

Project	AtlantOS – 633211				
Deliverable number	D2.8				
Deliverable title	SOOP Data System Upgrades				
Description	Report on data and connectivity upgrading, documenting system improvements to integrate observing systems, improve network infrastructure, near-real-time delivery of data and best practice for integrated observations to provide data useful for Marine Services and other users				
Work Package number	2				
Work Package title	Enhancement of ship-based observing networks				
Lead beneficiary	UiB, IMR				
Lead authors	Are Olsen, Henning Wehde				
Contributors					
Submission date	27/2/2019				
Due date	PM45				
Comments					



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement n^o 633211.

Stakeholder engagement <u>relating to this task</u>*

WHO are your most important stakeholders?	 Private company If yes, is it an SME or a large company ? X National governmental body X International organization NGO X others Please give the name(s) of the stakeholder(s): Integrated Carbon Observing System (ICOS) Communities of Ocean Action - implementation of SDG14 Copernicus Marine Environmental Monitoring Service (CMEMS) Output Description: X of the stakeholder (S) X of the stakeholder
WHERE is/are the company(ies) or organization(s) from?	 X Your own country X Another country in the EU Another country outside the EU Please name the country(ies): France, Germany, Belgium, Italy, UK etc .
Is this deliverable a success story? If yes, why? If not, why?	Yes, because it has contributed with critical developments towards making near-real-time delivery of data collected on board Ships of Opportunity possible. The developments include principles of automated quality assurance, of data corrections, and preparation of on-line tools for their implementation.
Will this deliverable be used? If yes, who will use it? If not, why will it not be used?	Yes, the developments are relevant for three communities dedicated to SOOP type of observations; the FerryBox, surface ocean CO ₂ and ADCP communities. Some of the methods and tools are already being implemented for operational use.

Table of Contents

E)	(ECUTIVE SUMMARY	1
1.	INTRODUCTION	2
	1.1. Background and objectives	2
2.	METHODOLOGY	2
	2.1.Ferrybox	2
	2.2. Carbon	3
	2.3. ADCP	4
3.	RESULTS AND DISCUSSION	5
	3.1 Ferrybox	5
	3.2 Carbon	6
	3.3 ADCP	7
4.	CONCLUSIONS AND OUTLOOK	9
5.	REFERENCES	9

EXECUTIVE SUMMARY

Our knowledge of the ocean is limited by our observational ability and the ocean continues to be severely under-sampled. To better understand and manage the ocean and coastal systems, there is a clear need for environmental data of high spatial and temporal resolution. Efforts within global and regional programmes to better coordinate observing efforts internationally are evolving. However, collecting the data can prove costly. Recent efforts have shown great promise in reducing this cost by taking advantage of ships of opportunity (SOOP) as platforms for environmental data collection. There are numerous advantages to the SOOP program: no ship running costs, no energy restrictions, regular maintenance is possible, transects are sampled repeatedly and problems with biofouling of sensors can be controlled by automated maintenance/cleaning procedures. The installed systems can integrate data on water quality and meteorological conditions with GPS information into a data stream that is automatically transferred from ship to shore. There is great potential for obtaining good data coverage using ferries and cargo ships sailing a fixed route on a regular basis.

Already in the 1930s observational systems were developed to be installed on ships-ofopportunity. As examples, the Sir Alistair Hardy or the activities on the Hurtigruten ships by IMR can be named. These provide long-term data for understanding variability in the ocean. In recent years the data transmission and quality assurance have become more and more operational and many SOOP data are now actually available in near real time through the Copernicus Marine Environmental Monitoring Services (CMEMS). Here we describe AtlantOS activities towards operationalizing the data streams and quality assurance of Ferrybox and Carbon SOOP data, and for shipboard current measurements from Acoustic Doppler Current Profilers (ADCPs).

