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# A Surface Ocean CO<sub>2</sub> Reference Network, SOCONET and Associated Marine Boundary Layer CO<sub>2</sub> Measurements

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The Surface Ocean CO<sub>2</sub> NETwork (SOCONET) and atmospheric Marine Boundary Layer (MBL) CO<sub>2</sub> measurements from ships and buoys focus on the operational aspects of measurements of CO<sub>2</sub> in both the ocean surface and atmospheric MBLs. The goal is to provide accurate pCO<sub>2</sub> data to within 2 micro atmosphere (μatm) for surface ocean and 0.2 parts per million (ppm) for MBL measurements following rigorous best practices, calibration and intercomparison procedures. Platforms and data will be tracked in near real-time and final quality-controlled data will be provided to the community within a year. The network, involving partners worldwide, will aid in production of important products such as maps of monthly resolved surface ocean CO<sub>2</sub> and air-sea CO<sub>2</sub> flux measurements. These products and other derivatives using surface ocean and MBL

CO<sub>2</sub> data, such as surface ocean pH maps and MBL CO<sub>2</sub> maps, will be of high value for policy assessments and socio-economic decisions regarding the role of the ocean in sequestering anthropogenic CO<sub>2</sub> and how this uptake is impacting ocean health by ocean acidification. SOCONET has an open ocean emphasis but will work with regional (coastal) networks. It will liaise with intergovernmental science organizations such as Global Atmosphere Watch (GAW), and the joint committee for and ocean and marine meteorology (JCOMM). Here we describe the details of this emerging network and its proposed operations and practices.

**Keywords: carbon dioxide, network, oceanography, fluxes, best practices**

## INTRODUCTION

Rising carbon dioxide (CO<sub>2</sub>) levels in the atmosphere and ocean are major issues of our time. Historically, the main focus in carbon cycle research has been on understanding the flow and partitioning of the excess carbon dioxide in the earth system components of atmosphere, ocean and terrestrial biosphere. Revelle and Suess (1957) stated “*Human beings are now carrying out a large scale geophysical experiment of a kind that could not have happened in the past nor be reproduced in the future.*” Roger Revelle subsequently wrote that “*People’s attitude toward the rise of CO<sub>2</sub> should probably contain more curiosity than apprehension.*” (Weart, 2008). The basic understanding of processes and impacts remains a priority in carbon cycle research but concerns and societal implications of the impacts of rising CO<sub>2</sub> have surpassed mere curiosity. Increasing emphasis in carbon cycle research is placed on monitoring and quantifying the sources and sinks of atmospheric CO<sub>2</sub>, and the interplay between the anthropogenic CO<sub>2</sub>, that is, CO<sub>2</sub> released by human activities such as fossil fuel burning and land-use changes, and the natural carbon cycle. This requires a systematic and sustained observational approach, well served by a closely coordinated network. The ocean is a significant sink of anthropogenic CO<sub>2</sub> capturing about 25% of the anthropogenic carbon from 1870–2017 (Le Quéré et al., 2018). Once sequestered by the ocean, the retention time is on the order of centuries to millennia, compared to decades for terrestrial systems. The uptake of CO<sub>2</sub> by the ocean is thus a critical element in understanding carbon dynamics and future trajectories of atmospheric CO<sub>2</sub> growth.

Accurate measurements of CO<sub>2</sub> concentrations in the surface ocean and atmospheric marine boundary layer (MBL) are critical factors to quantify the air-sea flux of CO<sub>2</sub>, along with the forcing function, called the gas transfer velocity,  $k$ . The air-sea CO<sub>2</sub> flux,  $F_{CO_2}$  [mol m<sup>-2</sup> yr<sup>-1</sup>] is commonly expressed in terms of a bulk formulation as:

$$F_{CO_2} = k s(pCO_{2w} - pCO_{2a}) = k s \Delta pCO_2 \quad (1)$$

where  $k$  [m yr<sup>-1</sup>] is parameterized with wind (Wanninkhof, 2014),  $s$  is the solubility [mol m<sup>-3</sup> atm<sup>-1</sup>],  $pCO_{2w}$  is the partial pressure of CO<sub>2</sub> in water [atm],  $pCO_{2a}$  is the partial pressure of CO<sub>2</sub> in air [atm], and  $\Delta pCO_2$  is the difference. The units for  $k$ ,  $s$ , and  $pCO_2$  are often reported as cm hr<sup>-1</sup>, mol l<sup>-1</sup> atm<sup>-1</sup>, and  $\mu$ atm, respectively, and appropriate conversions

need to be applied. The quantities measured are the mole fractions of CO<sub>2</sub> in water,  $xCO_{2w}$ , and air,  $xCO_{2a}$ , and these are converted to partial pressure with knowledge of the total pressure and water vapor pressure (Pierrot et al., 2009). While  $\Delta pCO_2$  over the open ocean can vary in time and space by about  $\pm 100 \mu$ atm, the average disequilibrium needed to sequester the current annual ocean uptake of 2.5 billion tons of anthropogenic carbon (2.5 Pg C yr<sup>-1</sup>) (Le Quéré et al., 2018) is only 7–14  $\mu$ atm, requiring accurate measurements of  $pCO_{2w}$  and  $pCO_{2a}$  with high spatiotemporal resolution. Due to the small average disequilibrium, measurements must be accurate. Bias, in particular, can be a major issue and thus well-calibrated measurements are a must. Of note is that in Eq. 1 the concentrations right at the interface are of relevance. The measurements, typically at 0.2–8 m depth and 1–20 m height, need to be corrected to surface conditions requiring adjustments for temperature, pressure, and chemical effects. The corrections are largest and most uncertain on the water-side of the interface.

The sequestration of anthropogenic CO<sub>2</sub> emissions by the ocean is of benefit as it curtails increasing atmospheric CO<sub>2</sub> level and its associated greenhouse effect, but the corresponding CO<sub>2</sub> increase in ocean surface waters also leads to ocean acidification (OA), which is detrimental to many marine organisms. Knowledge of the rate of CO<sub>2</sub> uptake and changes thereof are of importance for socio-economic assessments related to the fate of anthropogenic CO<sub>2</sub> and to ocean health.

Systematic measurement of atmospheric CO<sub>2</sub> concentrations began in the late 1950s (Keeling, 1958) to investigate the long-term atmospheric trend of this important greenhouse gas. The discovery of seasonal variability, resulting from terrestrial biosphere CO<sub>2</sub> uptake and release, prompted a small global network of measurements to assess the global distribution of the seasonal and long-term features in CO<sub>2</sub> (Keeling, 2008). As such, initial CO<sub>2</sub> measurements were made from locations where well-mixed MBL air could be sampled, usually coastal or island sites with prevailing onshore winds, so that the data were representative of the regional background CO<sub>2</sub> concentration, and not unduly influenced by localized sources and sinks.

Today, there are more than 100 sites where atmospheric scientists make sustained high-accuracy measurements of atmospheric CO<sub>2</sub>. However, the open ocean MBL remains undersampled. Many of these oceanic regions are visited by research vessels and commercial ships of opportunity (SOOP) equipped with underway  $pCO_{2w}$  systems that also make routine

measurements of CO<sub>2</sub> in the MBL. The atmospheric CO<sub>2</sub> data from these ocean community CO<sub>2</sub> systems do not, however, typically meet the rigorous standards of the atmospheric CO<sub>2</sub> measurement community, as set out in the World Meteorological Organization (WMO) Global Atmosphere Watch (GAW). Much of this data is currently not quality controlled. If the MBL CO<sub>2</sub> data from these ocean community measurement systems can be validated, and where necessary improved, this could lead to mutual benefits for both oceanographers and atmospheric scientists. As described below, based on initial comparisons and analyzer performance on underway systems, an accuracy of 0.2 ppm can be reached with these systems. While this is less accurate than the targets of global atmospheric CO<sub>2</sub> measurements, such calibrated measurements can be used effectively for constraining air-sea CO<sub>2</sub> fluxes, and in inverse models.

Surface ocean CO<sub>2</sub> measurements have been performed onboard ships for over 50 years (Takahashi, 1961; Keeling, 1965) using approaches that are similar to current measurements, but the observations have become increasingly more automated. Unattended measurements referenced against compressed air standards traceable to atmospheric CO<sub>2</sub> standards are now done routinely on ships and, since the 2000s, on moorings (Sutton et al., 2014). The measurements cover much of the global ocean, and allow regular access to regions of economic and environmental importance such as upwelling regions (González-Dávila et al., 2017). Many of the measurements are performed following standard operating procedures (e.g., Pierrot et al., 2009) and much of the data are submitted to global datasets and undergo independent secondary quality control. However, there is no global coordinated effort at the operational level for the data acquisition from ships and moorings as is proposed here for SOCONET.

This paper outlines the ongoing efforts to use established assets to create a reference network for high-quality surface ocean CO<sub>2</sub> observations from SOOP and moorings. As part of the effort we will assess current accuracy and develop protocols for improvement of MBL measurements. The effort is focused on the operational aspect, that is, the operations and tracking of the platforms; acquisition of the data; and their validation. The scientific justifications and resulting products are briefly described. While the need of global coordination has been highlighted over the last decade (Bender et al., 2002; Monteiro et al., 2010; Wanninkhof et al., 2012), the description and justification of doing so in a systems/network approach has been lacking. SOCONET is in developmental stages, and details have not been worked out and implemented. This community white paper was developed from two abstracts for the OceanObs'19 conference, one focused on MBL and the other on the surface ocean CO<sub>2</sub> measurements. The ideas described should be considered in a conceptual framework. The high-level scientific output and socioeconomic motivations are described first, followed by a discussion of the distributed network design, deliverables and challenges to establish the reference network. **Table 1** provides a list of the acronyms and abbreviations used in this work.

## SOCIETAL AND SCIENTIFIC IMPERATIVES FOR SOCONET

CO<sub>2</sub> is an important anthropogenic greenhouse gas, and a major driver of climate change that has, and will continue to have, far reaching consequences for our society. Its relevance is highlighted as an Essential Climate Variable (ECV) in the atmosphere and the ocean (as part of the inorganic carbon system), as well as a biogeochemical Essential Ocean Variable (EOV). CO<sub>2</sub> is produced by, for instance, the burning of fossil fuels, aerobic respiration, and oxidation of organic matter. At the most basic valuation this byproduct, or waste product, has an economic cost/value associated with it. Its cost/value has depended on speculation and has been affected by failures in the dedicated commodity markets. It currently is mostly traded as an “emission allowance” as part of a cap and trade system (re)instituted after the Paris Agreement. The largest trading system currently is the European Union (EU) emission trading scheme (ETS). The emission allowances in the EU ETS are equivalent to the right to emit one ton of CO<sub>2</sub> (or 270 kg of C). While ocean carbon uptake is currently not part of the trading scheme, at the valuation listed it would have an annual value of 170 billion US dollars (\$) (D’Maris and Andrew, 2017). This is based on a 2.5 Pg C yr<sup>-1</sup> ocean uptake and a price of \$19 per ton CO<sub>2</sub>.

While the uptake of CO<sub>2</sub> by the ocean is not included in ETS, its value is recognized as an ecosystem service. The sequestration comes at a cost though in that the resulting elevated CO<sub>2</sub> levels cause ocean acidification which impact ocean biota (see **Appendix A**). This, in turn, can have major effects on fisheries, tourism and other activities contributing to the marine economy. There are no estimates of the current dollar cost of the global impact of ocean acidification but an economic assessment of the impact of a future “OA catastrophe” ranges from a total cost of \$97 billion to \$301 billion (Colt and Knapp, 2016). While from an economic perspective the possible benefits of CO<sub>2</sub> uptake, expressed per annum above, are greater than the total ecosystem service losses, such an analysis is overly simplistic and does not take the significant societal impacts into account. The socio-economic take-home message is that the anthropogenic component of the carbon cycle translates into many billions of dollars, and impacts ecosystem health and human well-being. It thus requires thorough investigation and monitoring.

