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Work Package title	Data flow and data integration
Lead beneficiary	UiB, CNRS/LSCE
Lead authors	Siv K. Lauvset
Contributors	Are Olsen, Marion Gehlen, Anna Sommer
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Comments	

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Stakeholder engagement relating to this task*

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 ☐ others Please give the name(s) of the stakeholder(s): International Ocean Carbon Coordination Project (IOCCP) Global Carbon Project (GCP) WCRP Coupled Model Intercomparison Project (CMIP) Integrated Carbon Observing System (ICOS) Surface Ocean Lower Atmosphere Study (SOLAS) Integrated Marine Biosphere Research project (IMBER) Communities of Ocean Action - implementation of SDG14 National Oceanic and Atmospheric Administration (NOAA) Copernicus Marine Environmental Monitoring Service (CMEMS)
WHERE is/are the company(ies) or organization(s) from?	X Your own country X Another country in the EU X Another country outside the EU Please name the country(ies): The surface ocean carbon syntheses prepared within this deliverable are used globally.
Is this deliverable a success story? If yes, why? **If not, why?**	Yes, because it contributed critically to the production of the Surface Ocean CO2 Atlas (www.SOCAT.info), the most used data product for surface ocean carbon EOV data and further enabled development of a statistical model for carbon cycle EOVs, which will provide yearly updated reconstructions of monthly pCO_2 distributions as new releases of SOCAT become available.
Will this deliverable be used? **If yes, who will use it?** **If not, why will it not be used?**	Yes, SOCAT is heavily used by the global carbon cycle research community. For example these data directly feed into the annual assessments of the global carbon budget, published every year by the Global Carbon Project, released at the annual COP meeting. SOCAT is used in a total of 40-50 peer reviewed publications each year. Further, it is foreseen for the statistical reconstructions of pCO2 to be integrated to the

	CMEMS product catalogue. They are useful a benchmark for numerical models and priors for atmospheric inversions.

Table of Contents

Table of Figures

EXECUTIVE SUMMARY

Understanding the global ocean carbon sink is of key importance for understanding the future of the oceans. The oceans are a crucial source of food and energy, as well as being a large economic entity for tourism and transport. These ocean services are likely to be affected by changes in ocean carbon, especially ocean acidification.

AtlantOS deliverable 7.10 is a report on the AtlantOS synthesis work on the essential ocean variable (EOV) surface carbon. EOVs are defined based on their relevance to climate, ocean services, and ocean health, their high technical and scientific feasibility, cost efficiency, and high impact on knowledge and understanding. Inorganic carbon is an EOV and on the surface the most important component is pCO_2.

AtlantOS has contributed to the Surface ocean Carbon Atlas (SOCAT) through dissemination of best practices and quality control procedures, an active role in quality control of AtlantOS and other data in the Atlantic Ocean, and creating the annual SOCAT data products. Including AtlantOS data in SOCAT ensures their visibility and use globally.

AtlantOS has also developed a statistical model to reconstruct monthly pCO_2 distributions and air-sea flux of CO_2. The rationale for developing a novel statistical model is to enable the yearly release of carbon system EOVs and to contribute to the main AtlantOS objective to design an optimal multi-platform observing system for surface ocean pCO_2.

This report outlines the work AtlantOS has done for SOCAT (section 3.1) and how this has aided the development of a new statistical model (section 3.2). Relevance for the overarching AtlantOS objectives and ongoing and future work is provided in section 4.

1. INTRODUCTION

1.1. Background and objectives

The Voluntary Observing Ship network forms the backbone of the global observation system for the ocean CO_2 sink. Its data, sea surface fCO_2, are regularly integrated to a global product, the Surface Ocean Carbon Atlas (SOCAT, www.socat.info). The SOCAT database and products is a major international community effort for the assembly, quality control and distribution of surface ocean fCO_2 observations. In fact, over the course of the 10 years since its inception it has established itself as the most important and encompassing activity of its kind.

The objectives in AtlantOS deliverable 7.10 are to:

- (i) provide data from the network to SOCAT;
- (ii) subject those data to secondary QC according to SOCAT and ICOS protocols;
- (iii) make available synthesis products
- (iv) produce proof-of-concept that statistical technique can resolve seasonal and interannual variability

1.2. Essential Ocean Variables (EOV)

According to the International Ocean Carbon Coordination Project (IOCCP), which acts as the expert panel on ocean biogeochemistry for the Global Ocean Observing System (GOOS), an "Essential Ocean Variable is a sustained measurement or a group of measurements necessary to assess state and change at a global level, and to increase societal benefits from the ocean [on scales from global to regional]".

