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A Surface Ocean CO_2 Reference Network, SOCONET and Associated Marine Boundary Layer CO_2 Measurements

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The Surface Ocean CO_2 NETwork (SOCONET) and atmospheric Marine Boundary Layer (MBL) CO_2 measurements from ships and buoys focus on the operational aspects of measurements of CO_2 in both the ocean surface and atmospheric MBLs. The goal is to provide accurate pCO_2 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_2 and air-sea CO_2 flux measurements. These products and other derivatives using surface ocean and MBL

CO_2 data, such as surface ocean pH maps and MBL CO_2 maps, will be of high value for policy assessments and socio-economic decisions regarding the role of the ocean in sequestering anthropogenic CO_2 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_2) 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_2 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_2 have surpassed mere curiosity. Increasing emphasis in carbon cycle research is placed on monitoring and quantifying the sources and sinks of atmospheric CO_2, and the interplay between the anthropogenic CO_2, that is, CO_2 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_2 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_2 by the ocean is thus a critical element in understanding carbon dynamics and future trajectories of atmospheric CO_2 growth.

Accurate measurements of CO_2 concentrations in the surface ocean and atmospheric marine boundary layer (MBL) are critical factors to quantify the air-sea flux of CO_2, along with the forcing function, called the gas transfer velocity, k. The air-sea CO_2 flux, F_{CO2} [mol m^{-2} yr^{-1}] is commonly expressed in terms of a bulk formulation as:

$$F_{CO2} = k\,s(pCO_{2w} - pCO_{2a}) = k\,s\Delta pCO_2 \quad (1)$$

where k [m yr^{-1}] is parameterized with wind (Wanninkhof, 2014), s is the solubility [mol m^{-3} atm^{-1}], pCO_{2w} is the partial pressure of CO_2 in water [atm], pCO_{2a} is the partial pressure of CO_2 in air [atm], and ΔpCO_2 is the difference. The units for k, s, and pCO_2 are often reported as cm hr^{-1}, mol l^{-1} atm^{-1}, and μatm, respectively, and appropriate conversions need to be applied. The quantities measured are the mole fractions of CO_2 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 ΔpCO_2 over the open ocean can vary in time and space by about ± 100 μatm, the average disequilibrium needed to sequester the current annual ocean uptake of 2.5 billion tons of anthropogenic carbon (2.5 Pg C yr^{-1}) (Le Quéré et al., 2018) is only 7–14 μatm, 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_2 emissions by the ocean is of benefit as it curtails increasing atmospheric CO_2 level and its associated greenhouse effect, but the corresponding CO_2 increase in ocean surface waters also leads to ocean acidification (OA), which is detrimental to many marine organisms. Knowledge of the rate of CO_2 uptake and changes thereof are of importance for socio-economic assessments related to the fate of anthropogenic CO_2 and to ocean health.

Systematic measurement of atmospheric CO_2 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_2 uptake and release, prompted a small global network of measurements to assess the global distribution of the seasonal and long-term features in CO_2 (Keeling, 2008). As such, initial CO_2 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_2 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_2. 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_2 in the MBL. The atmospheric CO_2 data from these ocean community CO_2 systems do not, however, typically meet the rigorous standards of the atmospheric CO_2 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_2 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_2 measurements, such calibrated measurements can be used effectively for constraining air-sea CO_2 fluxes, and in inverse models.

Surface ocean CO_2 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_2 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_2 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 its 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_2 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_2 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_2 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_2 (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^{-1} ocean uptake and a price of $19 per ton CO_2.