Following the adage that anything of significant value needs to be tracked, many aspects of the global carbon cycle require monitoring. In particular, the stocks (inventories) of the major reservoirs and flows (fluxes) at the interfaces between the atmospheric, oceanic, and terrestrial boundaries need to be quantified. Many parts of the systems are monitored following well-developed network principles and data acquisition. The data from these networks are the cornerstone of increasingly sophisticated products benefitting from robust modeling frameworks. Of particular interest in developing SOCONET and MBL CO<sub>2</sub> monitoring has been the development of the European Integrated Carbon Observation System (ICOS) which is a distributed network primarily based on established research entities incorporating oceanic, atmospheric

**TABLE 1** | Acronyms and Abbreviations.

ACT	Alliance for Coastal Technologies, <a href="http://www.act-us.info/">www.act-us.info/</a>
CCL	Central Calibration Laboratory
CCGG	Carbon Cycle and Greenhouse Gas network <a href="http://www.esrl.noaa.gov/gmd/ccgg/mbll/index.html">www.esrl.noaa.gov/gmd/ccgg/mbll/index.html</a>
DBCP	Data Buoy Cooperation Panel of JCOMM
ERDDAP	Environmental Research Division Data Access Program, <a href="https://coastwatch.pfeg.noaa.gov/erddap/index.html">https://coastwatch.pfeg.noaa.gov/erddap/index.html</a>
ESRL	Earth System Research Laboratory of NOAA
EU	European Union
FOO	Framework for Ocean Observing of GOOS, <a href="http://www.oceanobs09.net/foo/">www.oceanobs09.net/foo/</a>
GAW	Global Atmosphere Watch of WMO, <a href="http://www.wmo.int/gaw">http://www.wmo.int/gaw</a>
GCOS	Global Climate Observing System
GCP	Global Carbon Project, <a href="http://www.globalcarbonproject.org">www.globalcarbonproject.org</a>
GMD	Global Monitoring Division of NOAA/ESRL
GOA-ON	The Global Ocean Acidification Observing Network
GOOS	Global Ocean Observing System
GOSUD	Global Ocean Surface Underway Data project
ICOS	Integrated Carbon Observation System, a European Research Infrastructure, <a href="http://www.icos-ri.eu">www.icos-ri.eu</a>
IG3IS	Integrated Global Greenhouse Gas Information System, <a href="http://www.wmo.int/pages/prog/arep/gaw/ghg/IG3IS-info.html">www.wmo.int/pages/prog/arep/gaw/ghg/IG3IS-info.html</a>
IOC	Intergovernmental Oceanographic Commission of UNESCO <a href="http://www.ioc-unesco.org/">www.ioc-unesco.org/</a>
IOCCP	International ocean carbon coordination project, <a href="http://ioccp.org">http://ioccp.org</a>
JCOMM	the Joint WMO-IOC Committee for Ocean and Marine Meteorology, <a href="http://www.jcomm.info">www.jcomm.info</a>
JMA	Japan Meteorological Agency
LDEO	Lamont-Doherty Earth Observatory of Columbia University
NOAA	National Oceanic and Atmospheric Administration
OCG	Observation Coordination Group of JCOMM
OCO-2	Orbiting CO <sub>2</sub> Observatory 2, <a href="https://co2.jpl.nasa.gov/#mission=OCO-2">https://co2.jpl.nasa.gov/#mission=OCO-2</a>
OPA	Observations Program Area of JCOMM
SOCAT	Surface Ocean CO <sub>2</sub> Atlas; <a href="http://www.socat.info">www.socat.info</a>
SOCOM	Surface Ocean pCO <sub>2</sub> Mapping intercomparison
SOCONET	Surface Ocean CO <sub>2</sub> reference Network, <a href="http://www.socnet.info">www.socnet.info</a>
TCCON	Total Carbon Column Observing Network, <a href="https://tccon-wiki.caltech.edu/">https://tccon-wiki.caltech.edu/</a>
TransCom	Atmospheric Tracer Transport Model Intercomparison Project, <a href="http://transcom.lscce.ipsl.fr/transcom.lscce.ipsl.fr/">transcom.lscce.ipsl.fr/transcom.lscce.ipsl.fr/</a>
WDCGG	World Data Centre for Greenhouse Gases, <a href="https://gaw.kishou.go.jp/">https://gaw.kishou.go.jp/</a>
WMO	World Meteorological Organization, <a href="https://public.wmo.int/en">https://public.wmo.int/en</a>
AI	Artificial Intelligence
ASV	Autonomous Surface Vehicles
BGC	Biogeochemistry
CO <sub>2</sub>	Carbon dioxide
DIC	(Total) Dissolved Inorganic Carbon
ECV	Essential Climate Variable, <a href="https://public.wmo.int/en/programmes/global-climate-observing-system/essential-climate-variables">https://public.wmo.int/en/programmes/global-climate-observing-system/essential-climate-variables</a>
EOV	Essential Ocean Variable, <a href="http://www.goosocean.org/eov">http://www.goosocean.org/eov</a>
ETS	Emission Trading Scheme
FAIR	Findable, Accessible, Interoperable and Reusable
H <sub>2</sub> O	Water (vapor)
MBL	Marine Boundary Layer
NN	Neural Network
OA	Ocean Acidification
OSE	Observing System Experiment
OSSE	Observing System Simulation Experiment
pCO <sub>2a</sub>	Partial pressure of carbon dioxide in air
pCO <sub>2w</sub>	Partial pressure of carbon dioxide in water
Pg C	Petagram of carbon (10 <sup>15</sup> g; 10 <sup>9</sup> ton)
ppm	Parts per million (10 <sup>-6</sup> )
REBS	Robust Extraction of Baseline Signal
SOM	Self Organizing Map
SOOP	Ship of Opportunity Program
SOP	Standard Operating Procedures
SSS	Sea Surface Salinity
SST	Sea Surface Temperature
TAlk	Total Alkalinity
TSG	(Surface ocean) therosalinograph
TT	Target Tank
VOS	Volunteer Observing Ship

*Organizations and programs including some of the associated websites.*



and terrestrial components. This approach of going from measurements in research projects to a sustained monitoring network following clear protocols can guide development of SOCONET.

Surface Ocean CO<sub>2</sub> NETWORK will be a major contributor of reference quality observations to quantify air-sea CO<sub>2</sub> fluxes on seasonal to interannual scales, and to determine trends in pCO<sub>2w</sub> levels over time. To deliver the global products on a regular and anticipated basis, it must be a global effort of sustained nature, and a network approach is most practical (Table 2). Networks are best established through a single source of funding/agency, with strong oversight and leadership, and uniform instrumentation. However, this is rarely achievable for global ocean networks focused on climate and environmental issues. The closest example in oceanography is the successful Argo profiling float network. SOCONET will be a distributed network involving many groups. It will provide coordination and homogenization of nationally funded efforts on a global level. The execution of the primary objectives rely on several other components and additional measurements. Besides accurate air and ocean water measurements provided by the SOCONET partners, data from other sources needs to be included through activities such as the Surface Ocean CO<sub>2</sub> Atlas, SOCAT (Bakker et al., 2016) and mapping efforts such as SOCOM (Rödenbeck et al., 2015; Figure 1).

Surface Ocean CO<sub>2</sub> NETWORK is largely an operational entity but must be justified through delivery of (improved) products of scientific and socio-economic value. The major products that SOCONET will contribute to are surface ocean pCO<sub>2</sub> maps and air-sea CO<sub>2</sub> fluxes on monthly scales and with spatial

resolution of 1°. The data need to be interpolated in time and space, and combined with other environmental parameters to create such maps (Figure 1). These maps rely on high-density data, often from satellite remote sensing (Shutler et al., 2019) and increasingly more sophisticated regression approaches, including machine learning such as neural networks (NN), and self-organizing maps (SOM) (Rödenbeck et al., 2015). Furthermore, possibilities of utilizing artificial intelligence (AI) approaches are being considered. Aside from application to determine the air-sea concentration difference (Eq. 1), the atmospheric CO<sub>2</sub> measurements will be used by atmospheric inverse modeling teams to generate improved estimates of CO<sub>2</sub> fluxes over oceans and adjacent continents (Jacobson et al., 2007; Gaubert et al., 2019).

These products and inputs are the cornerstones of derivatives, such as estimates of trends in uptake. The F<sub>CO<sub>2</sub></sub> estimates are currently used to test and benchmark carbon sink estimates derived from “bottom-up” ocean process models, many of which are used to predict future scenarios of global and regional climate change. The creation of surface pH maps using pCO<sub>2w</sub> as a primary variable, as part of the verifying targets of Sustainable Development Goal 14.3 is another important product. The needs for the products are articulated at high levels, such as the Global Carbon Project (GCP) that produces annual data-based estimates of fluxes between the major carbon reservoirs (Le Quéré et al., 2018), and the Global Climate Observing System (GCOS) that has called ocean acidification a headline indicator of changes in biogeochemistry in the ocean due to climate change.

## THE ESTABLISHMENT OF SOCONET

### Network Principles

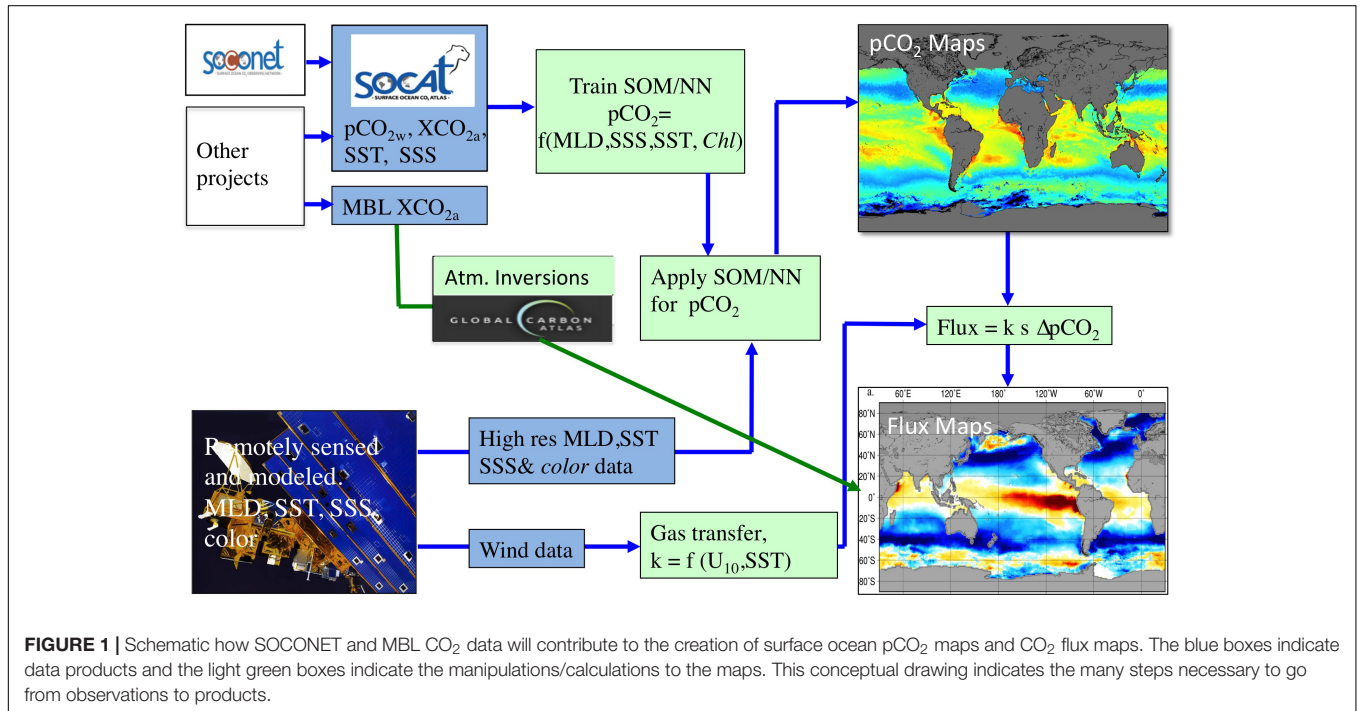
The SOCONET network development follows the network attributes proposed by the Observation Coordination Group (OCG) of JCOMM. This will facilitate incorporation of SOCONET within the JCOMM construct (Table 2). From an operational network perspective, a multi-PI distributed international network is challenging but benefits from human capital including expertise, innovation and oversight. The development of SOCONET relies heavily on established interactions in SOCAT. SOCAT is a well-designed data collation, quality check and distribution system of surface ocean pCO<sub>2</sub> measurements (Bakker et al., 2016). SOCAT is not directly involved in the operational aspects of data acquisition that is the focus of SOCONET. A schematic of the interaction of SOCONET and SOCAT and the more informal product development efforts, such as the surface ocean pCO<sub>2</sub> mapping intercomparison project, SOCOM is shown in Figure 2. Admission to SOCONET is selective based on meeting the network criteria. SOCONET will initially only include platforms that meet the data quality and release schedule as outlined in Table 3. The full details of SOCONET, that is focused on the operations of surface ocean CO<sub>2</sub> measurements, can be found in the SOCONET prospectus (Wanninkhof et al., 2018) with a brief summary below.