The EOVs were determined and defined by identifying which scientific and societal challenges facing us in the coming decade rely on observation of ocean biogeochemistry. One of the biogeochemistry EOVs that have been defined is named "inorganic carbon" and contains the sub-variables necessary to constrain the ocean carbon cycle at a point in time and space. Table 1 gives more detailed information on this EOV and its sub-variables.

The sub-variable of particular interest in this deliverable is the partial pressure of carbon dioxide (pCO_2), or CO_2 fugacity (fCO_2), which has been corrected for the non-ideality of CO_2 gas. These are very similar, and both terms have been used in this report. pCO_2 data are important to answer scientific challenges relating to air-sea CO_2 fluxes and ocean acidification, and societal challenges relating to the size of the ocean carbon sink and impacts of ocean acidification on ecosystem services.

Table 1. Information about the essential ocean variable (EOV) "inorganic carbon". From the GOOS Biogeochemistry panel's description: http://www.ioccp.org/images/10FOO/BGC-EOV-Spec-Sheets_Aug-2017/03-EOV-BGC_Inorganic-Carbon_20170825.pdf.

Table 1: EOV Information	
Name of EOV	Inorganic Carbon
Sub-Variables	Dissolved Inorganic Carbon (DIC), Total Alkalinity (TA), Partial pressure of carbon dioxide (pCO_2) and pH. *[At least two of the four Sub-Variables are needed.]*
Derived Products	Saturation state (aragonite, calcite), Dissolved carbonate ion concentration, Air-sea flux of CO_2, Anthropogenic carbon, Change in total carbon
Supporting Variables	Surface and subsurface Temperature, Surface and subsurface Salinity, Ocean vector stress (wind speed), Atmospheric column-averaged dry-air mole fraction of CO2 (xCO_2), Barometric pressure, Oxygen, Calcium concentration, Transient tracers, Oxygen to argon ratio (O_2/Ar)
Responsible GOOS Panel	GOOS Biogeochemistry Panel Contact: ioccp@ioccp.org

2. METHODOLOGY

2.1. SOCAT

The AtlantOS activities towards SOCAT have taken place over the entire project period to support the annual releases of SOCAT. Prior to the AtlantOS funding new versions of SOCAT were released every few years, but with the decision of the SOCAT coordination group to proceed to annual releases of SOCAT, we decided that it was preferable to support the actual annual SOCAT releases rather than to pursue intermediate products on the same schedule.

Work in AtlantOS has specifically gone towards ingesting data into the SOCAT system, performing the actual quality control of the data, and preparing the final SOCAT synthesis product. AtlantOS has so far contributed in this way to SOCATv4 (released June 2016, described in Bakker et al. (2016), Figure 1) and SOCAT v5 (released June 2017, Figure 2). AtlantOS is also contributing towards SOCAT v6 (ongoing and planned for June 2018, Figure 3) and will contribute in the same way towards SOCATv7 (planned for June 2019).

2.2. Statistical model

We developed a statistical model for the *reconstruction of monthly surface ocean pCO_2 from 2001 to 2016 at a global resolution of 1°x1°*. The approach is based on a two-step non-linear feed forward neural network (FFNN). Driver data (predictors) are provided by the 'Copernicus Marine Environment Monitoring Service (CMEMS)' for (1) the reprocessed monthly global observed (all at 0.25°x0.25°) for sea surface salinity (SSS), sea surface temperature (SST), sea surface height (SSH); and (2) chlorophyll a (Chl) from GLOBCOLOUR. Mixed layer depth (MLD) is taken from the "Estimating the Circulation and Climate of the Ocean, Phase II (ECCO2)" project at 0.25°x0.25° resolution. The set of predictors is completed by the atmospheric CO_2 mole fractions (xCO2, atm) from the Jena atmospheric CO_2 inversion, s76_v4.1, on a 5°x5° grid. Finally, a mask is applied over sea-ice covered regions based on daily Operational Sea Surface Temperature and Sea Ice Analysis (OSTIA) (0.05°x0.05° horizontal resolution). All driver data are averaged in space or interpolated on

the 1°x1° grid used by SOCAT. Monthly averages are computed if necessary. For algorithm training, predictors are co-localized at the SOCAT data positions.
In a first step, the model is trained to reproduce climatological distributions of surface ocean pCO_2 based on Takahashi et al. (2014). Month to month anomalies of surface ocean pCO_2 are added to the climatological distribution in a second step. Gridded surface ocean CO_2 fugacity measurements from SOCATv5 (Bakker et al., 2016; https://www.socat.info/index.php/data-access/) provide the target for step 2. The SOCATv5 data set includes data from moorings, ship tracks and drifters. Data are distributed irregularly over the global ocean with 188274 individual measurements over the Northern hemisphere and 76065 over the Southern hemisphere. The period of reconstruction of surface ocean pCO_2 (2001-2016) represents ~77% of all data included in SOCATv5.