While the uptake of CO_2 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_2 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_2 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_2 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, www.act-us.info/
CCL	Central Calibration Laboratory
CCGG	Carbon Cycle and Greenhouse Gas network www.esrl.noaa.gov/gmd/ccgg/mbl/index.html
DBCP	Data Buoy Cooperation Panel of JCOMM
ERDDAP	Environmental Research Division Data Access Program, https://coastwatch.pfeg.noaa.gov/erddap/index.html
ESRL	Earth System Research Laboratory of NOAA
EU	European Union
FOO	Framework for Ocean Observing of GOOS, www.oceanobs09.net/foo/
GAW	Global Atmosphere Watch of WMO, http://www.wmo.int/gaw
GCOS	Global Climate Observing System
GCP	Global Carbon Project, www.globalcarbonproject.org
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, www.icos-ri.eu
IG3IS	Integrated Global Greenhouse Gas Information System, www.wmo.int/pages/prog/arep/gaw/ghg/IG3IS-info.html
IOC	Intergovernmental Oceanographic Commission of UNESCO www.ioc-unesco.org/
IOCCP	International ocean carbon coordination project, http://ioccp.org
JCOMM	the Joint WMO-IOC Committee for Ocean and Marine Meteorology, www.jcomm.info
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_2 Observatory 2, https://co2.jpl.nasa.gov/#mission=OCO-2
OPA	Observations Program Area of JCOMM
SOCAT	Surface Ocean CO_2 Atlas; www.socat.info
SOCOM	Surface Ocean pCO_2 Mapping intercomparison
SOCONET	Surface Ocean CO_2 reference Network, www.soconet.info
TCCON	Total Carbon Column Observing Network, https://tccon-wiki.caltech.edu/
TransCom	Atmospheric Tracer Transport Model Intercomparison Project, transcom.lsce.ipsl.fr/transcom.lsce.ipsl.fr/
WDCGG	World Data Centre for Greenhouse Gases, https://gaw.kishou.go.jp/
WMO	World Meteorological Organization, https://public.wmo.int/en
AI	Artificial Intelligence
ASV	Autonomous Surface Vehicles
BGC	Biogeochemistry
CO_2	Carbon dioxide
DIC	(Total) Dissolved Inorganic Carbon
ECV	Essential Climate Variable, https:public.wmo.int/en/programmes/global-climate-observing-system/essential-limate-variables
EOV	Essential Ocean Variable, http://www.goosocean.org/eov
ETS	Emission Trading Scheme
FAIR	Findable, Accessible, Interoperable and Reusable
H_2O	Water (vapor)
MBL	Marine Boundary Layer
NN	Neural Network
OA	Ocean Acidification
OSE	Observing System Experiment
OSSE	Observing System Simulation Experiment
pCO_{2a}	Partial pressure of carbon dioxide in air
pCO_{2w}	Partial pressure of carbon dioxide in water
Pg C	Petagram of carbon (10^{15} g; 10^9 ton)
ppm	Parts per million (10^{-6})
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) thermosalinograph
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_2 NETwork will be a major contributor of reference quality observations to quantify air-sea CO_2 fluxes on seasonal to interannual scales, and to determine trends in pCO_{2w} 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_2 Atlas, SOCAT (Bakker et al., 2016) and mapping efforts such as SOCOM (Rödenbeck et al., 2015; **Figure 1**).

Surface Ocean CO_2 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_2 maps and air-sea CO_2 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_2 measurements will be used by atmospheric inverse modeling teams to generate improved estimates of CO_2 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_{CO2} 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_{2w} 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.

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.

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_2 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_2 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_2 measurements, can be found in the SOCONET prospectus (Wanninkhof et al., 2018) with a brief summary below.

Surface Ocean CO_2 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_2 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:

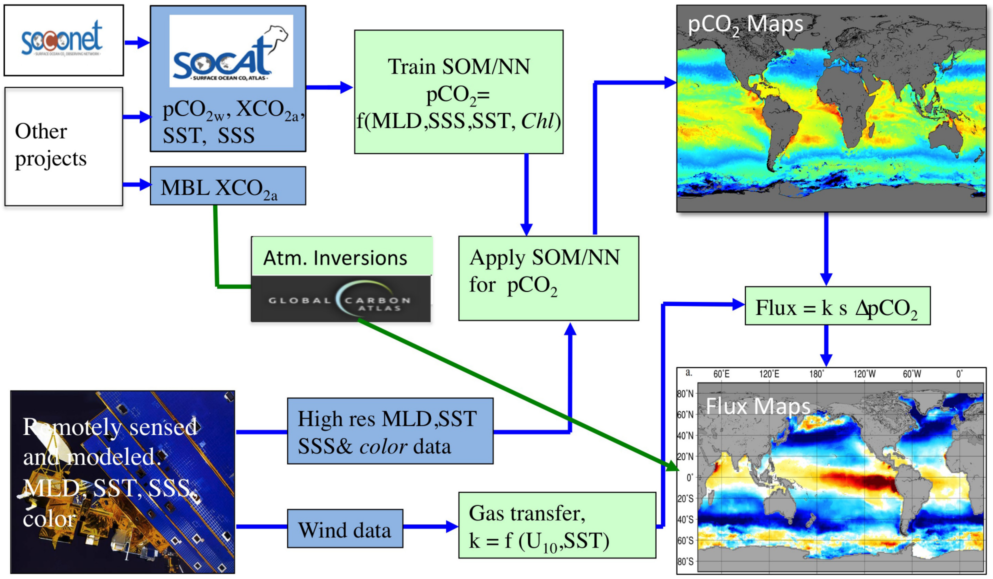


FIGURE 1 | Schematic how SOCONET and MBL CO_2 data will contribute to the creation of surface ocean pCO_2 maps and CO_2 flux maps. The blue boxes indicate data products and the light green boxes indicate the manipulations/calculations to the maps. This conceptual drawing indicates the many steps necessary to go from observations to products.

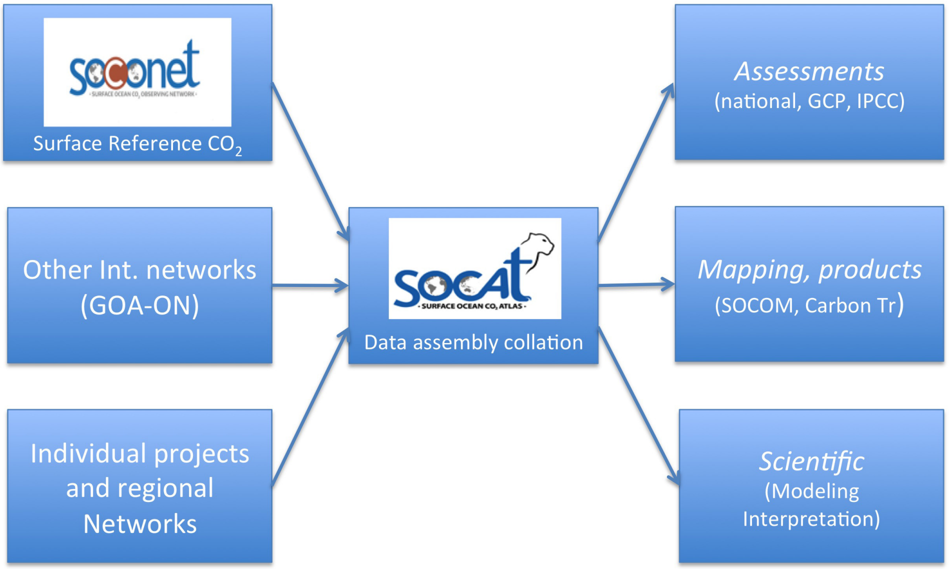


FIGURE 2 | Flow diagram that shows the relationship between SOCONET, SOCAT and other activities.

"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_2 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).

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_2 measurements are better than 2 μatm for water (pCO_{2w}) and 0.2 ppm for air (xCO_{2a}).
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.