**TABLE 2** | Attributes of a JCOMM Network.

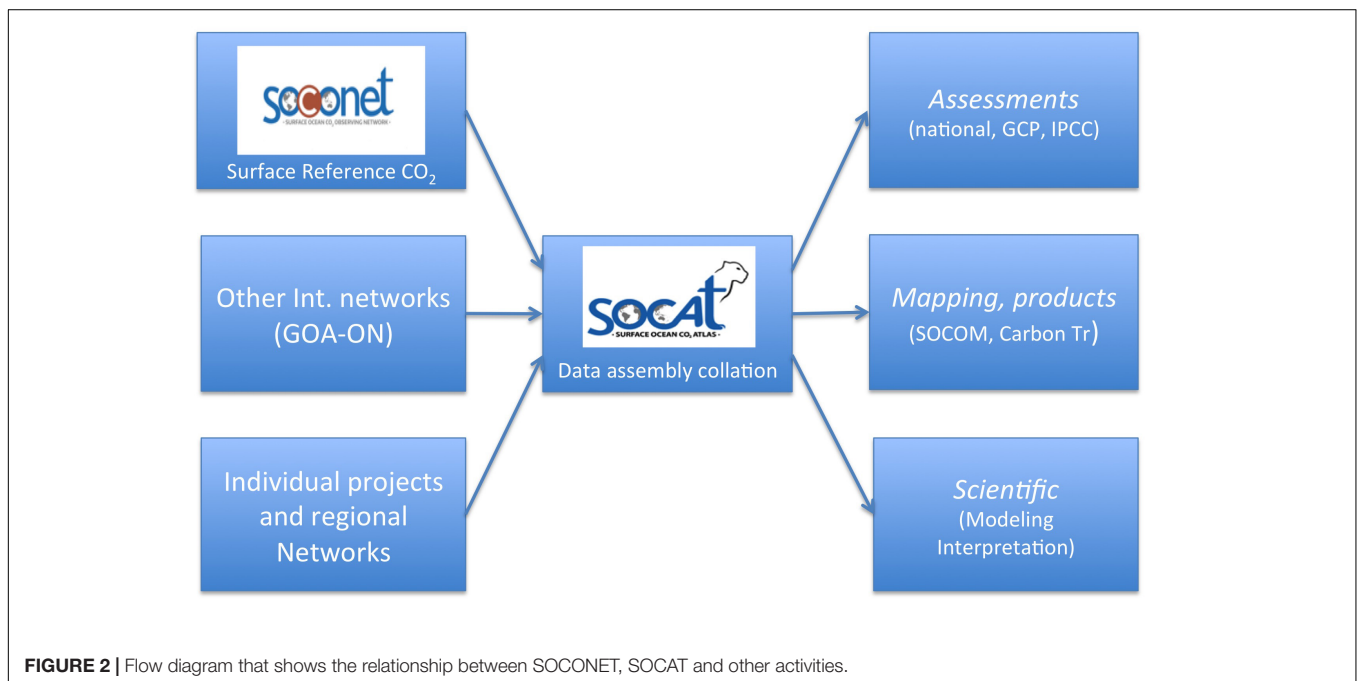
Global in scale	Greater than regional, and as far as feasible, intention to be global.
Sustained observations	Sustained over multiple years, beyond time-span of single research or experimental projects.
Community of practice	Has an identified community governance structure that provides a means of developing a multi-year strategy, implementation plans and targets, and standards and best practices.
Delivers data that are free, open, and available in a timely manner	Has a defined data management infrastructure that delivers interoperable and inter-comparable data in real-time and/or with minimal delay after becoming available.
Observes one or more Essential Ocean Variable or Essential Climate Variable	Contributes to meeting requirements through observing one or more of the GOOS EOVS or GCOS ECVs.
Maintains network mission and targets	The role in GOOS is defined and progress toward targets can be tracked and progress assessed.
Develops, updates and follows standards and best practices	Provides standard operating procedures that are readily accessible and citable.

Surface Ocean CO<sub>2</sub> NETWORK will cover key regions of the ocean (Figure 3) with data of specified quality. It will perform measurements following documented procedures and network practices including: common protocols, similar instrumentation, and standardization. It will provide standard operating procedures (SOPs) for acquiring the data. Data will be appropriately documented with metadata compliant with international protocols, and accuracy and precision

requirements. Surface water pCO<sub>2</sub> data from SOCONET will be submitted through the established SOCAT data system. The platforms will be tracked through the JCOMMOPS platform management system and tagged as SOCONET reference network data. The network will be constructed within the Framework for Ocean Observing (FOO) of the Global Ocean Observing System (GOOS) and in accord with FOO mission statement:



**FIGURE 1 |** Schematic how SOCONET and MBL CO<sub>2</sub> data will contribute to the creation of surface ocean pCO<sub>2</sub> maps and CO<sub>2</sub> flux maps. The blue boxes indicate data products and the light green boxes indicate the manipulations/calculations to the maps. This conceptual drawing indicates the many steps necessary to go from observations to products.



**FIGURE 2 |** Flow diagram that shows the relationship between SOCONET, SOCAT and other activities.

*“A framework for moving global sustained ocean observations forward in the next decade, integrating feasible new biogeochemical, ecosystem, and physical observations while sustaining present observations, and considering how best to take advantage of existing structures.”*

The objectives and criteria of the SOCONET reference network are provided in **Table 3**.

## Platform Types

Surface Ocean CO<sub>2</sub> NETWORK is envisioned as a multi-platform EOV-based network, but currently only includes instruments on moorings and ships. The differences and attributes of the platforms are shown in **Table 4**. The strengths and weaknesses of each platform listed are generalities, and vary for each individual platform, but it serves to show issues and challenges that require further attention. There are several other autonomous platforms and instruments that could be part of SOCONET in the future. However, each needs to be fully vetted in meeting the criteria specified in **Table 3**. Of particular use in this respect are instrument intercomparison exercises, and side-by-side comparisons to assure new platforms and instruments meet the requirements. Regular intercomparison activities are envisioned in collaboration with national and regional efforts, and coordination groups such as the alliance for coastal technologies (ACT) and the International Ocean Carbon Coordination Project (IOCCP).

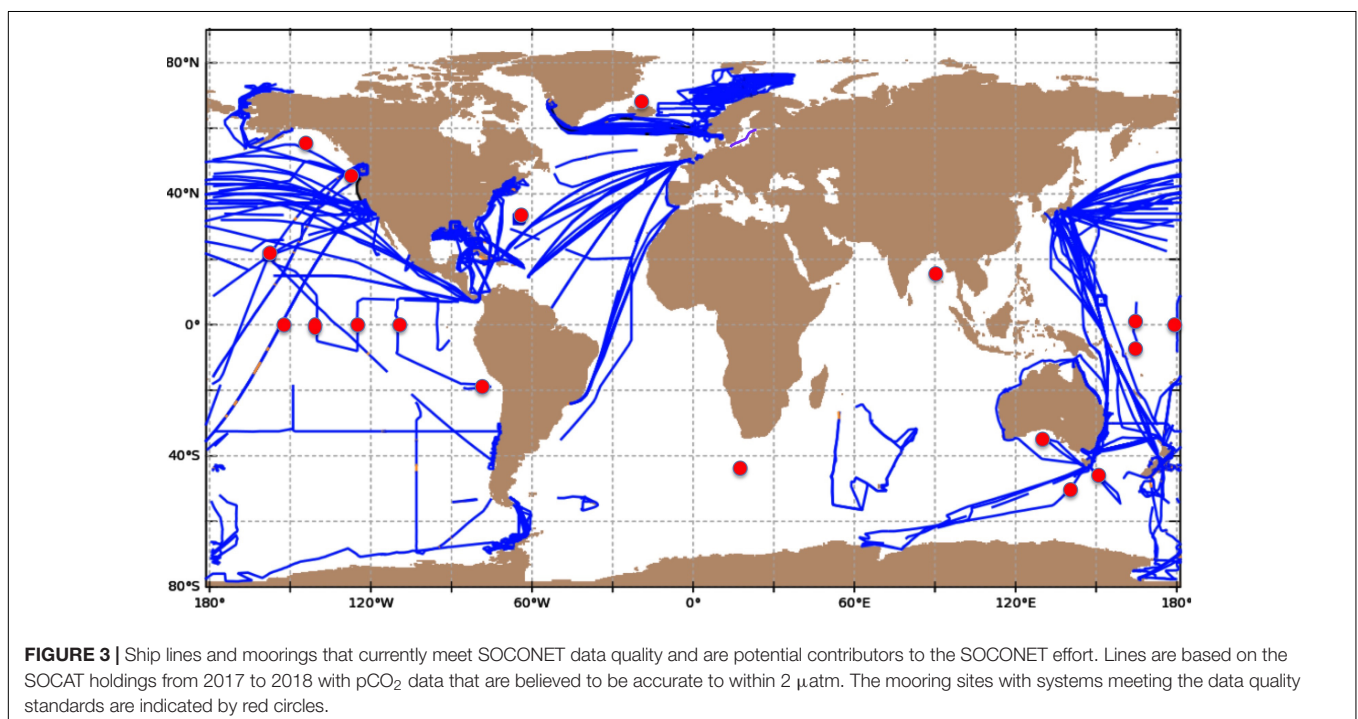
## Data Management, Access and Quality Control

The data management framework developed under SOCAT (Pfeil et al., 2013; Bakker et al., 2016) will also serve as the data

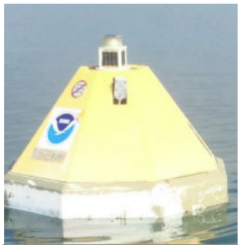
**TABLE 3** | Synopsis of SOCONET objectives and criteria.

Activity	Criteria
Membership	Partners have a track record of operations and will follow agreed upon procedures to obtain quality measurements.
Observational target	The compatibility (i.e., the allowable difference from a recognized scale) CO <sub>2</sub> measurements are better than 2 μatm for water (pCO <sub>2w</sub> ) and 0.2 ppm for air (xCO <sub>2a</sub> ).
Data delivery	Quality controlled reference data in 6 to 12 months.
Tracking	Near real-time platform tracking with location updates at least once a day.
Oversight	Metrics on data quality and quantity are provided on an annual basis.
Quality assurance	Quality assessment intercomparison exercises are performed to assure that standards are met.
Quality assurance	Instruments checked before installation, during operation, and after recovery of systems.
Deliverables	A dataset of reference network data will be created once a year.
Collaborate	Mutual aid, exchange and assistance are provided by SOCONET members for addressing technical issues in operations.
Outreach	Scientific outreach focuses on elevating quality and providing assistance to other groups in sustaining quality observations with a goal to entrain additional platforms into the network.
Outreach	The SOCONET members provide input and guidance to the community on new platforms, measurements, and protocols with a vision toward implementing a biogeochemical network and supporting marine boundary layer atmospheric measurements.
Connection to WMO/IOC/JCOMM	The network funders will provide resources toward tracking platforms through JCOMMOPS and other agreed upon mutual services.