3. RESULTS AND DISCUSSION

3.1 SOCAT

Understanding the global ocean carbon sink is of key importance for understanding future climate change due to human CO_2 emissions. Key research questions include how much CO_2 is taken up by the ocean, how much excess carbon is stored in the ocean, how much the ocean pH is changing (ocean acidification), and on which time scales the ocean carbon sink adapts and changes.
One of the major reasons that we are able to quantify the size of the ocean carbon sink is that we for the past several decades have observed rising CO_2 in the surface ocean. These observations make it clear that the partial pressure of CO_2 in the ocean is increasing at approximately the same rate as the partial pressure in the atmosphere (Figure 5). While it is a good thing for the atmosphere that the ocean is removing CO_2, the uptake by the ocean is the direct cause of ocean acidification.
The ocean carbon system is in a delicate balance, which is being disrupted by human activities. The observations of the EOV inorganic carbon in the ocean, and changes happening to this EOV, are crucial for full understanding of several critical phenomena in the earth system. In order for that understanding and knowledge to come about, continued high level quality control of the observations will be required for a long time. The support AtlantOS has provided towards this task is invaluable.
AtlantOS quality controlled 207 data files for SOCATv4 and 391 data files for SOCATv5. So far, AtlantOS has also quality controlled 275 data files for SOCATv6.

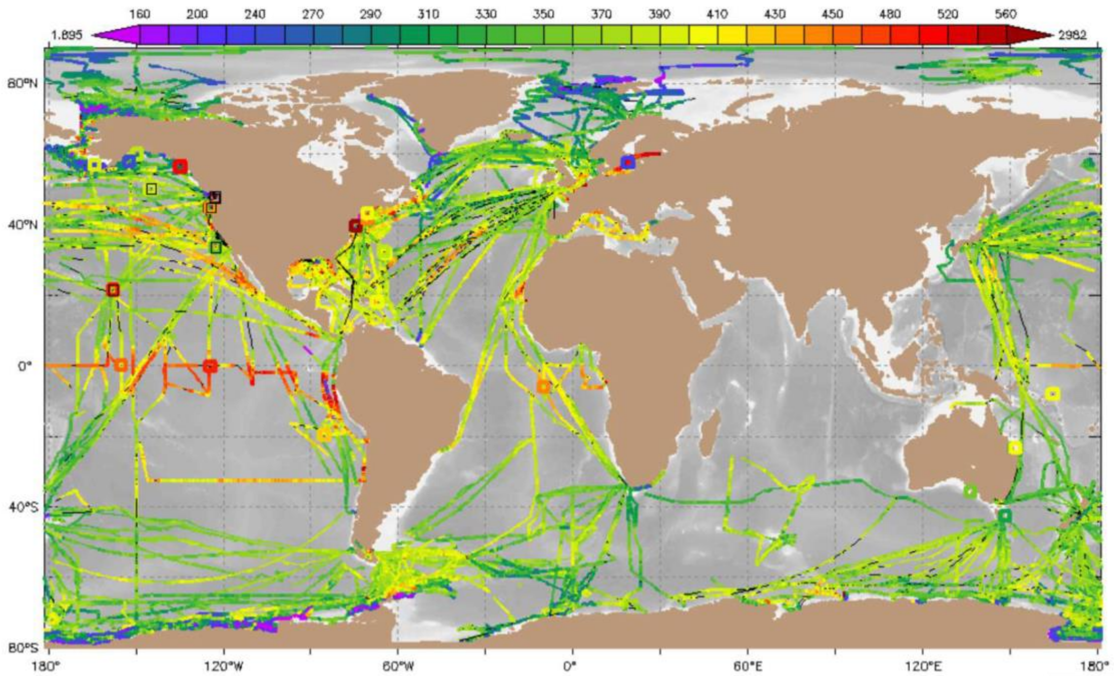

Figure 1. Map showing all new data in SOCATv4. SOCATv4 was released for public use in June 2016. Figure from www.socat.info