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 depository for SOCONET surface water CO_2 data (**Figure 2**), and likely for the MBL CO_2 taken in conjunction with surface ocean pCO_2. Over the last several years, the SOCAT data

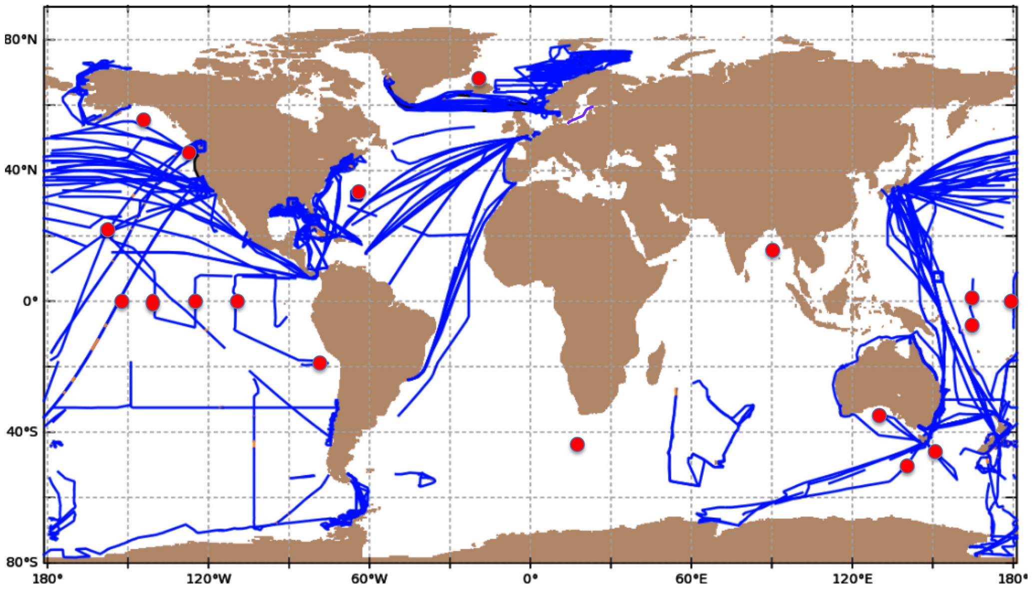
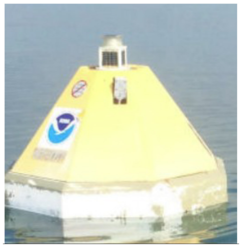


FIGURE 3 | Ship lines and moorings that currently meet SOCONET data quality and are potential contributors to the SOCONET effort. Lines are based on the SOCAT holdings from 2017 to 2018 with pCO_2 data that are believed to be accurate to within 2 μatm. The mooring sites with systems meeting the data quality standards are indicated by red circles.

TABLE 4 | Platforms used in SOCONET[1].

	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_2 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_2 systems. Other science projects often take place and provide value added both for interpretation of pCO_2 and for the projects.

[1] *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 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_2 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_2 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_2 exchange (e.g., Zappa et al., 2004); the impact of the biological pump on surface ocean CO_2 levels (e.g., Merlivat et al., 2015); feedbacks of calcifying organisms on surface water CO_2 (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_2 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_2 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_2 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_2 derived from pH sensors from profiling floats to estimate CO_2 values (Williams et al., 2017). While the derived pCO_2 data from pH provide good precision, the accuracy of the derived pCO_2 is not well constrained and this can be uniquely addressed by validation with accurate *in situ* pCO_2 data.

Network Design

To date there has not been a formal design of a global surface ocean CO_2 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_2 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_2 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_{2w} to Estimate Other Inorganic Carbon Parameters and Develop Products

In addition to using pH to estimate pCO_{2w} (Williams et al., 2017), the reverse needs to be investigated as well (**Appendix A**). The utilization of surface ocean pCO_2 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_2 map based on a SOM/NN approach. The pCO_{2w} 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_2 fluxes. As described above, there are several other data streams required to determine air-sea CO_2 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_2 OBSERVATIONS

Surface Ocean CO_2 NETwork has a strong focus on accurate pCO_{2w} measurements (**Table 3**), but offers a unique opportunity to contribute to (air) MBL CO_2 data, which are undersampled over the open ocean. Most of the underway pCO_2 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_2 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_2 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_2. Since the accuracy of MBL CO_2 data from underway CO_2 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.