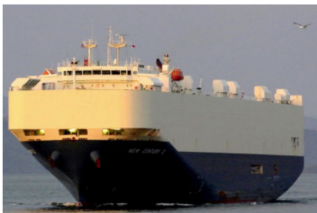
depository for SOCONET surface water CO<sub>2</sub> data (**Figure 2**), and likely for the MBL CO<sub>2</sub> taken in conjunction with surface ocean pCO<sub>2</sub>. Over the last several years, the SOCAT data





**TABLE 4** | Platforms used in SOCONET<sup>1</sup>.

Moorings provide high-resolution temporal coverage and provide measurements closest to *in situ* conditions, they currently operate with a span gas but no target gas to verify concentrations such that accuracies are estimated from intercomparisons and pre- and post-cruise calibration/verification. Moored air CO<sub>2</sub> measurements have not yet been validated to meet a target of 0.2 ppm.



Cargo ships provide regular observations with weekly to bimonthly repeat occupations offering seasonal resolution. Observations are along commerce routes, but miss coverage of key areas such as the South Indian and high latitude oceans. Instruments are often placed in inhospitable environments such as engine rooms degrading their performance. Water and air intakes depend on established infrastructure and are not always optimal.



Cruise ships and ferries provide high quality observations with weekly to biweekly repeats often with better installation options than cargo ships. The ships provide good outreach opportunities and exposure.



Research ships have infrastructure and support for quality measurements. Instrument locations are good. The ships often travel beyond shipping lanes and to regions of physical and biogeochemical interest (such as "hotspots"). Other projects provide added value. Cruise tracks are not frequently occupied and other activities can compromise (air) measurements.



Ice breakers and polar supply ships travel to regions of high interest, often at regular intervals. Infrastructure of ships facilitate operations of underway pCO<sub>2</sub> systems. Other science projects often take place and provide value added both for interpretation of pCO<sub>2</sub> and for the projects.

<sup>1</sup> These are examples of platforms with instruments that meet SOCONET criteria based on intercomparisons and guidelines (see **Table 3**). The comments are generalities. For example, some installations on cargo ships are superior to research ships.

team has improved the submission, quality control, access and archival processes that support the annual releases of the SOCAT data products. These data products are available to the public through the web site, [www.socat.info](http://www.socat.info) and are archived with persistent identifiers (doi's) provided. In addition, the SOCAT data products are made available through the ERDDAP data platform, providing interoperable access to the datasets through a wide variety of tools and machine-to-machine services. Discovery and visualization services are provided for the SOCAT data through NOAA's Live Access Server. By leveraging this framework, SOCAT, and therefore SOCONET, supports the FAIR (Findable, Accessible, Interoperable and Reusable) data principles for improved levels of data interoperability and reuse. The automated system used by SOCAT demonstrates a method to efficiently manage the larger volumes of data expected with the future of new ocean observing efforts and can support the emerging SOCONET.

## CONTRIBUTIONS OF SOCONET

### Improved Understanding, Basic Research

Surface Ocean CO<sub>2</sub> NETwork is, in part, a research network that delivers data for basic discovery and understanding of processes and mechanisms. Thus, the network will be used for more than the operational production of maps. This is important as there is a lack of understanding of the effect of variations and change in climate and ocean condition on CO<sub>2</sub> levels, including the possibility of thresholds, tipping points, and feedbacks. The high quality needs and challenges of making the exacting measurements require extensive basic understanding, instrumental expertise and manual quality control requires a firm knowledge of the processes and instrumental analysis.

Research questions relating to climate and ecosystem changes benefit from sustained observations. There are a series of research questions that can, in part, be addressed with data from SOCONET platforms including quantifying the physical parameters impacting air-sea CO<sub>2</sub> exchange (e.g., Zappa et al., 2004); the impact of the biological pump on surface ocean CO<sub>2</sub> levels (e.g., Merlivat et al., 2015); feedbacks of calcifying organisms on surface water CO<sub>2</sub> (e.g., Frankignoulle et al., 1994); the control and changes of biogeochemical process (e.g., Schneider and Müller, 2018); and the response of surface ocean CO<sub>2</sub> levels to changes in atmospheric forcing (e.g., Arora et al., 2013). The latter is of great importance in the socio-economic arena to assess the efficacy of fossil fuel CO<sub>2</sub> reductions in meeting climate accords (Peters et al., 2017) that will require observational validation.

The data from SOCONET platforms will be used to improve the quantification of air-sea CO<sub>2</sub> fluxes through timely updates to algorithms such as those established in SOCOM (Rödenbeck et al., 2015). The observations can also be used in data withholding exercises that provide an independent estimate of the accuracy of the results. The rapid release of data can inform and serve as an early warning to changing patterns and trends, in particular those that are not fully captured in the regression approaches. The data will be critical to validate the results of new sensors and new platforms. Of note is the validation of pCO<sub>2</sub> derived from pH sensors from profiling floats to estimate CO<sub>2</sub> values (Williams et al., 2017). While the derived pCO<sub>2</sub> data from pH provide good precision, the accuracy of the derived pCO<sub>2</sub> is not well constrained and this can be uniquely addressed by validation with accurate *in situ* pCO<sub>2</sub> data.

## Network Design

To date there has not been a formal design of a global surface ocean CO<sub>2</sub> network. Bender et al. (2002) provide a broad view of network needs based on de-correlation analyses which were fine-tuned by Li et al. (2005). Regional observing requirements for the Southern Ocean are described in Majkut et al. (2014), and an observing system design for biogeochemistry for this region is described in Kamenkovich et al. (2017). A global surface ocean CO<sub>2</sub> network design has been lacking, in part because there have been no formal collaborations between operators of systems. Moreover, because of the paucity of data, and their many applications, any new data is considered a significant contribution.

Instrument deployment for accurate CO<sub>2</sub> measurements is currently limited to platforms such as ships and moorings, but autonomous surface vehicles (ASV) have the potential to expand the means to obtain data. Data, particularly from the ASVs and research ships that often visit remote ocean regions, will be useful in observing system design. Several approaches such as observing system simulation experiments (OSSE), and observing system experiments (OSE) are available that utilize *a priori* knowledge of the global fields to optimize sampling strategy. These network design approaches, as well as approaches using mapping and data denial experiments will be necessary to justify and implement a comprehensive SOCONET network.

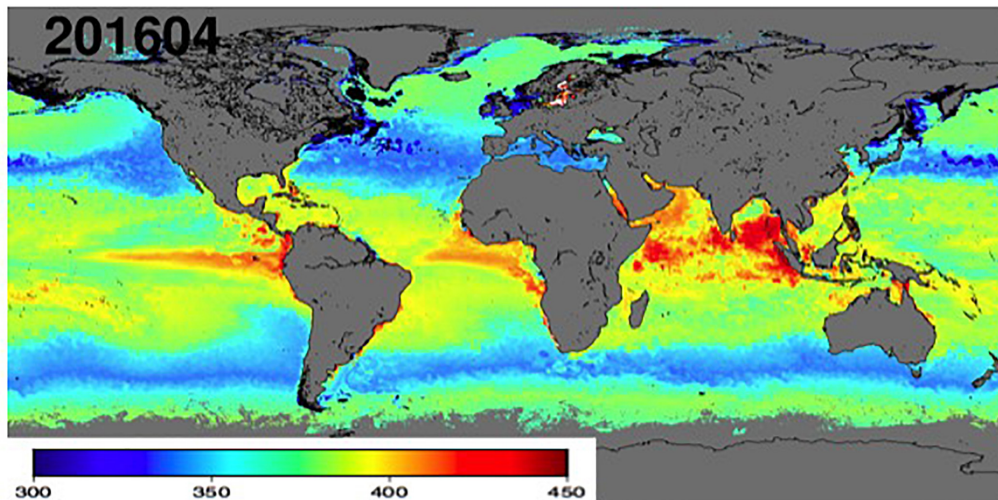
## Using pCO<sub>2w</sub> to Estimate Other Inorganic Carbon Parameters and Develop Products

In addition to using pH to estimate pCO<sub>2w</sub> (Williams et al., 2017), the reverse needs to be investigated as well (**Appendix A**). The utilization of surface ocean pCO<sub>2</sub> to aid in creating surface ocean pH maps will be an important use of SOCONET data (Lauvset et al., 2015). This is of particular relevance to determine longer-term trends in surface OA that need high accuracy data as called out in UN Sustainable Development Goal (SDG) 14.3 Ocean acidification and climate change. Much of the dedicated OA data are of lower quality focused on larger excursions of pH on sub-seasonal and local scales. These measurements are generally not suited for determining longer-term trends in OA. The Global Ocean Acidification Observing Network, GOA-ON will rely, in part, on SOCONET observations to estimate global patterns and trends. **Figure 4** is an example of a high-resolution monthly pCO<sub>2</sub> map based on a SOM/NN approach. The pCO<sub>2w</sub> data, along with measurements or estimates of TALK or DIC, can be used to calculate pH from which surface ocean pH maps can be created applying similar mapping approaches (Takahashi et al., 2014). A major deliverable of SOCONET will be data for improved near-term estimates of air-sea CO<sub>2</sub> fluxes. As described above, there are several other data streams required to determine air-sea CO<sub>2</sub> fluxes, such as remotely sensed winds for estimating the gas transfer velocity, and different parameters to aid interpolation, most notably sea surface temperature (SST) (**Figure 1**).

## CONTRIBUTION OF MBL CO<sub>2</sub> OBSERVATIONS

Surface Ocean CO<sub>2</sub> NETWORK has a strong focus on accurate pCO<sub>2w</sub> measurements (**Table 3**), but offers a unique opportunity to contribute to (air) MBL CO<sub>2</sub> data, which are undersampled over the open ocean. Most of the underway pCO<sub>2</sub> systems used in SOCONET take 5 air measurements, 1-min apart, from an intake at the bow or bridge of the ship, at intervals of about 3 h.

Moored pCO<sub>2</sub> systems in SOCONET take an air measurement every 4 h from 0.5 to 1 m on the buoy tower. By developing proper measurement protocols and quality control procedures, these data will be useful for improved MBL and air-sea CO<sub>2</sub> flux products. Here we focus on these measurements and means to verify their accuracy. In addition, there are dedicated instruments on some ships that meet GAW accuracy requirements. These efforts should be expanded, and having both types of instruments on select ships will provide critical information on the quality of the air data from the systems measuring surface water pCO<sub>2</sub>. Since the accuracy of MBL CO<sub>2</sub> data from underway CO<sub>2</sub> systems has not been fully investigated, and dedicated MBL systems meeting GAW accuracy requirements are costly, the air MBL requirements for SOCONET are under discussion and development. Below we describe the justification and current status.



**FIGURE 4** | Monthly map of  $p\text{CO}_{2w}$  for April 2016 created by a NN/SOM method showing the high fidelity of the output taking advantage of high-resolution remote sensing data. This example uses SOCAT data as the training set (units:  $\mu\text{atm}$ ) (J. Triñanes, pers. com.).