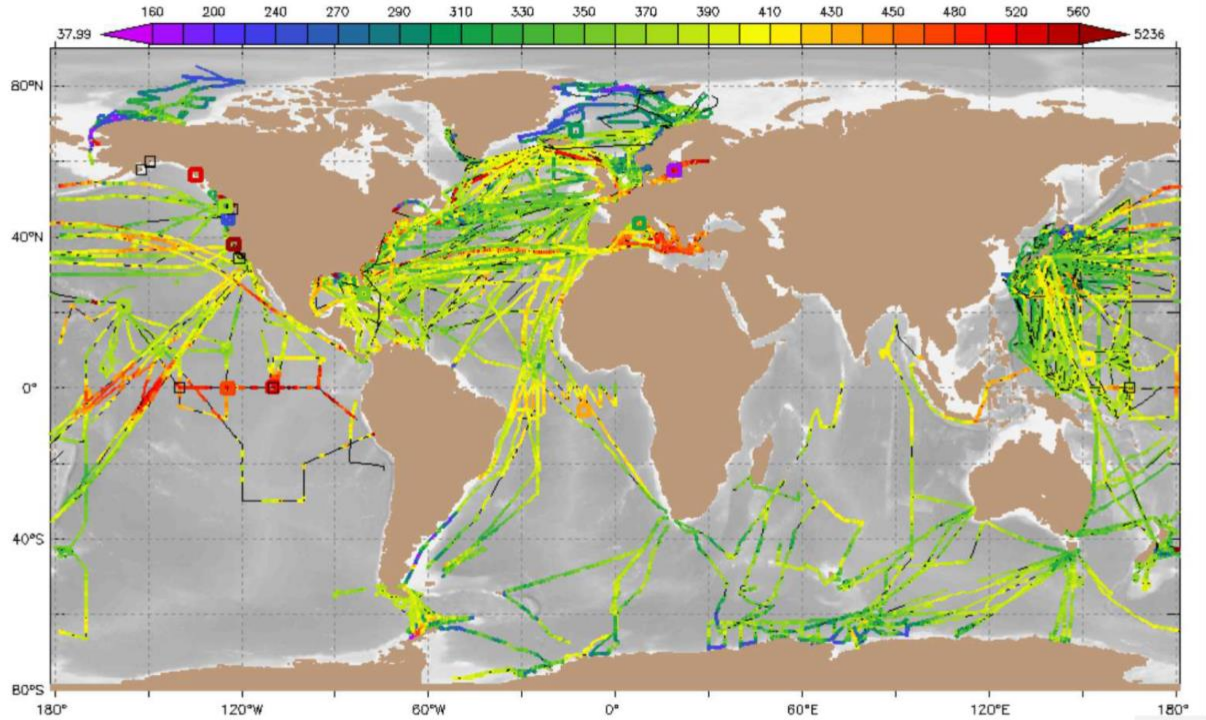

Figure 2. Map showing all new data in SOCATv5. SOCATv5 was released for public use in June 2017. Figure from www.socat.info

