewer provides access to the two kind of available products:
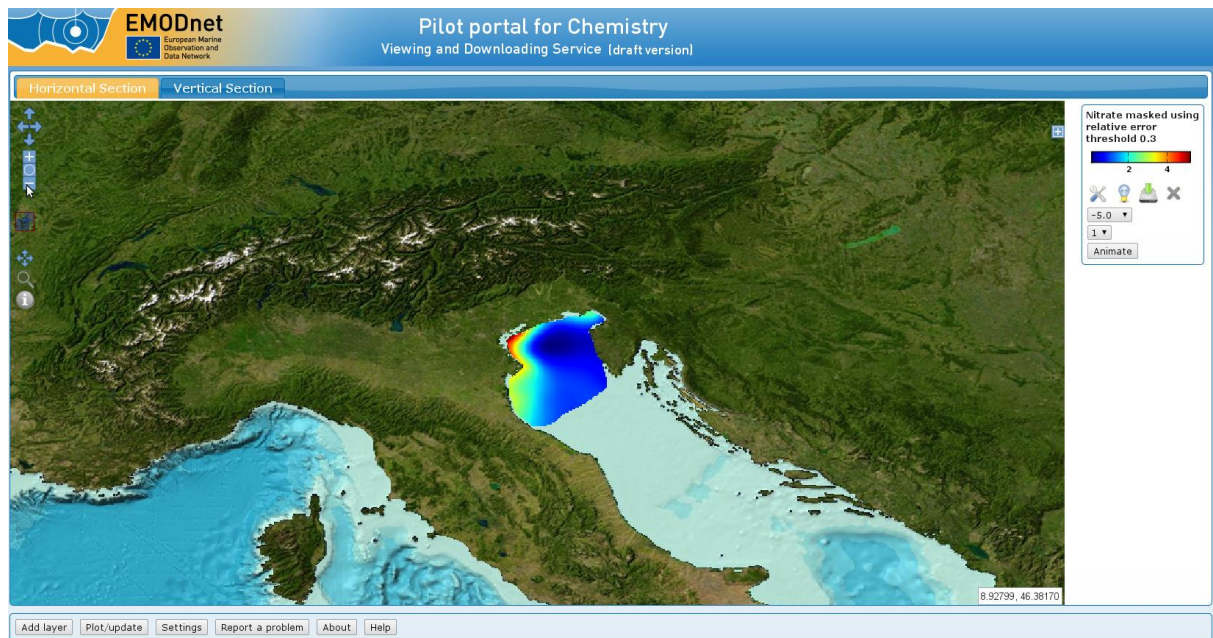
-DIVA interpolated maps. Output images available as horizontal sections and vertical sections. These can be drawn by the selection of an appropriate transept.
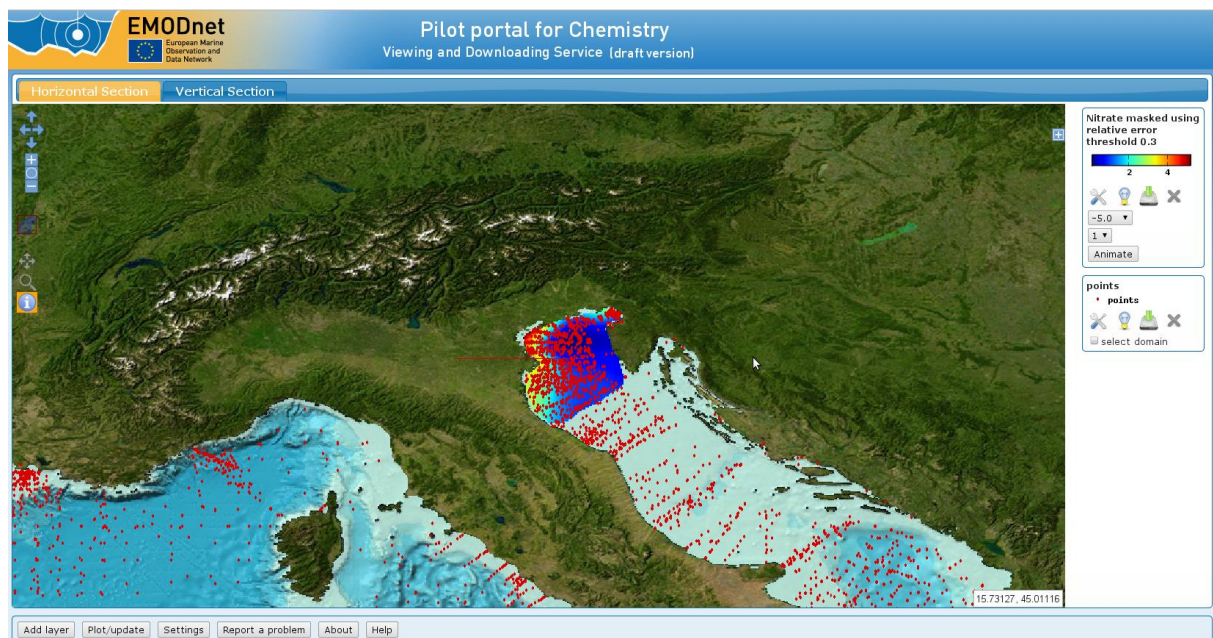
-Time series plots.