## Justification for Making Calibrated Accurate MBL $\text{CO}_2$ Observations From Ships

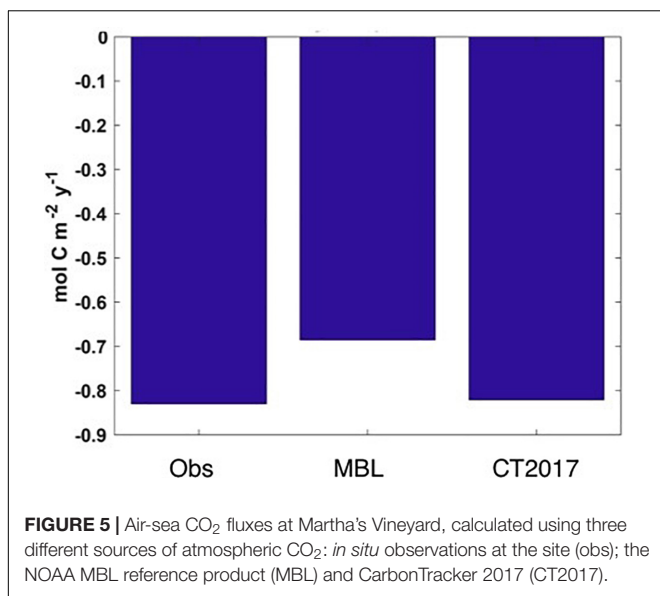
Here, calibrated accurate  $\text{CO}_2$  measurements are those that are compatible to within  $\pm 0.2$  ppm of the global  $\text{CO}_2$  scale maintained by the WMO/GAW Central Calibration Laboratory (CCL). We propose that this is the quality standard to which ocean community MBL  $\text{CO}_2$  measurements should strive. The term accuracy is used instead of precision/repeatability in recognition that imprecise measurement systems can still be sufficiently accurate if the noise in the data is randomly distributed around the “true” value and therefore does not bias the mean values. The MBL  $\text{CO}_2$  variability over the ocean interior is smaller than atmospheric  $\text{CO}_2$  variability over land, and MBL  $\text{CO}_2$  from the relatively imprecise measurements from systems focused on  $p\text{CO}_{2w}$  should be able to achieve the needed levels through averaging if these systems are appropriately optimized for atmospheric  $\text{CO}_2$  measurement and kept well-maintained, but this has not been fully tested. It should be noted that the WMO/GAW  $\pm 0.1$  ppm compatibility goal ( $\pm 0.05$  over the Southern Hemisphere) will likely not be attained by the systems measuring  $p\text{CO}_{2w}$ . Moored air  $\text{CO}_2$  measurements have not been validated to yet meet the  $\pm 0.2$  ppm goal and this should be an area of focus for improving accuracy of existing moorings. Data of such accuracy from sparsely sampled oceanic regions will be beneficial to atmospheric inverse modelers as long as their accuracy is quantified and described in the metadata. Moreover, this level of accuracy will not introduce a significant error in the air-sea fluxes where the uncertainty in the concentration gradient is dominated by the  $p\text{CO}_{2w}$  measurements that are good to within  $\pm 2 \mu\text{atm}$ .

Validating and improving the quality of oceanic MBL  $\text{CO}_2$  measurements is mutually beneficial to both the ocean and

atmospheric research communities. One of the key advantages for the ocean community is the improvement of air-sea  $\text{CO}_2$  fluxes ( $F_{\text{CO}_2}$ ). While most ships make *in situ* MBL  $\text{CO}_2$  measurements,  $F_{\text{CO}_2}$  is not usually calculated using these data. Instead, values for  $p\text{CO}_{2a}$  (from Eq. 1) are most commonly derived from the MBL reference data product provided by the Global Monitoring Division (GMD) of NOAA/ESRL. This data product is generated from a subset of NOAA atmospheric  $\text{CO}_2$  measurement sites near the coast that predominantly experience MBL air. These data are filtered, interpolated, and smoothed prior to being fit at latitudinal intervals of 0.05 sine of latitude from  $90^\circ\text{S}$  to  $90^\circ\text{N}$  and joined to create a 2-dimensional matrix (time versus latitude) of weekly  $\text{CO}_2$  values (Conway et al., 1994; EW Team, 2005). Thus, while this data product is useful for identifying large-scale trends, it does not reflect the full spatial or temporal variability of MBL  $\text{CO}_2$  that exists in the atmosphere, as explained in the online documentation and demonstrated previously (Pickers et al., 2017). The implications for  $F_{\text{CO}_2}$  calculated using this product are that in some regions, particularly coastal margins where the effects of continental airflow on MBL  $\text{CO}_2$  are not included in the NOAA MBL data product, biases will arise in the air-sea  $\text{CO}_2$  fluxes.

Comparing  $F_{\text{CO}_2}$  calculated using different sources of MBL  $\text{CO}_2$  data is useful for demonstrating the potential impacts of using inaccurate atmospheric data to calculate fluxes. **Figure 5** shows that air-sea  $\text{CO}_2$  fluxes calculated using the observed MBL  $\text{CO}_2$  values at the Martha’s Vineyard site in Massachusetts, United States ( $41.3^\circ\text{N}$ ,  $70.6^\circ\text{W}$ ) can differ by up to 15% compared to those calculated using the NOAA MBL product. Mean annual differences between atmospheric  $\text{CO}_2$  from the CarbonTracker 2017 modeling system (Peters et al., 2007) and the NOAA MBL reference product can be as high as 20 ppm within coastal seas near industrial centers, which translates into flux differences for these regions that can exceed  $0.5 \text{ mol m}^{-2} \text{ yr}^{-1}$  (**Figure 5**). Moored  $p\text{CO}_2$  systems, which measure air  $\text{CO}_2$ , also show





that these measurements can differ from the MBL reference data product in annual mean and seasonal variability due to local and regional effects (Northcott et al., 2019; Sutton et al., 2019). Although the uncertainty associated with pCO<sub>2a</sub> is often not considered to be significant compared to other sources of uncertainty in Eq. 1, **Figures 5, 6** indicate that inaccurate atmospheric CO<sub>2</sub> values can lead to significant biases in F<sub>CO<sub>2</sub></sub> at both local and regional scales. Using the *in situ* atmospheric CO<sub>2</sub> data from ships and moorings will likely eliminate these F<sub>CO<sub>2</sub></sub> biases, provided that the MBL CO<sub>2</sub> data are sufficiently accurate and devoid of ship contamination.

Other benefits to the oceanic community from improving or validating shipboard and mooring MBL CO<sub>2</sub> data include increased confidence in CO<sub>2</sub> flux data products that include data from multiple different ships/measurement platforms, and better traceability of pCO<sub>2</sub> data to the Central Calibration Laboratory (CCL) of WMO/GAW currently housed at NOAA/ESRL. The process of upgrading current shipboard CO<sub>2</sub> measurement systems and protocols to facilitate high-accuracy atmospheric CO<sub>2</sub> data from oceanic regions has an associated financial cost. This will require a significant oceanic community effort that should be supported by the collaboration of the atmospheric measurement community.

High-accuracy MBL CO<sub>2</sub> data from ships will benefit the atmospheric research community by substantially augmenting the atmospheric CO<sub>2</sub> measurement network in regions that are currently undersampled. Such data will be of value to the atmospheric inverse modeling community, who estimate surface CO<sub>2</sub> fluxes using a “top-down” approach, an alternative methodology for the calculation of global air-sea CO<sub>2</sub> fluxes to the bulk flux approach (Eq. 1) that utilizes surface ocean pCO<sub>2</sub> measurements (e.g., Takahashi et al., 2009; Landschützer et al., 2013, 2014). The “top-down” approach combines measurements of atmospheric CO<sub>2</sub> (e.g., provided by the surface sampling network of NOAA-GMD) and other global

contributors together with information on atmospheric transport (usually from atmospheric transport models), process-based prior flux estimates, and an inverse Bayesian optimization methodology (e.g., Rodgers, 2000). The current generation of such top-down inverse analyses often employ data assimilation or variational methods (e.g., Peters et al., 2007; Chevallier et al., 2010; Kang et al., 2011) and can provide grid-resolved flux-estimates at spatial-scales of ~10 km to 100 km (e.g., Broquet et al., 2013; Babenhauserheide et al., 2015). While top-down methods provide valuable alternative constraints on surface CO<sub>2</sub> fluxes, they are subject to significant uncertainties in regions of sparse sampling, most notably, in open ocean regions with few fixed sites (Rödenbeck et al., 2006), as well as significant uncertainties relating to atmospheric transport and the data assimilation methodology.

Given the additional cost involved in improved MBL CO<sub>2</sub> data from ships and moorings, interaction with the inverse modeling and observing system design communities will be used to identify regions where the added data have highest impact on uncertainty reduction. Within the European ICOS Network, pilot studies for the acquisition of MBL CO<sub>2</sub> data matching the standards of the atmospheric community are currently underway. SOCONET can make use of these investigations for the design of a network of high-accuracy MBL CO<sub>2</sub> measurement platforms with the aim to maximize the scientific return of investment.

## High-Accuracy Atmospheric CO<sub>2</sub> Measurement Approaches and Data Validation

The task of improving oceanic community MBL CO<sub>2</sub> measurements will be approached in two ways: by upgrading existing measurement systems that are not currently optimized for atmospheric CO<sub>2</sub> measurements; and, investment in new, purpose designed measurement systems that employ more modern technologies such as laser-based techniques. It is likely that some ocean community MBL CO<sub>2</sub> data are already sufficiently accurate to be used in F<sub>CO<sub>2</sub></sub> calculations and in inverse modeling studies where highest-accuracy is not required.

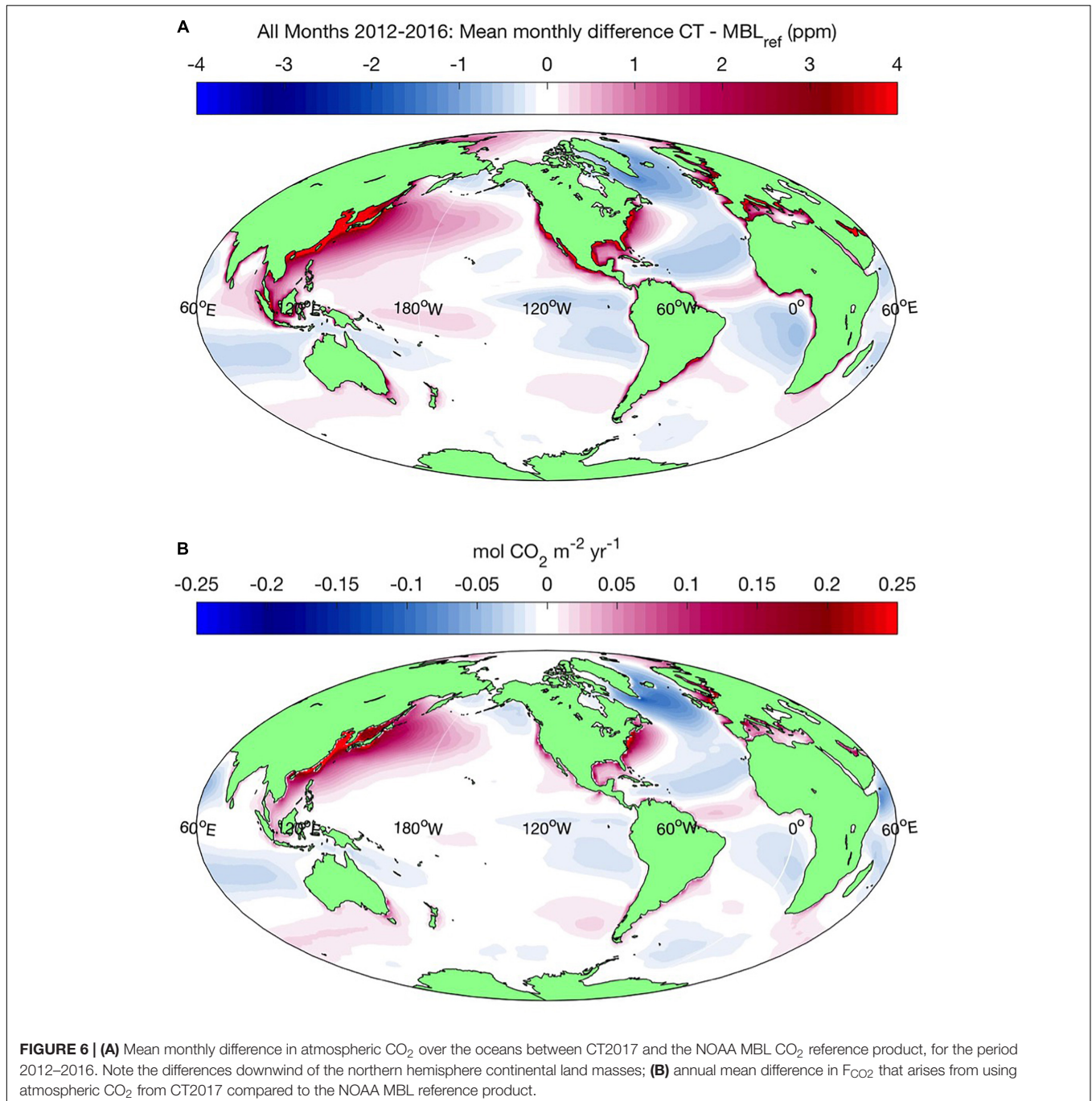
However, without validation this cannot be determined at present. Two approaches for improving MBL CO<sub>2</sub> are discussed, as well as the importance of data validation and quality control. Detailed technical information regarding atmospheric CO<sub>2</sub> measurement can be found in WMO/GAW Report 229 (2016) and in the ICOS atmospheric stations specifications document (Laurent, 2017).