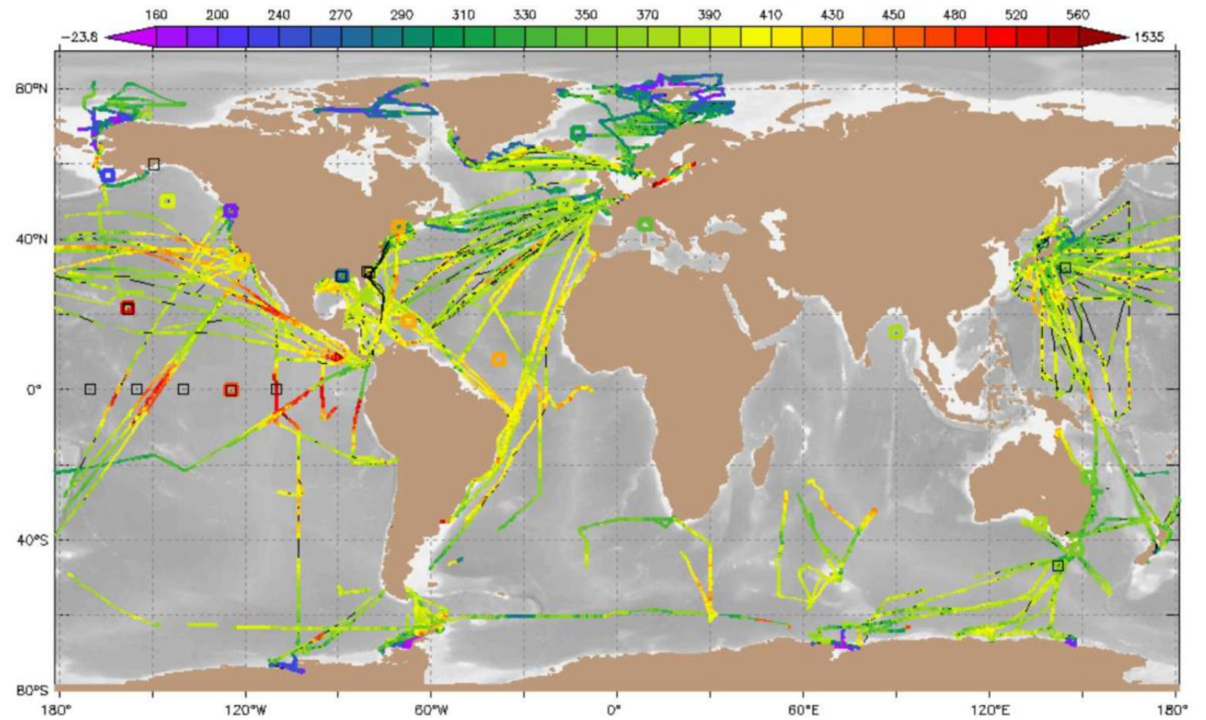

Figure 3. Map showing all new data in SOCATv6. SOCATv6 will be released for public use in June 2018. Figure from www.socat.info

SOCAT is also provided as a gridded data synthesis product (Figure 4), developed in co-operation with the National Oceanic and Atmosphere Administration (NOAA) Pacific Marine Environmental Laboratory (PMEL) in the US.

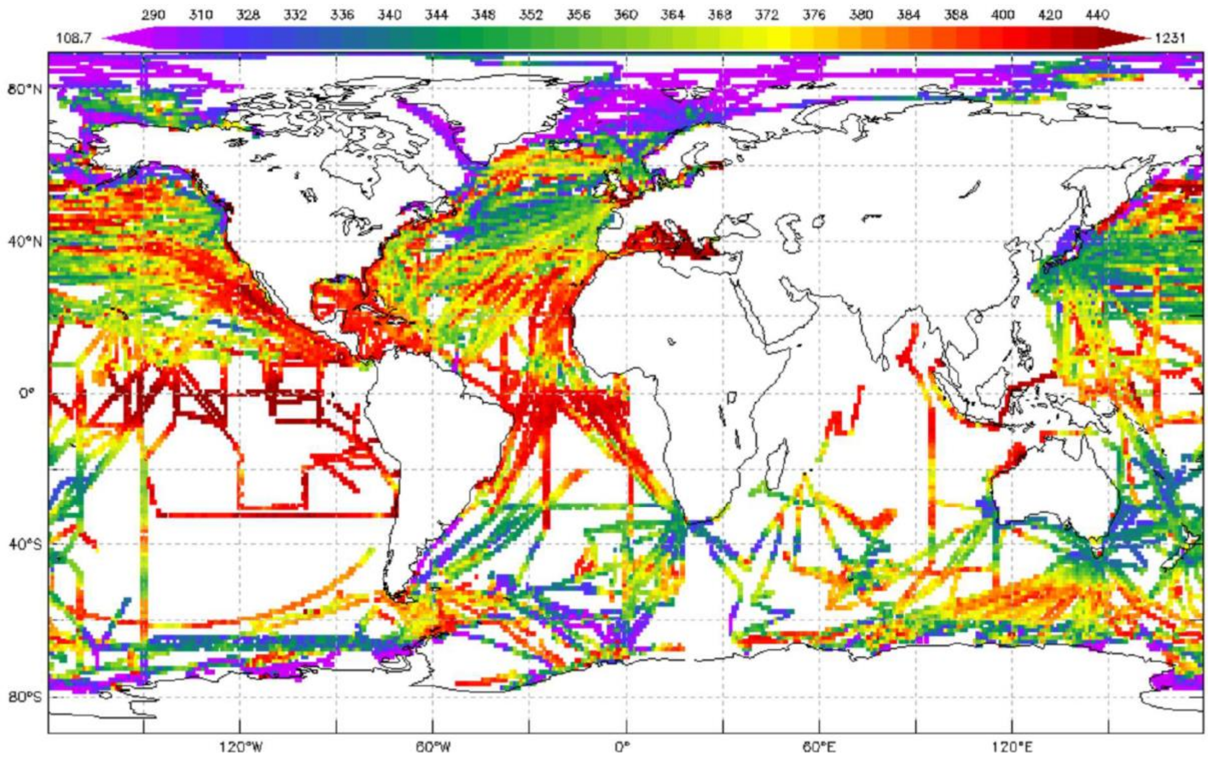

Figure 4. Map showing the gridded version of SOCATv5. This is the 1°x1° decadal fCO_2 in 2015.