1. INTRODUCTION

1.1. Background and objectives

Scientific instruments deployed on commercial vessels form an important part of the global observing system. These instruments provide large amounts of data, for instance on temperature and salinity, ocean currents (Petersen and Colijn, 2017; Petersen et al., 2008; Vindenes et al., 2018) and surface carbon (Bakker et al., 2016). While some observations (T and S) are operationalized to a large degree and their data relayed in near real time to user groups, the situation at the beginning of the AtlantOS project for Ferrybox, surface CO₂, and ADCP data was far less advanced. This is the result of many factors; the instruments are complex, many different types exist, the types of data they deliver vary, and as a consequence the procedures for working up the data to a useable and interpretable level are manifold. Within the course of the AtlantOS project this situation has improved and near real time data streams for the Ferrybox data and the CO₂ data have been implemented in order to make the data available within the CMEMS and in the EmodNet and GOOS/EuroGOOS activities. For the underway measurements of ocean currents with ADCP, development and application of methodology to detrend the measurements from, for example tidal motions, was emphasised as this is prerequisite for providing current and transport estimates in an operational mode.

This report describes the efforts undertaken in the course of the project period in terms of improving near real time data availability, quality control, integration and network infrastructure.

2. METHODOLOGY

2.1.Ferrybox

FerryBox technology is used for taking automated measurements aboard ships of opportunity. The core ocean parameters measured are temperature, salinity, turbidity, and chlorophyll-a fluorescence. In addition, non-standard sensors provide data on currents and sediment transport, pH, oxygen, nutrients, and algal species on specific SOOPs. Currently, Ferrybox systems are installed on many vessels by a network of Ferrybox contributors, mainly national marine research institutes and environmental agencies. The main actors of the Ferrybox community are working together to improve the Ferrybox approach in the EuroGOOS task team Ferrybox. The readers are refered to their website (http://www.ferrybox.org) in order to obtain recent news, publications on updates on improvement of the systems and network).

The principal idea of the Ferrybox approach is to use ships of opportunity like ferries on fixed routes to make automated measurements of important oceanographic parameters. Those measurements are made in a flow-through system where different sensors are applied to continuously measure parameters. Many Ferryboxes are equipped with automatic cleaning systems so that the effort for manual maintenance is reduced. The sensors installed offer the opportunity to measure a variety of important physical (Temperature, Conductivity (Salinity), turbidity,..), chemical (nutrients, pH, DOC, oxygen, ...), and biological (Chlorophyll, phytoplankton composition, dominant/harmful species) parameters .

The near real time quality control procedures used in the CMEMS data streams are based on Schuckmann et al. (2009), but further developed especially to consider the improvement of the near real time quality control for biological data in the recent years

Ferrybox systems have evolved with a set of standard sensors to a mature observational system

- FB systems allow cost-effective measurements with high resolution in space and time along a certain route;
- FB data may strongly support the validation of numerical ocean models;
- FB data can be used as ground truth measurements for satellite remote observations;
- New developments of biogeochemical sensors enable full insight into ocean acidification and the impact of coastal oceans on atmospheric CO₂;
- Continuous and long-term observations of the carbon cycle enable the detection of climate relevant changes in coastal and open ocean waters;
- FB systems enable discrete water sampling on certain positions for specific compounds (e.g. contaminants, micro plastics, etc.) without extra cost;
- A common European FB database including data quality control increases the availability of FB data and supports the activities of CMEMS and EMODnet;
- FB systems are still operated mainly by research money and suffer from unsustainable funding in the long term;
- New FB lines must be developed, especially in the Mediterranean and Black Sea;
- There is a further need for discussions with all potential stakeholders on which type of data products are needed to fulfil science or societal requirements e.g. for environmental assessments.