Most existing underway pCO<sub>2</sub> measurements are currently made using instrumentation following ocean surface water pCO<sub>2</sub> community design (Pierrot et al., 2009). The systems have been built in-house at different laboratories and are currently available from General Oceanics Ltd. They have both seawater and atmospheric CO<sub>2</sub> measurements capabilities using a non-dispersive infrared (NDIR) analyzer (typically those manufactured by LI-COR Inc.), the traditional method for continuous atmospheric CO<sub>2</sub> measurement. Ocean community MBL CO<sub>2</sub> measurements are typically only required to be



accurate to about  $\pm 1$  ppm in order to calculate air-sea  $\text{CO}_2$  fluxes to specifications (Bender et al., 2002); hence, these measurement systems are not designed for atmospheric  $\text{CO}_2$  measurement, with the priority instead focused upon ensuring the highest possible quality of near-continuous  $\text{pCO}_{2\text{w}}$  measurements. As such, the setups of these measurement systems are not optimized for obtaining high-accuracy MBL  $\text{CO}_2$ . For example, the wetted parts (i.e., the surfaces of components, such as pumps, valves and tubing, that are in contact with the sample air stream) might not be suitable for precise

atmospheric  $\text{CO}_2$  measurement, sample air drying might not be sufficient (insufficient drying can lead to  $\text{CO}_2$  dilution, pressure broadening effects, and surface effects with tubing walls, all of which can bias  $\text{CO}_2$  measurement), and there may be small undetected leaks, which can cause non-negligible  $\text{CO}_2$  biases owing to the rigorous precision requirements of atmospheric  $\text{CO}_2$  measurement. Furthermore, calibration protocols are currently not sufficiently rigorous to meet the compatibility standards aspired to by the atmospheric  $\text{CO}_2$  measurement community as outlined in WMO/GAW report



no. 229. Nevertheless, with careful adherence to established protocols and procedures, it appears possible to obtain well-calibrated, accurate atmospheric CO<sub>2</sub> data using these existing systems.

Moored pCO<sub>2</sub> measurements in SOCONET are made using an equilibrator- and NDIR-based methodology similar to the underway systems described above. The detector is spanned using WMO-traceable CO<sub>2</sub> reference gas and zeroed using air stripped of CO<sub>2</sub>, prior to every measurement. The sample air is not as completely dried as in the underway pCO<sub>2</sub> method (Sutton et al., 2014). Current development efforts are focused on improving accuracy through incorporation of a higher-quality NDIR or other CO<sub>2</sub> analyzer, further drying of air sample, and incorporation of a CO<sub>2</sub> reference/target gas.

The advent of commercial CO<sub>2</sub> analyzers that employ laser-based spectroscopic technology, such as off-axis integrated cavity output spectroscopy (Baer et al., 2002), Fourier transform infrared spectroscopy (Esler et al., 2000), and cavity ring-down spectroscopy (Crosson, 2008) have opened up new opportunities for high-accuracy CO<sub>2</sub> measurement on ships. These spectroscopic analyzers are typically stable for longer periods of time compared to NDIR-based analyzers, thus significantly reducing reference gas (required for differential analyzers) and calibration gas demands. Spectroscopic analyzers usually also have the provision to make sufficiently accurate water vapor corrections compared to NDIR-based analyzers that are not very accurate for H<sub>2</sub>O, which can allow for the relaxation of sample air drying requirements. It is important to note, however, that partial drying is normally still required with spectroscopic analyzers, as maintaining a high-accuracy water correction in the field over the full range of ambient atmospheric H<sub>2</sub>O concentrations is challenging.

The use of ships for MBL measurements using the new technology is gaining traction with the WMO recognizing the first mobile research station in the GAW in May 2018 on the Australian ship, RV *Investigator*. This ship is equipped with a purpose-built atmospheric monitoring laboratory that reports 1-min measurements of atmospheric CO<sub>2</sub> using a cavity ring down spectrometer. The ship is also equipped with an array of meteorological, radon and carbon particulate sensors that are useful for identifying land-based or ship-stack sources of CO<sub>2</sub>. These newer spectroscopic analyzers are much more expensive than NDIR analyzers; they can, however, be used for pCO<sub>2w</sub> measurement as well as MBL CO<sub>2</sub> measurement, preventing the need to double up on equipment, as demonstrated by Becker et al. (2012). Depending on the model, they are also capable of other underway measurements of interest to the carbon cycle community, such as the stable carbon isotope ratio of CO<sub>2</sub> (<sup>13</sup>C/<sup>12</sup>C) in water and air (Cheng et al., 2019).

To make an informed decision about how best to obtain high-accuracy MBL CO<sub>2</sub> data (i.e., using existing equipment or investing in new instrumentation), one needs to take into consideration both the scientific goals and logistical constraints (such as space, power requirements, and frequency of maintenance). It is also necessary to address the following question: just how good are the existing data? Verifying the quality of MBL CO<sub>2</sub> data is an important and on-going part of

making such measurements, and there are several approaches that can be employed. A highly recommended way is the use of a Target Tank (TT). A TT is a cylinder of dry, natural air that has been measured for CO<sub>2</sub> against the CCL maintained scale before and after it is deployed in the field. The TT is not used to calibrate the system, but is run periodically as a quality control check (e.g., Kozlova and Manning, 2009), to check if the TT CO<sub>2</sub> value obtained from the shipboard measurement system matches the CCL declared value, thus enabling the compatibility of the pCO<sub>2</sub> system to be quantified relative to the laboratory where the TT CO<sub>2</sub> value was declared. The main limitation of TTs is that they usually do not pass through the whole gas handling system (it is generally not practical to feed TT gas through the inlet lines, for example), and so only provide a partial test of the system. The TT can also be used to assess drift of the onboard calibration cylinders.

Other methods that provide a more independent check consist of comparisons with co-located measurements, either from flask samples, which are collected *in situ* and sent to a laboratory for subsequent analysis, or by making use of a “traveling instrument”: a completely independent, high-precision continuous measurement system that is installed alongside the existing measurement system for a limited time. The latter approach is used as part of the WMO/GAW station audits in the atmospheric measurement community (Zellweger et al., 2016). Using the flask approach is logistically much easier and can be continued periodically, but does not necessarily help to identify the source of discrepancy in cases where measurements do not agree. Conversely, a traveling instrument can be impractical to implement for a shipboard system and is usually a one-time operation lasting only a few weeks, but is more likely to be able to assist in diagnosing CO<sub>2</sub> offsets.

Employing at least one of the methods mentioned above to regularly validate MBL CO<sub>2</sub> measurements is fundamental to maintaining good data quality, regardless of whether an investigator uses existing equipment or new instrumentation.

A separate issue is that ships are moving platforms that generate their own CO<sub>2</sub> emissions; thus, shipboard CO<sub>2</sub> measurement differs from land-based CO<sub>2</sub> measurement, where stations are typically located remotely from local sources of pollution to avoid data contamination. While efforts are made to locate measurement system inlets as far away as possible from ship exhaust stacks, it is usually unavoidable that some CO<sub>2</sub> emissions from the ship itself will be observed and will need to be filtered out of the dataset, or “flagged,” during post-processing. Even if exhaust CO<sub>2</sub> emissions are not often detected (as on some of the larger container ships), any data that is deemed to be “non-background,” such as when ships are close to the coast, will also need to be identified. Moorings and wind- or wave-powered ASVs avoid this CO<sub>2</sub> contamination, except when in proximity to a ship or to the coast.

A simple and effective method for flagging non-background values in a MBL CO<sub>2</sub> dataset is to assess the  $\pm 1\sigma$  standard deviation (sd) of the CO<sub>2</sub> values over a specific time period, often an hour (but sometimes a shorter or longer time period is used, depending on the measurement frequency). Other, more sophisticated statistical flagging methods also exist, such as

the “REBS” method from El Yazidi et al. (2018), but are not necessarily any better than the sd approach. For ships, it is also often prudent to combine a statistical flagging method with meteorological flagging, whereby data that are measured when the relative wind direction originates from the exhaust stack of the ship and when the absolute wind speed is low are flagged as polluted (e.g., Chapter 3 of Pickers, 2016).

Regardless of the automated flagging method used, some manual quality control/validation of shipboard MBL CO<sub>2</sub> measurements is desirable if these data are to be made available to the wider scientific community via online databases such as SOCAT. Details on quality control activities and who would be responsible are currently being worked out.

## PERSPECTIVE AND STATUS OF PRODUCT DEVELOPMENT

The need for ocean carbon networks was articulated in a previous Ocean Observing Conference, OceanObs09 paper (Monteiro et al., 2010) and in an Integrated Ocean Observing System (IOOS) Summit manuscript (Wanninkhof et al., 2012). SOCONET is a refinement of the concepts discussed in these proceedings with more focus on network design, required instrumental accuracy and deliverables. SOCONET aims to contribute data of known high-quality and at regular intervals for three main products: surface ocean CO<sub>2</sub> maps; the global air-sea CO<sub>2</sub> fluxes at monthly resolution and 1° by 1° grid that will be served annually; and MBL CO<sub>2</sub> data to constrain inverse models. These products are in development in research mode by different groups. The inverse models and assimilation approaches such as CarbonTracker are quasi-operational but results can be improved with quality MBL CO<sub>2</sub> data.

Surface maps of ocean acidification can be created in a similar fashion as surface ocean CO<sub>2</sub> maps, utilizing surface ocean pCO<sub>2</sub> data, and estimates or measurements of DIC or TALK.