The SOCAT data synthesis products allow us to evaluate changes in surface ocean carbon over the past five decades using basic statistical analyses of the observational data. Here we have used SOCATv4, which includes 18.5 million surface ocean carbon dioxide fugacity (fCO_2) measurements globally, spanning the years 1957-2015, to show a clear fCO_2 shift towards higher values decade by decade between 1970 and 2015 (Figure 5). This shift aligns with the decadal increase in atmospheric CO_2 (black solid line in Figure 5).

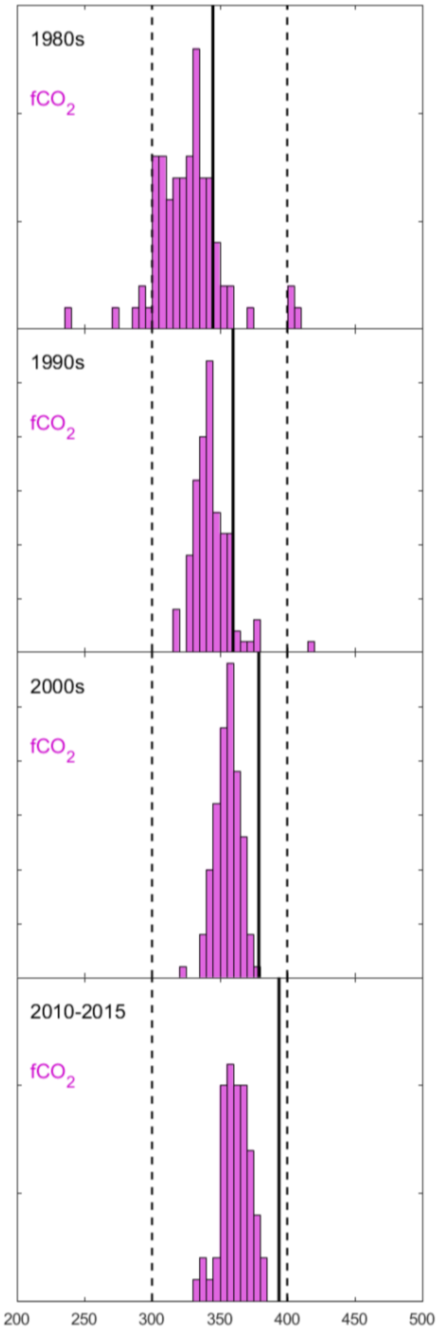

Figure 5. Figure showing how surface ocean fCO2 has changed globally over the past four decades. The histogram shows the observations in SOCATv5 and the black line shows the atmospheric concentration in the given decade. Figure from Lauvset et al. (in preparation)

3.2. Statistical model

The rationale for developing a novel statistical model is twofold: (1) to enable the yearly release of carbon system EOVs (pCO_2, air-sea flux of CO_2, pH) and (2) to contribute to the design of an optimal multi-platform observing system for surface ocean pCO_2 (WP1).
The two-step FFNN was applied to reconstruct monthly surface ocean pCO_2 distribution at 1°x1° spatial resolution from 2001 to 2016. Figure 6 illustrates the performance of the model for the reconstruction of climatological pCO_2 fields during step 1.