2.2. Carbon

Surface ocean carbon observations are conducted by a loosely coordinated network of commercial and research vessels where instruments that measure the sea surface CO₂ fugacity (fCO₂, this is the CO_2 partial pressure corrected for the non-ideal behaviour of the CO_2 gas) are installed. Over the recent years, the management and wider distribution of these data has been significantly improved, in particular in the framework of SOCAT, the Surface Ocean CO_2 Atlas (Bakker et al., 2016). SOCAT provides annual synthesis products of surface ocean fCO_2 data. However, this is a delayed-mode product; up to a year can pass between data collection and release. There are several rate limiting factors, the two most important are ship-to-shore data transfer and processing software that can handle delivered data with no or little human input and pass them on to user groups in NRT. One of the suggested activities in the grant agreement was implementing the Iridium Short Burst Data (SBD) service for ship-to-shore transfer to deal with the first. However, we have since discovered that (i) an Iridium based protocol for data transfer already exists, and more importantly (ii) the recent developments towards digitalization of society also occur for the fleet of merchant and research vessels, so most ships now have regular (several times a day) or continuous internet access and data transfer via their email systems are becoming the norm. Therefore we have focussed on the second suggested activity in the grant agreement, developing processing software for such data.

The processing software, QuinCe is based on the fCO_2 data reduction routines described in Pierrot et al. (2009), which are based of the Guide to Best Practices for Ocean CO_2 measurements (Dickson et al., 2007). These are implemented in the Java programming language with additional tools for quality checking (QC) the data. The quality checks are in principle fully automatic, but can be refined through user input.

Briefly, the steps to reduce the data are:

-calibration of the CO_2 mole fractions, xCO_2 , reported by the infrared sensor using its measurements of standard gasses;

-conversion of the calibrated xCO₂ data to pCO₂ including a water vapour correction;

-correcting for the non-ideal behaviour of pCO₂, so that data on fCO₂ are obtained;

-corrections for the temperature difference between the seawater and the equilibrator where the measurements are done.

Automatic quality control routines by QuinCE include:

- file format checks;
- time stamp checks;
- range checks (bad/impossible and questionable);
- constant value checks (may indicate instrument malfunction);
- outlier checks (standard deviation range checks);
- checks for excessive gradients during a certain period;

Following these automated QC routines the data are made available for NRT distribution. In addition, the principal investigator of the line receives a notification and can perform additional quality checks, resulting in fully quality controlled delayed mode data. A range of QC tools are available, and the PI can accept or override the automatic QC flags, or provide additional. These tools include maps, graphs and tables for visual checks, performs QC on the external gas standards, and provides an overview of system diagnostics.

2.3. ADCP

In order to provide realistic current and transport data from ADCPs installed on board SOOPs, the tidal current component has to be corrected for. A methodology was developed and applied (Vindenes et al., 2018). This methodology now allows the analysis of the data set for realistic current and transport estimations (Vindenes et al., 2019), enabling the provision of a realistic current data set in near real time. The ADCP-instruments transmit sound, commonly referred to as pings, of a known frequency along four beams down into the water column. The ping returns to the instrument with a change in frequency depending on the velocity of the ocean, the doppler shift. For example, if there is an oncoming current, the return frequency is increased. The measurements from all four beams are combined to determine the ocean velocity in three dimensions relative to the instrument. Absolute ocean velocities are determined by subtracting the velocity of the ship. For each ping the velocity is determined and grouped in vertical bins. During processing, velocity determined from each ping are averaged over a set time increment to create ensembles. The exemplary ADCP dataset used within the AtlantOS activity consists primarily of 3 min and some 5 min ensembles. For this activity we are focusing on the data from the MV Nuka Arctica traveling from Aalborg (Denmark) and Nuuk (Greenland), and MV Norröna travelling from Hirtshals (Denmark) via Torshavn (Faroese) to Seyðisfjörður (Iceland), partly the Norrøna have had Bergen (Norway) as its harbour instead of Hirtshals. Both the vessels have cruising speeds of approximately 15 to 20 knots, so the horizontal resolution of the ADCP data varies from around 1400–3100 m. Vertically the ADCP data are separated into 8 m bins. When the vessels are sailing in the North Sea, the instruments are predominantly run in broadband mode with bottom tracking. The navigation source on both ships is the Ashtech ADU5 with a 4-antenna array.