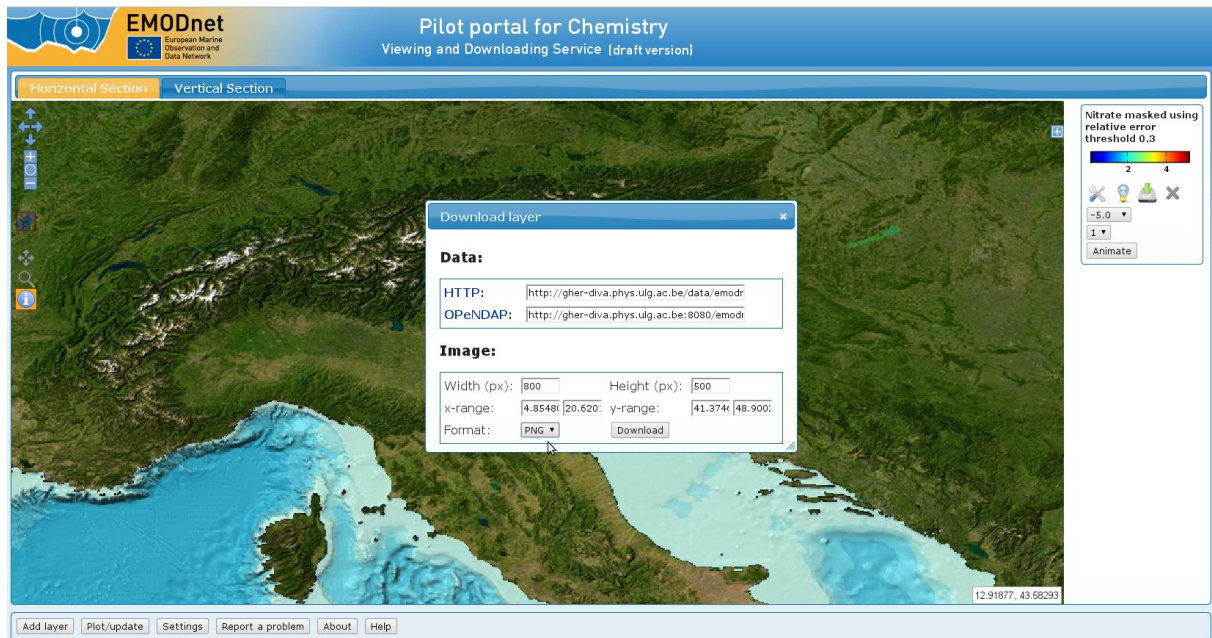*OceanBrowser viewing service with the selection list window of the available products*

An example about interpolated maps:

OceanBrowser viewing service with the selected DIVA interpolated map

OceanBrowser viewing service with the CDI layer overlapped to the selected DIVA interpolated map, obtained thanks to the "Add Server" function.