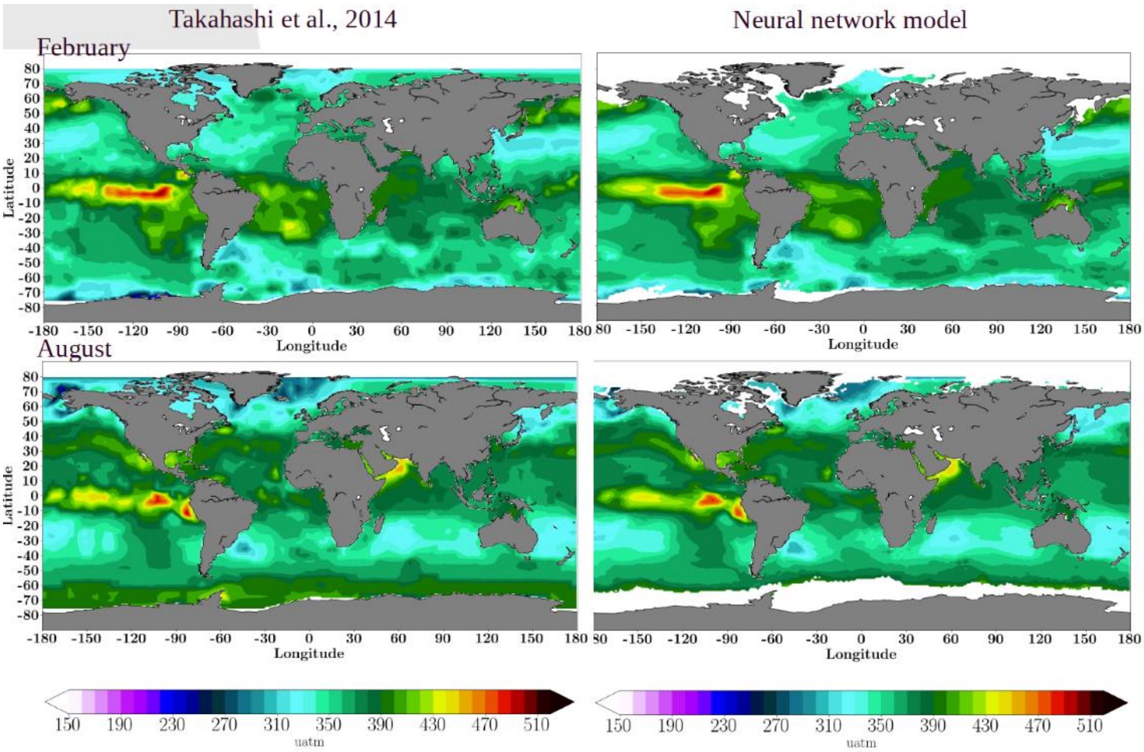

Figure 6: Climatological pCO_2 distributions for February and August: left column, Takahashi et al. (2014); right column, FFNN model developed in AtlantOS (step 1).

Figure 6 presents a comparison between climatological pCO_2 distributions for February and August from Takahashi et al. (2014) and those reconstructed by the non-linear FFNN. Large-scale structures are in good agreement. The seasonal modulation of outgassing in major upwelling regions is well reproduced by the FFNN, in particular in the Arabian Sea. Differences at high latitude correspond to the sea-ice mask used during the reconstruction.

The full FFNN is applied for the reconstruction of interannually varying monthly surface ocean pCO_2. When compared to the target data from SOCAT, the models yields a root-mean-squared error of 18.03 μatm, a correlation coefficient (r^2) of 0.76 and a bias of 11.58 μatm. The performance of the model is similar to other previously published methods (Rödenbeck et al., 2015). Model output is compared to four alternative approaches included in Rödenbeck et al., (2015), in Figure 7. Results of the model developed within AtlantOS are within the range of these 4 previous models. The quality of pCO_2 reconstructions is further evaluated at the regional level following the breakdown in biomes proposed by Fay and McKinley (2014). The regional analysis highlights the convergence of all five models in terms of seasonal cycle and interannual variability over areas with sufficient data coverage (e.g. North Atlantic subtropical gyre), as opposed to regions with poor data density (e.g. Equatorial North Atlantic).