3. RESULTS AND DISCUSSION

3.1 Ferrybox

In the course of the AtlantOS project the Ferrybox data availability has become much more operational. In collaboration with the EuroGOOS task team Ferrybox an online Common European Ferrybox database and data portal have been developed and made available. In addition are data from all Ferrybox lines included in the CMEMS and available in real time. The EModNet data portal is also including the Ferrybox data, via a data stream from the CMEMS.



Figure 1: Schematic diagram of the European Ferrybox database. (Taken from Petersen and Colijn, 2017)

While in the period prior to the implementation of the operational CMEMS, i.e. during era of the MyOcean projects, the efforts were geared towards the improvement of the physical parameters of the Ferrybox observations, during recent years priority has been given to improving quality control of biogeochemical parameters, in order to enable their real time data flow. Acceptable data ranges have been refined especially for the coastal regions, where now more and more data become available through the Ferrybox measurements. Those ranges are now implemented and used for the detection of erroneous data in the real time data flow, for example in the CMEMS. Figure 2 shows the ocean provinces in which the ranges for the biological parameters are much improved.



Figure 2. Ocean provinces used to define allowable ranges for Ferrybox measurements, based on Spalding et al. (2007, 2012). The different colours indicate type of province, e.g. green is coastal.

3.2 Carbon

QuinCe officially was released in August 2018 and is available at GitHub (https://github.com/BjerknesClimateDataCentre/QuinCe) under a GNU General Public License v3.0. It was deployed for first live use in December 2018 and was tested locally. Daily data are being received from one station, which can be submitted as soon as the final deployment is complete. Work towards retrieving data from a second station is under way.

In practice, the users upload a data file and identifies/confirm its format, in particular in terms of the columns in which the various measured variables occur (e.g. time, position, xCO₂, sea surface temperature, etc.). This step is crucial as the output from the various available instruments varies in format and content, and the set-up is saved by the system for automatic data handling. QuinCe then preforms the automatic QC as described in Sect 2.2, and passes the data onwards to various NRT user groups and notifies the PI of the data, that they are ready for delayed mode QC. Detailed documentation is available at GitHuB.

QuinCe is currently being implemented for the stations that are part of the network coordinated by the Integrated Carbon Observing System (ICOS) under the Ocean Thematic Centre (OTC). It is made available and can be deployed by any other group or network that collects underway fCO₂ data. A screenshot of a QuinCe Session is provided in Figure 3.

GOFL2015041	0 – Qualit	y Control									
				Reykja	vik	470 460 00 10 10 10 10 10 10 10 10 10 10 10 10	h, M	~~~n~~n	- Harris		1 17/5 ₁ ,
					5	13 Ap	pr	14 Apr Date/Time	15	Apr	16 Apr
K 🔘 🖫	Q					E © SE	Q				
Date	Longitude	Latitude	Intake Temperature	Salinity	Equilibrator Temperature	Equilibrator Pressur	re (differential)	Ambient Pressure	CO2 fCO2	Automatic QC	Manual QC
2015-04-15 03:07:58	-30.450	61.176	5.745	34.177	4.880)	-2.260	997.980 4	419.980 460.067	Bad	Good
2015-04-15 03:09:02	-30.456	61.175	5.743	34.175	4.880)	-2.190	998.310 4	419.720 459.968	Bad	Good
2015-04-15 03:10:06	-30.461	61.175	5.743	34.175	4.860)	-2.650	997.330 4	419.370 459.356	Bad	Good
2015-04-15 03:11:11	-30.466	61.174	5.740	34.173	4.850)	-2.580	997.790 4	419.000 459.391	Bad	Good
2015-04-15 03:12:15	-30.472	61.173	5.742	34.174	4.840)	-2.440	997.260 4	419.180 459.612	Bad	Good
2015-04-15 03:13:19	-30.477	61.173	5.743	34.175	4.820)	-3.020	998.310 4	418.950 460.019	Questionable	Questionab
2015-04-15 03:14:23	-30.483	61.172	5.742	34.174	4.810)	-2.280	997.830 4	418.710 460.087	Bad	Good
2015-04-15 03:15:27	-30.488	61.172	5.741	34.174	4.820)	-2.560	998.060 4	418.680 459.819	Bad	Good
2015-04-15 03:16:52	-30.495	61.171	5.739	34.170	4.840)	-2.610	998.400 4	418.680 459.525	Bad	Good
2015-04-15 03:17:56	-30.500	61.170	5.739	34.170	4.860)	-2.380	997.540 4	418.940 459.074	Bad	Good
2015-04-15 03:19:01	-30.506	61.170	5.734	34.167	4.870)	-2.740	997.700 4	419.180 458.929	Bad	Good