OceanBrowser downloading the map with the "download layer" window. Format available are: PNG, PDF, EPS, SVG, KML.

An example about time series plots:
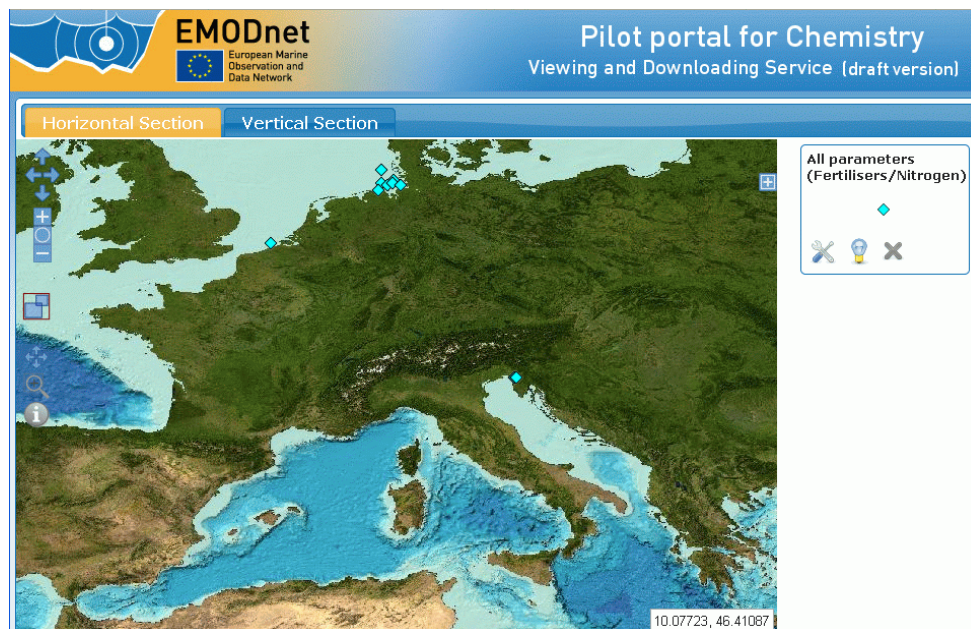
OceanBrowser viewing service with the stations for the selected Fertiliser/Nitrogen parameter

After the parameter was selected, using the "info mode" by clicking on the blue i, it is possible to identify the features of the stations.

OceanBrowser viewing service with the features of the stations: plots and linked CDIs.