These include pH maps but also carbonate ion concentrations and aragonite/calcite saturation state maps. A synopsis of the interrelationships between pCO<sub>2</sub> and inorganic carbon parameters as they pertain to OA are provided in **Appendix A**. The global climatological maps of pH by Jiang et al. (2015) were produced from measurements and interpolation of the relevant ocean acidification parameters calculated from total alkalinity (TALK) and total dissolved inorganic carbon (DIC). SOCONET will provide data for products that more closely follow the approach of Takahashi et al. (2014) and Lauvset et al. (2015). It uses surface ocean pCO<sub>2</sub> data together with estimates of TALK based on salinity to determine climatological OA products. The Takahashi et al. (2014) effort includes interpolation and is on monthly resolution and 4° by 5° spacing, and is based on a climatology referenced to year 2010 excluding the Pacific. By creating pCO<sub>2</sub> fields using remotely sensed sea surface temperature (SST) and sea surface salinity (SSS) fields and other high-resolution data, the OA products derived from SOCONET can be created at higher temporal and spatial resolution (Salisbury et al., 2015; Shutler et al., 2019). The approach of assessing OA from pCO<sub>2</sub> measurements may be

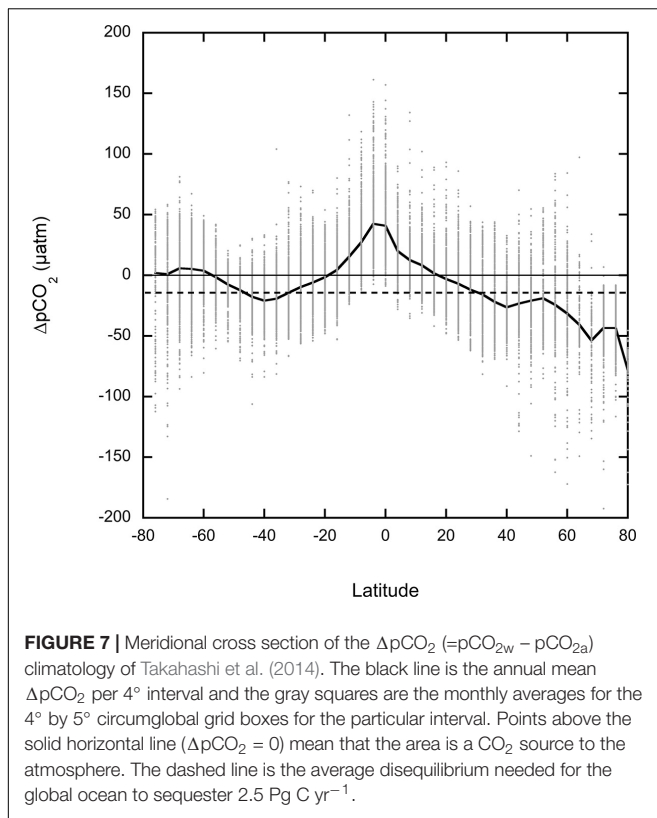
hindered in coastal settings, such as the Baltic Sea where TALK and TALK-SSS relationships may change on similar timescales as pCO<sub>2</sub> (Müller et al., 2016).

There are several efforts to create air-sea CO<sub>2</sub> flux maps. Monthly climatologies at 4° by 5° grids referenced to a particular year are provided in Takahashi et al. (2009). The temporal and spatial gap filling, which is a major consideration in the production of maps, was aided by using a surface velocity field from an ocean circulation model. Lee et al. (1998) and Park et al. (2010) used these pCO<sub>2w</sub> climatologies to determine changes in time and space by establishing correlations between pCO<sub>2</sub> and SST for each 4° × 5° pixel. This provided the first observation-based estimate of interannual changes in air-sea CO<sub>2</sub> fluxes. More sophisticated approaches have been developed in the last decade, most notably NN and SOM approaches, and data constrained inverse methods. Eleven of the pCO<sub>2</sub> products have been evaluated in a project called SOCOM (Rödenbeck et al., 2015). The detail and complexity of interpolation schemes differ significantly between the various approaches but they all aim to create pCO<sub>2</sub> fields at high resolution from relatively sparse data (**Figure 4**).

Advances in collation of data from groups worldwide have aided the product development. First initiated by Taro Takahashi of LDEO, Columbia University, largely as a single investigator effort, it was communalized under the auspices of IOCCP as the Surface Ocean CO<sub>2</sub> Atlas (SOCAT) effort that provides annual releases of data voluntarily submitted and quality controlled by groups around the globe (Bakker et al., 2016). The value added to the collated dataset is that the data undergo secondary quality control, and pertinent external parameters are added. Standardized metadata and common methods of data acquisition are encouraged, in part, through a ranking of datasets from A through F. Since data sets rated as A and B meet the accuracy standards for SOCONET pCO<sub>2w</sub> data (**Table 3**), the SOCAT data can be used as an initial screening of platforms. Data products averaged at 1° by 1° for the open ocean and 1/4° by 1/4° for the coastal ocean are provided by SOCAT as well.

A challenge in producing accurate global surface ocean CO<sub>2</sub> and flux maps is that the magnitudes of longer-term trends in pCO<sub>2w</sub> are small compared to spatial and temporal variability but their assessments are critical in evaluating the trends of the flux on decadal time-scales (Schuster and Watson, 2007; Landschützer et al., 2014; Iida et al., 2015). Ocean acidification and long term changes in air-sea CO<sub>2</sub> fluxes are driven by increases in atmospheric CO<sub>2</sub> and the resulting disequilibrium between marine air and surface ocean, which is small. This small disequilibrium is difficult to discern. Atmospheric CO<sub>2</sub> values that are currently increasing by 2.4 ppm yr<sup>-1</sup> and seasonal changes in pCO<sub>2w</sub> that can be greater than 150 μatm. Regional annual mean differences are over 50 μatm (**Figure 7**). Moreover, near-surface gradients in CO<sub>2</sub> caused by temperature and other physical and chemical effects can influence the CO<sub>2</sub> gradient and flux across the interface. This requires more investigation and could influence operational aspects of SOCONET in the future. An underappreciated fact in view of the large variability is that small systematic biases in pCO<sub>2</sub> measurements and biases





caused by the interpolations over time will have a large impact on quantification of uptake.

It is envisioned that the production of near real-time surface ocean  $\text{CO}_2$  maps and  $\text{CO}_2$  flux maps will rely heavily on the SOCONET effort. Currently the maps are not created in an operational fashion but tools to do so are under development. The closest to an operational product are the SOM/NN approaches. Summaries of the methodologies to determine surface  $\text{CO}_2$  fields and  $\text{CO}_2$  fluxes are provided in Rödenbeck et al. (2015) and Zeng et al. (2017). In these efforts the fidelity of the different approaches are critically and objectively investigated, and visualized through, for example, Taylor diagrams such that a concise statistical summary is obtained of how well patterns match each other in terms of their correlation, their root-mean-square difference, and the ratio of their variances (Taylor, 2001; National Center for Atmospheric Research Staff [NCAR], 2013).

All current surface ocean  $\text{CO}_2$  mapping efforts rely on interpolation and/or creating algorithms of  $p\text{CO}_2$  with environmental fields that are available with high space/time coverage. The ability to create realistic, near real-time maps will depend on the amount of  $p\text{CO}_2$  data available, its timeliness, and, because the fluxes are greatly influenced by bias, on the accuracy of  $p\text{CO}_{2w}$  and  $p\text{CO}_{2a}$  values. The MBL and surface ocean  $\text{CO}_2$  values are systematically changing with time due to emission of anthropogenic  $\text{CO}_2$  into the atmosphere, such that obtaining values in a timely fashion is critical.

The need for up-to-date  $\text{CO}_2$  values for accurate and timely products is emphasized as current approaches rely on creating relationships of  $p\text{CO}_2$  with variables that can be obtained

in near real-time through remote sensing, models or from autonomous platforms. The NN and SOM methods that are increasingly used are based on machine learning of patterns and correlations. The relationships are created with different input parameters but generally include SST, location, mixed layer depth, and sometimes SSS, and ocean color. In some approaches there is partitioning based on biogeographic provinces that are effective for the changing ocean (Oliver and Irwin, 2008; Fay and McKinley, 2014). The independent variables change with time, and can change in a different fashion than surface ocean  $\text{CO}_2$ , such that continued updates using recent  $p\text{CO}_{2w}$  data are important in order to produce accurate products. Once the correlations in machine learning approaches are established, the approach can be used in absence of actual  $p\text{CO}_{2w}$  data. However, the products can become biased over time if the algorithms are not updated.

Maps can be created as soon as the independent variables are available; this is in near real-time and within a year with quality control. It is *a priori* assumed that over annual time period the relationship between  $p\text{CO}_{2w}$  and independent variables is invariant. If  $p\text{CO}_2$  data are available in a prompt fashion, these can be used for validation and for updating the parameterizations. A proper collation and quality control mechanisms of recent SOCONET data, and an approach to easily ingest the SOCONET data into algorithms will be essential. Being able to provide up-to-date information of anticipated data through real-time data tracking will facilitate the routine development of products.

## CONNECTIVITY TO OTHER SCIENTIFIC EFFORTS AND NETWORKS

Surface Ocean  $\text{CO}_2$  NETWORK will contribute to other surface ocean networks and the MBL measurements can contribute to atmospheric efforts. This includes the full surface ocean  $p\text{CO}_2$  network, whose data are largely captured by SOCAT, and contains  $p\text{CO}_2$  data obtained by different types of instruments. Networks that focus on other carbon variables, often associated with OA and ocean health under the GOA-ON purview, will benefit from the SOCONET effort. In addition, the SOCONET effort is closely aligned with GO-SHIP, executed on research ships. Accurate surface ocean and air  $\text{CO}_2$  values can be used to constrain  $\text{CO}_2$  fluxes in a similar fashion as heat and momentum fluxes (Edson et al., 2004). The MBL  $\text{CO}_2$  measurements are part of a broader effort of greenhouse gas measurements over the ocean including nitrous oxide and methane in ICOS.

The network is focused on the infrastructure to deliver accurate  $p\text{CO}_2$  data. It is envisioned that the JCOMM Observations Program Area (OPA) structure will facilitate the operational interactions with other networks. The interactions are largely synergistic, and include the needs for implementing SOCONET, and benefits of SOCONET to other efforts.

## Efforts and Networks That Are of Direct Benefit to SOCONET

The surface ocean thermosalinograph (TSG) network and data management by the Global Ocean Surface Underway Data



project, GOSUD provide sea surface temperature and salinity data. TSGs are integral support instruments for surface ocean CO<sub>2</sub> observations and interpretation, and are often critical for their transformation to OA parameters. All underway and mooring CO<sub>2</sub> systems have TSGs but these data do not undergo quality control as part of the pCO<sub>2</sub> data reduction. While TSG data are captured in the pCO<sub>2</sub> files, it is at lower temporal resolution congruent with the pCO<sub>2</sub> measurements. Interactions with JCOMM/SOT/SOOP should facilitate that the TSG data on SOOP-CO<sub>2</sub> and Mooring-CO<sub>2</sub> are quality controlled and served to the community. The quality control of salinity data would be coordinated through GOSUD. Automated routines for TSG data are available but access and flagging routines are cumbersome.

The Volunteer Observing Ship (VOS) Meteorological observations and moorings under the Data Buoy Cooperation Panel (DBCP) benefit SOCONET as barometric pressure is a key variable to calculate pCO<sub>2</sub> in air and water. These measurements are made routinely on VOS for weather applications, and barometers are calibrated by the national weather services. Wind speeds used to calculate air-sea CO<sub>2</sub> fluxes are generally obtained from remote sensing or numerical weather models but anemometer on ships or buoys are useful for comparison or validation of wind products.

## Contributions of SOCONET to Other Research and Network Efforts

Measurements of pCO<sub>2a</sub> from SOCONET platforms can be used to improve the NOAA/GMD MBL CO<sub>2</sub> reference product; to validate of MBL CO<sub>2</sub> in support of remote sensing (Chatterjee et al., 2017); and ground-based networks, such as TCCON (the Total Carbon Column Observing Network). An example of current satellite capacity to obtain synoptic global column XCO<sub>2</sub> based on the OCO2 mission values on global scales is provided in **Figure 8**.

The value of underway pCO<sub>2</sub> system MBL CO<sub>2</sub> measurements with inaccuracies of up to 0.2 ppm still needs to be fully investigated; although these data would not meet the WMO CCL compatibility goal of  $\pm 0.1$  ppm, but they still offer potential to be included in the collation/distribution efforts of the atmospheric measurement community because they help to fill gaps in the atmospheric measurement network. The World Data Centre for Greenhouse Gases (WDCGG), operated by the Japan Meteorological Agency (JMA) under GAW/WMO, and NOAA ObsPack products are two such atmospheric measurement community data distribution efforts that MBL CO<sub>2</sub> data from pCO<sub>2</sub> systems on ships could potentially contribute to. The atmospheric inverse modeling community as potential users of MBL CO<sub>2</sub>, for example, those involved in the TransCom and IG3IS initiatives, is another way the underway pCO<sub>2</sub> community could forge and strengthen links with other scientists looking a similar carbon cycle issues from different angles.