Sensors Calculations Diagnostics

Selection: 0 🗵 Accept Automatic QC Override Automatic QC | Finish

Figure 3 Screenshot of a QuinCe session on an underway CO₂ cruise. Notice columns "Automatic QC" (done by QuinCE) and "Manual QC" (by the PI).

QuinCe is key for integrating NRT and delayed mode data into networks like CMEMS. Currently it handles underway fCO_2 and accompanying physical oceanographic and atmospheric measurements but expansion to include further underway data on seawater CO_2 chemistry so to comply with EOV Inorganic Carbon specification, where at least 2/4 variables are required, is envisioned.

3.3 ADCP

In order to improve the availability of current measurements and transport estimates the existing datasets from the Nuka Arctica and Norrøna vessels were exemplarily analysed to extract the tidal compartments of the current system for the northern North Sea. The developed methodology provides tidal ellipses for the regions, for example as displayed in Figure 4 for the depth of 53 meters. Those ellipses can be used for the evaluation of numerical models and for general information (Vindenes et al., 2018)



Fig. 4. Tidal ellipses of the two main semi-diurnal tidal constituents M2(A), and S2(B), and the two main diurnal tidal constituents K1(C), and O1(D). Ellipse parameters are calculated from ADCP current measurements from 53m depth. Note that reference ellipse in (A) and (B) has a 10cm/s radius, while in (C), and (D) it has a radius of 5cm/s. Blue ellipses rotate clockwise, red ellipses rotate counter clockwise.

This extraction enables the estimation of the depth-averaged mean current along the most traversed routes with the ADCPs and shows realistic circulation features for the northern North Sea (Figure 5)



Figure 5: Map of the Northern North Sea with depth-averaged current estimates from the ADCP measurements. Contour lines show bottom depth in 50 m increments, while the colour scale is set at 25m increments. (Taken from Vindenes et al., 2019)

4. CONCLUSIONS AND OUTLOOK

After a couple of decades Ferrybox, Carbon, and ADCP observational systems have been developed into a stage of maturity. The loosely coordinated networks of commercial and research vessels where instruments are installed and the different parameters are measured have been able to strengthen their efforts in order to provide the community with near real time data for the physical and biogeochemical parameters from the Ferryboxes and the CO₂ instruments on board the SOOPs. The main challenge remaining is for the near real time delivery of the full range of current measurements and transport estimates. Here the analysis of the data was strongly improved during the AtlantOS period, but the near real time delivery is still challenging because of the transmission of large data volumes from the acoustic devices that are necessary in order to transmit all the information needed. Major achievements are undertaken in general in terms of the data quality assurance, which provides the community with quality information that is necessary to assess the uncertainty of the data obtained.

For all the measurements obtained from the SOOP and VOS activity the implementation into the actual common data flow systems has been highly improved and the inclusion of the data stream into the CEMS provides the large opportunity of an extensively increased use of the data in future.