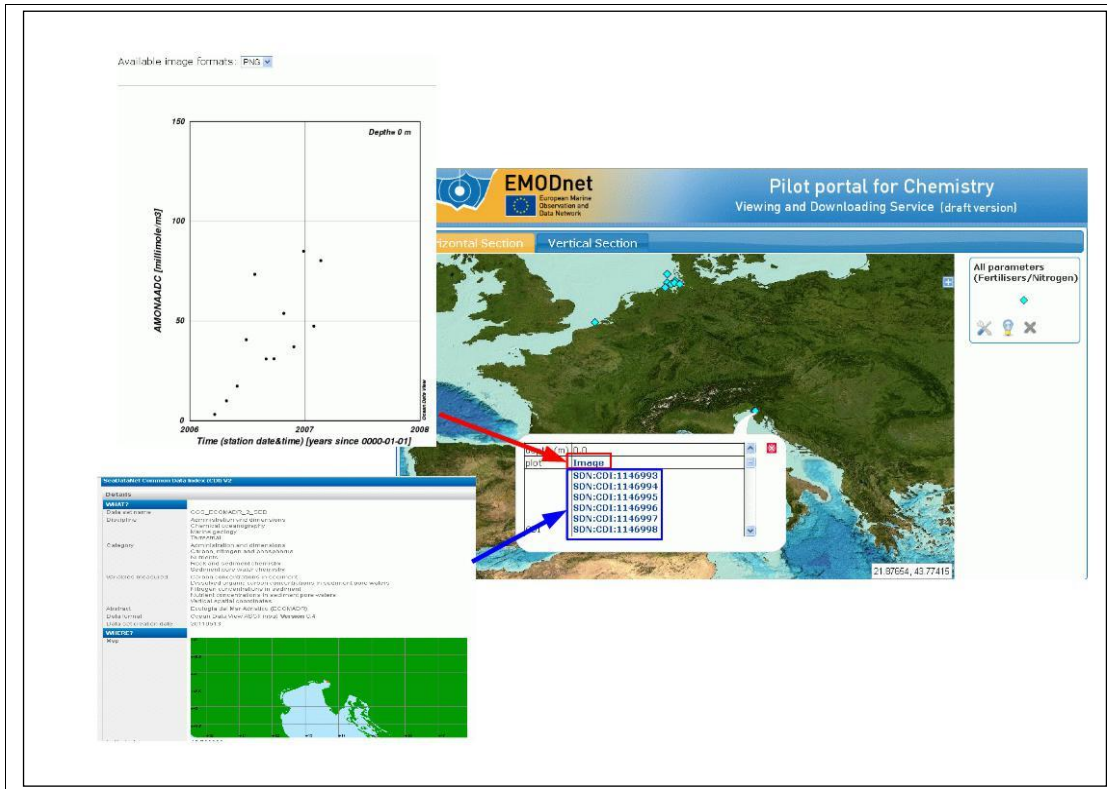Available outputs are images that can be exported in: png, svg, kml and eps formats. The service lets the user to customize the products by choosing some available graphic styles. The stations used to produce the plots are synchronized with the SeaDataNet Common Data Index (CDI), so the metadata are consulted by the portal.

SEXTANT PRODUCTS METADATA CATALOGUE

Sextant catalogue is used to describe the data product: for each data product it is required to populate metadata and its generation, because that will facilitate the exchange and use of data products in various portals.
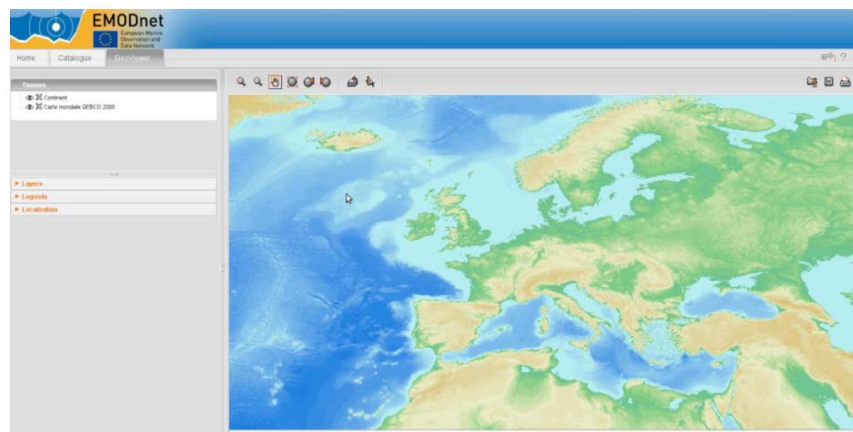
Sextant web interface

LESSONS LEARNED

1 The main barriers to the provision of data and a plan outlining how to overcome those barriers.

With regard to the main barriers to the provision of data, the financial barrier (effort required to prepare data) turned out to be very important as database preparation has been highly time-consuming due to the lack of standardized data formats, collection protocols, measurement units. The amount of resources required could be reduced by agreement and adoption of common standardized procedures/formats. Institutional (willingness of bodies to share data) and legal (rules to limiting access to data) barriers were also of high importance. Formal requests directly from the EEA and EC to the member state policy departments may be effective in removing legal or institutional barriers to the provision of data. In addition, setting mandatory reporting duties on data collection in EC projects and promoting new ways of data publications and of citation of data should be developed and promoted by the EU.