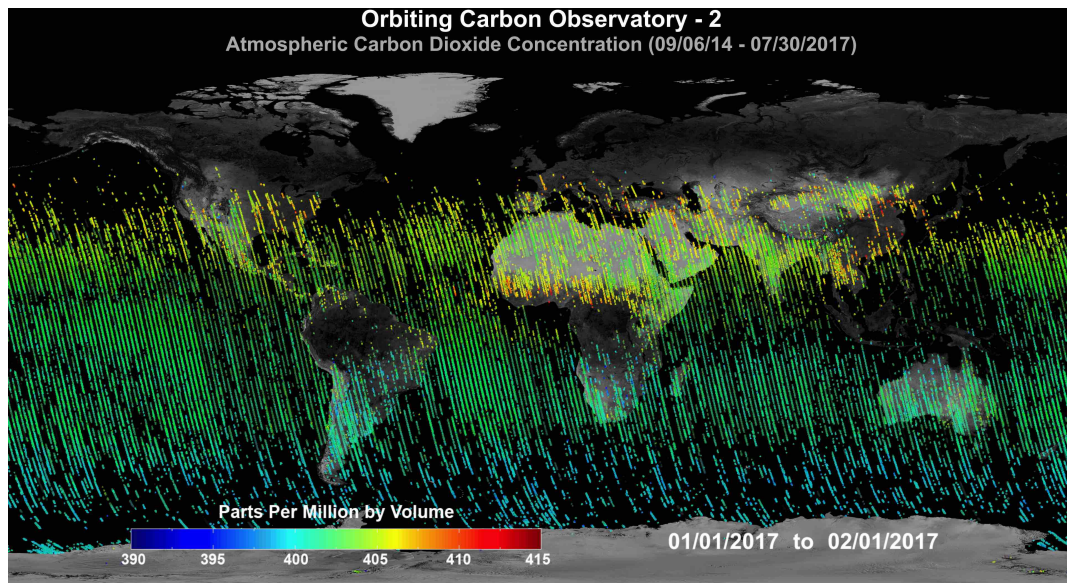
The data from the SOCONET effort can be used to validate pCO<sub>2</sub> estimates from BGC (biogeochemical) Argo floats. The development of biogeochemical sensors for Argo floats will greatly enhance our observational capabilities of the ocean, including the possibility of using the pH data from Argo to

calculate surface ocean pCO<sub>2</sub>. The current estimated accuracy for pCO<sub>2w</sub> values derived from pH is about 7  $\mu$ atm (Williams et al., 2017; Gray et al., 2018). However, the pH sensors cannot be calibrated once deployed, and pCO<sub>2w</sub> estimates need to be validated to evaluate how systematic errors evolve with time. This can be accomplished with ships in SOCONET. For example, cross-overs between SOCCOM BGC floats and the ARSV *Laurence M. Gould* have been evaluated by Fay et al. (2018). Strategies for targeting of BGC floats with SOCONET ships could enhance validation efforts by increasing the number and quality of cross-overs. As the reference network includes research ships that deploy the BGC Argo floats, co-located measurements are also possible at the site and time of deployment. A rapid return of quality-controlled data is desirable for this application.

Surface Ocean CO<sub>2</sub> NETWORK could be used to build out of a BGC network in the essential ocean variable (EOV) framework. Inorganic carbon is an EOV and pCO<sub>2</sub> is a key component of the inorganic carbon system. Monitoring pCO<sub>2</sub> from surface platforms will provide key insights on ocean acidification. It is a core measurement that can be used in conjunction with other developing BGC observations to study biological productivity in the ocean. The SOCONET reference network and its infrastructure have the potential to be the backbone of the surface ocean BGC observing system.

## OUTLOOK AND RECOMMENDATIONS

Surface Ocean CO<sub>2</sub> NETWORK is a partnership of many investigators that have as major goal measuring surface ocean CO<sub>2</sub> and MBL CO<sub>2</sub> levels on an operational basis following agreed upon procedures. The accurate measurements will be disseminated within a year of measurement. Platform and instrument metadata tracking would occur in near-real time. The current list of platforms and participants that expressed interest in being part of SOCONET can be found at [www.aoml.noaa.gov/ocd/gcc/SOCONET](http://www.aoml.noaa.gov/ocd/gcc/SOCONET). The measurements are key inputs to products addressing important social, policy, and economic issues of our time as they pertain to marine health and anthropogenic carbon sequestration. The SOCONET activities are not the sole effort of most partners who are involved in a variety of related research activities. This will facilitate interactions with other networks and research efforts. While the surface ocean and MBL measurements are automated, the data reduction and quality control for the level of accuracy required for SOCONET are labor intensive, adding to the challenges of timeliness and cost of operation of the network. From an organizational perspective, securing and maintaining resources in these international distributed networks is critical, and means need to be explored to accomplish this. This holds true particularly for the communal aspects, including network design, data tracking, and coordination. A procedure of securing equitable national contributions must be developed for SOCONET (and many other network activities as described in this volume). Working through intergovernmental entities such as JCOMM and GOOS will be of benefit. SOCONET can serve as



**FIGURE 8** | Column  $x\text{CO}_2$  measurement from the Observations from the Orbiting Carbon Observatory-2 (OCO-2) for January 2017. These data were produced by the OCO-2 project at the Jet Propulsion Laboratory, California Institute of Technology, and obtained from the OCO-2 data archive maintained at the NASA Goddard Earth Science Data and Information Services Center.

an example how networks will transition from platform-based to EOVS-based entities addressing stakeholder needs.

The recommendations evolve around the establishment of the network for accurate  $p\text{CO}_{2w}$  and MBL  $\text{CO}_2$  measurements following GOOS/JCOMM network principles that include utilizing the approaches of technical readiness level and addressing current impediments for execution. The following recommendations for implementing SOCONET and MBL measurements are the general steps necessary to develop and maintain a sustained network of surface ocean observations:

### Resource Requirements

Determine the cost and agency contributions for a sustained reference network and develop strategies to maintain such a network including common operational facilities. Sustained support for technical coordination through JCOMMOPS needs to be sought.

### Labeling of All Platforms in SOCONET

Labeling is a term used in ICOS referring to a station providing the required metadata and readiness of the measurements. For SOCONET the labeling and tracking of platforms would occur through JCOMMOPS.

### Protocols for Quality Control and Verification of SOCONET Data

Surface Ocean  $\text{CO}_2$  NETWORK instruments should be operated with a means to verify quality through a series of steps including shoreside checks, side-by-side comparisons, crossover checks, traceable gas standards and periodic calibration or calibration checks of system components.

### Network Performance Checks

The network performance would be evaluated based on number of platforms acquiring data, initial quality assessment, data loss and causes thereof, and network stability based on number of platforms and location of measurements. Implementing these checks will require creating a set of metrics based on the delivery surface ocean and MBL  $\text{CO}_2$  data to specified accuracy and density.

### MBL Air Measurements From SOCONET Platforms

Verify accuracy of current systems and determine protocols to determine quality of data including use of target gases and intercomparisons. Determine if accuracy meets community needs, and assess alternative arrangements such as different sampling frequency, sensors or stand-alone systems.

### Utility of Measurements

Determine and track users and uses of measurements. This includes outreach and new applications focused on societal importance. In particular determine new customers of the reference data such as those who are involved in greenhouse gas verification schemes.

Surface Ocean  $\text{CO}_2$  NETWORK and associated MBL  $\text{CO}_2$  measurements is an emerging network utilizing established instruments and platforms. It is focused on applying best practices for reference quality measurements, rapid data delivery, and platform tracking. The coordinated effort should aid development of timely and routine data products delivery in support of quantifying air-sea  $\text{CO}_2$  fluxes, trends and variability in MBL and surface ocean  $p\text{CO}_2$ . It should lead

to positive exposure and stability of funding for all the participants who rely on national resources for operation of their systems.

## AUTHOR CONTRIBUTIONS

All authors listed have made direct and intellectual contributions to the work, and approved it for publication. RW and PP were the lead on the surface ocean and MBL components, respectively. MH performed a thorough proofreading of the galley proofs.

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## SUPPLEMENTARY MATERIAL

The Supplementary Material for this article can be found online at: <https://www.frontiersin.org/articles/10.3389/fmars.2019.00400/full#supplementary-material>

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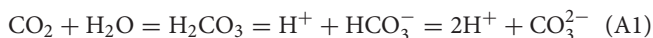
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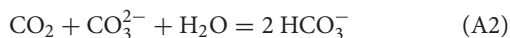
## APPENDIX A: OCEAN ACIDIFICATION AND PCO<sub>2</sub>

A direct impact of increasing pCO<sub>2</sub> levels in the ocean is the phenomenon of ocean acidification. While the definitions of OA vary to some extent most are in line with the following: “Ocean acidification refers to a reduction in the pH of the ocean over an extended period of time, typically decades or longer, which is caused primarily by uptake of carbon dioxide (CO<sub>2</sub>) from the atmosphere.” (Field et al., 2011). With increasing emphasis on changes in ocean inorganic carbon chemistry in addition to pH decrease, the definition is broadened to: “reduction of seawater pH and changes ocean chemistry that are collectively referred to as ocean acidification.”

Surface Ocean CO<sub>2</sub> NETWORK thus addresses the key forcing components of OA involving the uptake of anthropogenic CO<sub>2</sub> and changing surface ocean CO<sub>2</sub>. There is a strong correlation between pCO<sub>2</sub> and pH as can be seen from the hydration reaction and dissociation of CO<sub>2</sub> summarized by the chemical equation:



The changes in inorganic carbon speciation can impact the biogeochemical and biological responses. In particular, increasing CO<sub>2</sub> concentrations lower carbonate ion concentrations through the major net buffering reaction in the oceanic inorganic carbon system that can be summarized as:



An example of the correlation between pCO<sub>2</sub> and pH for surface water is shown in **Supplementary Figure S1** using surface

ocean measurements from a GO-SHIP cruise P18 in the SE Pacific. The strong correspondence is apparent, and deviations from a singular relationship are due to differences in the buffering of the seawater that will impact the equilibria in A1 and A2.

Increasing CO<sub>2</sub> leads to a decrease in carbonate levels and resulting decrease of calcium carbonate saturation state (Bates et al., 2014). This is of concern for calcifying organisms that are abundant in the ocean. The biological production of corals, as well as calcifying phytoplankton and zooplankton will be inhibited or slowed. The dissolution of biotic and abiotic calcium carbonate in the water column and the ocean floor will be enhanced.

Species containing aragonite, and meta-stable forms of calcium carbonate produced by corals and plankton, such as pteropods will be particularly susceptible to a reduction of CO<sub>3</sub><sup>2-</sup> in seawater.

Ocean acidification also impacts organisms that do not fix calcium carbonate. Increasing seawater CO<sub>2</sub> levels and lower pH can weaken metabolic processes for organisms, from feeding to respiration to reproduction and change the chemical speciation of trace metals essential for their needs. While predicting the precise response of ocean ecosystems is challenging for scenarios of increased CO<sub>2</sub> levels, it is likely the ecosystems will be less productive, less diverse and less resilient. In addition, the synergistic impacts of other climate and human impacts on the ocean, including ocean warming and de-oxygenation, will exacerbate the impacts of elevated CO<sub>2</sub> levels and associated acidification. SOCONET data will provide critical input on the trends of the major factors influencing OA and air-sea CO<sub>2</sub> fluxes, and resulting decreases in pH and carbonate levels.