5. REFERENCES

- Bakker, D.C.E., Pfeil, B., Landa, C.S., Metzl, N., O'Brien, K.M., Olsen, A., Smith, K., Cosca, C., Harasawa, S., Jones, S.D., Nakaoka, S.I., Nojiri, Y., Schuster, U., Steinhoff, T., Sweeney, C., Takahashi, T., Tilbrook, B., Wada, C., Wanninkhof, R., Alin, S.R., Balestrini, C.F., Barbero, L., Bates, N.R., Bianchi, A.A., Bonou, F., Boutin, J., Bozec, Y., Burger, E.F., Cai, W.J., Castle, R.D., Chen, L., Chierici, M., Currie, K., Evans, W., Featherstone, C., Feely, R.A., Fransson, A., Goyet, C., Greenwood, N., Gregor, L., Hankin, S., Hardman-Mountford, N.J., Harlay, J., Hauck, J., Hoppema, M., Humphreys, M.P., Hunt, C.W., Huss, B., Ibánhez, J.S.P., Johannessen, T., Keeling, R., Kitidis, V., Körtzinger, A., Kozyr, A., Krasakopoulou, E., Kuwata, A., Landschützer, P., Lauvset, S.K., Lefèvre, N., Lo Monaco, C., Manke, A., Mathis, J.T., Merlivat, L., Millero, F.J., Monteiro, P.M.S., Munro, D.R., Murata, A., Newberger, T., Omar, A.M., Ono, T., Paterson, K., Pearce, D., Pierrot, D., Robbins, L.L., Saito, S., Salisbury, J., Schlitzer, R., Schneider, B., Schweitzer, R., Sieger, R., Skjelvan, I., Sullivan, K.F., Sutherland, S.C., Sutton, A.J., Tadokoro, K., Telszewski, M., Tuma, M., van Heuven, S.M.A.C., Vandemark, D., Ward, B., Watson, A.J., Xu, S., 2016. A multi-decade record of high-quality fCO₂ data in version 3 of the Surface Ocean CO2 Atlas (SOCAT). Earth Syst. Sci. Data 8 (2), 383-413.
- Dickson, A. G., Sabine, C. L., Christian J. R., 2007. Guide to Best Practices for Ocean CO₂ measurements. PICES Special Publication 3., 191 pp.
- Petersen, W. and Colijn, F., 2017, Ferrybox White Paper, EuroGOOS Publication, available at http://eurogoos.eu/download/publications/EuroGOOS_Ferrybox_whitepaper_2017.pdf
- Petersen, W., Wehde, H., Krasemann, H., Colijn, F., F. Schroeder, 2008. FerryBox and MERIS Assessment of coastal and shelf sea ecosystems by combining in situ and remotely sensed data Estuarine, Coastal and Shelf Science, 77, 296-307.
- Pierrot, D., Neill, C., Sullivan, K., Castle, R., Wanninkhof, R., Luger, H., Johannessen, T., Olsen, A., Feely. R. A., Cosca, C. E., 2009. Recommendations for autonomous underway pCO₂ measuring systems and data-reduction routines, Deep-Sea Res. II, 56, 512-522.
- Spalding, M.D., Fox, H.E., Allen, G. R., Davidson, N., Ferdaña, Z. A., Finlayson, M., Halpern. B. S., Jorge, M. A., Lombana, A., Lourie, S. A., Martin, K. D., McManus, E., Molnar. J., Recchia, C. A., Robertson, J., 2007.
 Marine Ecoregions of the World: A Bioregionalization of Coastal and Shelf Areas. BioScience, 57, 573– 583.

Spalding, M. D., Agostini, V. N., Rice, J., Grant, M. S., 2012. Pelagic provinces of the world: A biogeographic classification of the world's surface pelagic waters', Ocean and Coastal Management, 60, 19–30.

Vindenes, H., Orvik, K. A., Søiland, H., Wehde, H., 2018. Analysis of tidal currents in the North Sea from shipboard acoustic doppler current profiler data. Continental Shelf Research, 162, 1 – 12.

- Vindenes, H., Orvik, K. A., Søiland, H., Wehde, H., 2019. Mean current and volume transport estimation derived by shipborne measurements. In submission to Continental Shelf Research.
- Von Schuckmann, K., Garau, B., Wehde, H., Gies T., Durand, D., Reseghetti, F., 2009. Real Time Quality Control of temperature and salinity measurements, MyOcean document. Adopted as EuroGOOS recommendation document.