2 The challenges to rendering data interoperable.

The challenge due to the complex data structure which includes several matrices, different analytical protocols, lack of standardized vocabularies and measurement units was approached/tackled by adopting the SeaDataNet infrastructure as technical set up. The setting up/adoption of common standards, common and upgraded vocabularies and standardized QA guidelines will guarantee the interoperability, the homogeneity and the cross-comparability of data.

3 The challenges to producing contiguous data over a maritime basin.

DIVA Standard Interpolated Maps were produced for parameters with homogeneous distribution and suitable data coverage in time and space. For not homogeneous datasets with fragmented coverage, time series plots were produced for single stations were repeated data were available.

4 The fitness for purpose of the data for measuring ecosystem health.

EMODnet Chemistry Lot provides data that can be used for measuring ecosystem health through descriptors 5, 8 and 9 indicated by the MSFD. In particular, the use of the chemistry data in combination with EMODnet biology data and supporting information from the other lots, will enable the assessment of ecosystem health. However, the chemistry portal in its current state of development is unable to provide information strictly comparable between different maritime basins and particular efforts should be dedicated to guarantee homogeneity and standardization of protocols.

5 The priorities and effort required for improving the accuracy, precision and coverage of the data.

Further information on accuracy, precision and limit of detection of chemical methods needs to be added to the portal in order for the user to make correct interpretation of the data. Furthermore, establishing a common quality assurance process for the entire chemical inventory for the EU basins and intercomparison among QA systems already adopted at a national level would be a major priority.

6. The performance of the chosen portal technology in terms of speed of response, user-friendliness.

Feedback on the EMODnet portal were mainly positive, indicating ease of use and navigation, speed of response and reasonable license conditions.

CONCLUSIONS

The EMODnet Chemical pilot has represented a great challenge. In fact, the main difficulties were related to:

- The complexity of the measurements covering 8 groups of parameters (pesticides, antifoulants, pharmaceuticals, heavy metals , hydrocarbons, radionuclides, fertilisers, organic matter) collected on 3 matrices (sediment, water column and biota);

- The geographic heterogeneity of the data distribution (coastal points time series Vs homogeneous sampling at basin level) and of measurement methods (instrument, method, target species, target basis, grain sizes).

To address the first point, data collection was approached with a priority list to proceed over successive steps, starting with a first release ready at the end of the first year (as a proof of concepts), a process that continued throughout the course of the project and the final release at the end of the project.

To address the second point, as highlighted during the Venice expert meeting (organised in September 2010) two main subsets of data products were identified depending upon the available data distribution:

- ➢ DIVA Standard Interpolated Maps, to be produced only for parameters with homogeneous distribution and suitable data coverage in time and space (measured on basin scale),

- ➢ Time series plots, to be produced for not homogeneous datasets as coastal points repeated in time and/or datasets with fragmented coverage.

In fact, it is clear that the use of DIVA standard interpolation is suitable only for the more "classic" sets of parameters measured in the water column. For the parameters measured in the other two matrices such as Biota and Sediment the spatial and temporal distribution of available data highlighted the need of a different commonly agreed analysis approach.

Also, great attention was put on the collection and management of data, providing the best metadata available describing for example: sediment fraction measured, dry/wet weights measurements, measurement methodology. This was considered fundamental in order to help a correct comparison between different data sets. The continuous update and upgrade of SDN common vocabularies was the helping tool to manage this.

A summary of the lessons learned during the three years of activities are:

- Source data are not always easily accessible, there is the need to improve data flow. This also for the Marine Strategy Framework Directive reporting needs;

- For some areas there is a huge work of data/metadata standardization from source datasets (heterogeneous formats, scarcity of metadata);

- The complexity of the measurements need to focus efforts on the collection of a wide metadata description and to continue with the adapting process of SeaDataNet adopted standards;

- The heterogeneity of the measurements highlighted the need to split subsets of homogeneous datasets to generate suitable products;

- The so called "exotic parameters" (contaminants) need an ad hoc QC protocol (no spikes, difficult to apply ranges);

- Products need to have an local group of experts for regular revision.