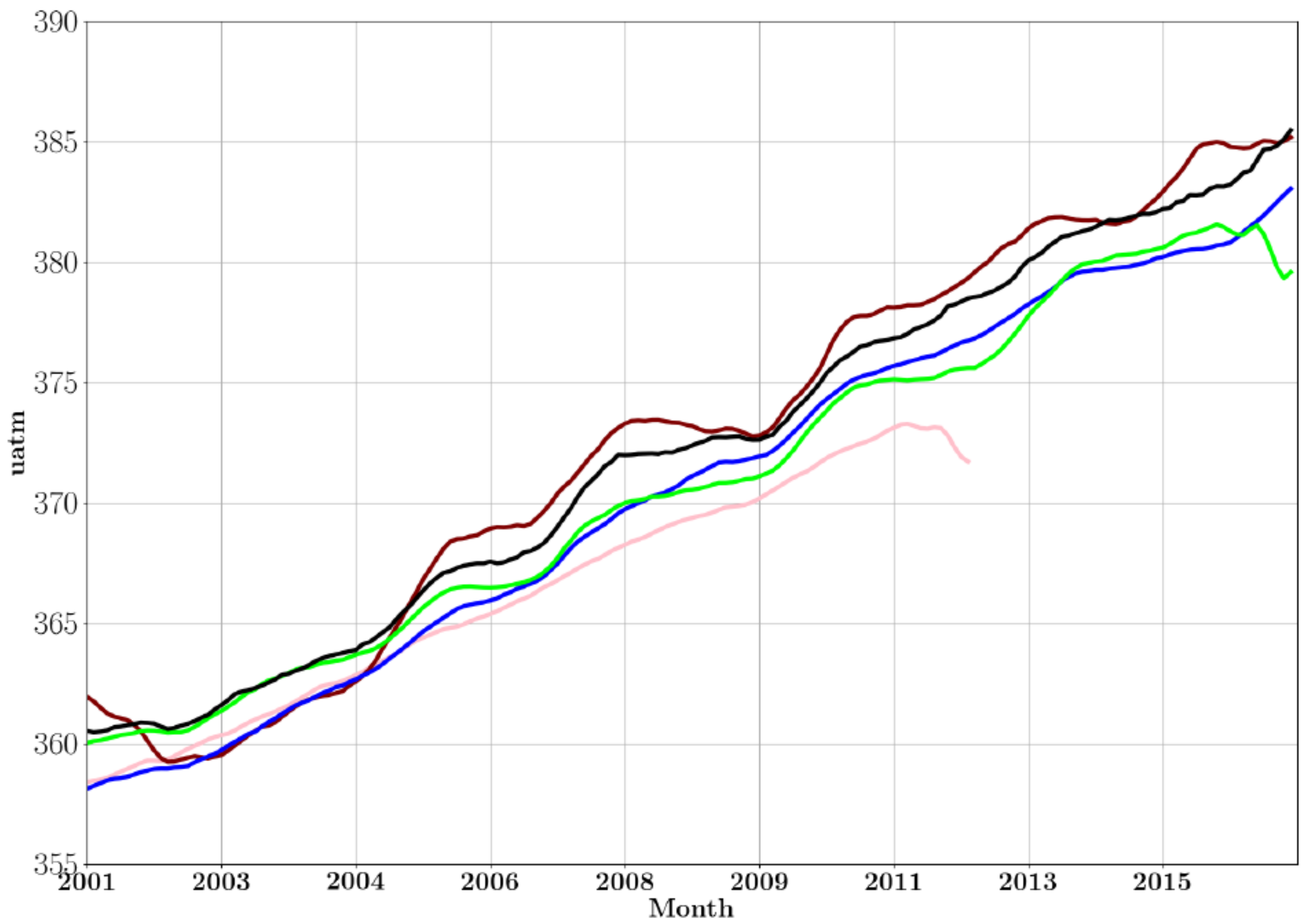

Figure 7: Time series of average global surface ocean pCO_2 from 2001 to 2016: Comparison between the new FFNN model developed under AtlantOs (black line) and 4 published models (pink, UEA-SI; brown, Jena-MLS13; blue, JMA-MLR; green, ETH-SOMFFN) that contributed to Rödenbeck et al. (2016).

4. CONCLUSIONS AND OUTLOOK

According to the project description “the overarching objective of AtlantOS is to achieve a transition from a loosely-coordinated set of existing ocean observing activities producing fragmented, often monodisciplinary data, to a sustainable, efficient, and fit-for-purpose Integrated Atlantic Ocean Observing System (IAOOS)”. To aid this objective eleven sub-objectives are defined and the work in deliverable 7.10 supports objectives 3 and 11:

Objective 3) Support Atlantic observing communities within existing networks observing EOVs including international expertise in the design and development, operation and maintenance of IAOOS networks, and disseminate best practices, harmonizing data processing and quality control procedures.

The work done in deliverable 7.10 has in particular contributed towards dissemination of best practices and quality control procedures. The next steps include a full revision of the quality control procedures for SOCAT, which in great part comes about through new developments initiated by AtlantOS work. AtlantOS is also contributing quality control towards SOCAT v6 (ongoing and planned for June 2018, Figure 3) and will contribute in the same way towards SOCATv7 (planned for June 2019).

Objective 7) Provide new information products in several societal benefit areas (i.e. climate, disasters, ecosystems, health and fresh water) including increased safety for offshore activities and coastal communities.

The statistical model for carbon cycle EOVs developed within AtlantOS will provide yearly updated reconstructions of monthly pCO_2 distributions as novel releases of SOCAT become available. pCO2 distributions will be completed by air-sea flux of CO2 and pH by the end of 2018. Data will be distributed as part of CMEMS. Results presented below are for pCO_2 only, but the FFNN system will be extended to cover air-sea fluxes of CO_2 and pH over the coming four months.

Objective 11) Enable free and open access to all data.

SOCAT is open to the public for free use and distribution, only requiring a proper citation. Including AtlantOS data in SOCAT ensures their visibility and use globally. A SOCAT fair use statement has been developed, and can be found here: https://www.socat.info/wp-content/uploads/2017/04/Fair_Data_Use_Statement-for-SOCAT_v5.pdf

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