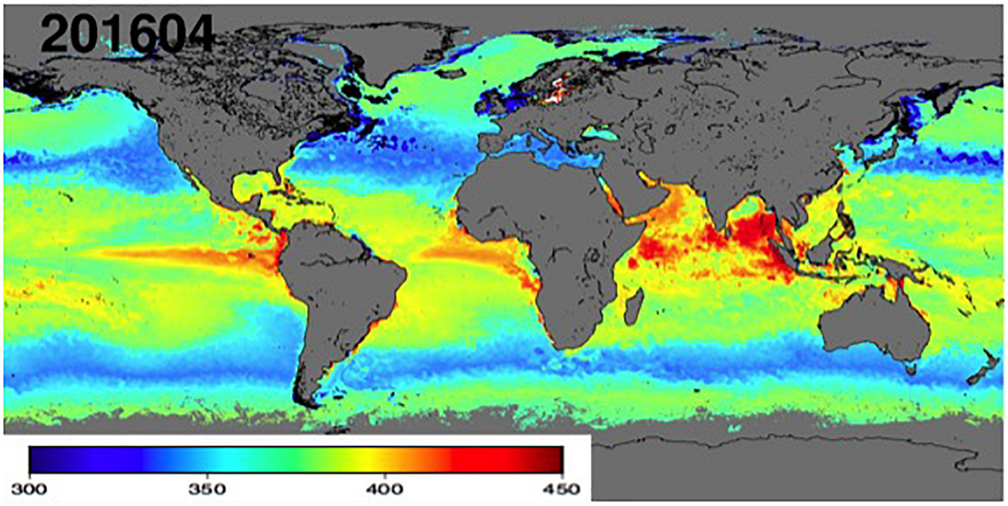


FIGURE 4 | Monthly map of pCO_{2w} for April 2016 created by a NN/SOM method showing the high fidelity of the output taking advantage of high-resolution remote sensing data. This example uses SOCAT data as the training set (units: μatm) (J. Triñanes, pers. com.).

Justification for Making Calibrated Accurate MBL CO_2 Observations From Ships

Here, calibrated accurate CO_2 measurements are those that are compatible to within ± 0.2 ppm of the global 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 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 CO_2 variability over the ocean interior is smaller than atmospheric CO_2 variability over land, and MBL CO_2 from the relatively imprecise measurements from systems focused on pCO_{2w} should be able to achieve the needed levels through averaging if these systems are appropriately optimized for atmospheric CO_2 measurement and kept well-maintained, but this has not been fully tested. It should be noted that the WMO/GAW ± 0.1 ppm compatibility goal (±0.05 over the Southern Hemisphere) will likely not be attained by the systems measuring pCO_{2w}. Moored air CO_2 measurements have not been validated to yet meet the ± 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 pCO_{2w} measurements that are good to within ± 2 μatm.

Validating and improving the quality of oceanic MBL 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 CO_2 fluxes (F_{CO2}). While most ships make *in situ* MBL CO_2 measurements, F_{CO2} is not usually calculated using these data. Instead, values for pCO_{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 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°S to 90°N and joined to create a 2-dimensional matrix (time versus latitude) of weekly 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 CO_2 that exists in the atmosphere, as explained in the online documentation and demonstrated previously (Pickers et al., 2017). The implications for F_{CO2} calculated using this product are that in some regions, particularly coastal margins where the effects of continental airflow on MBL CO_2 are not included in the NOAA MBL data product, biases will arise in the air-sea CO_2 fluxes.

Comparing F_{CO2} calculated using different sources of MBL CO_2 data is useful for demonstrating the potential impacts of using inaccurate atmospheric data to calculate fluxes. **Figure 5** shows that air-sea CO_2 fluxes calculated using the observed MBL CO_2 values at the Martha's Vineyard site in Massachusetts, United States (41.3°N, 70.6°W) can differ by up to 15% compared to those calculated using the NOAA MBL product. Mean annual differences between atmospheric 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 mol m^{-2} yr^{-1} (**Figure 5**). Moored pCO_2 systems, which measure air CO_2, also show

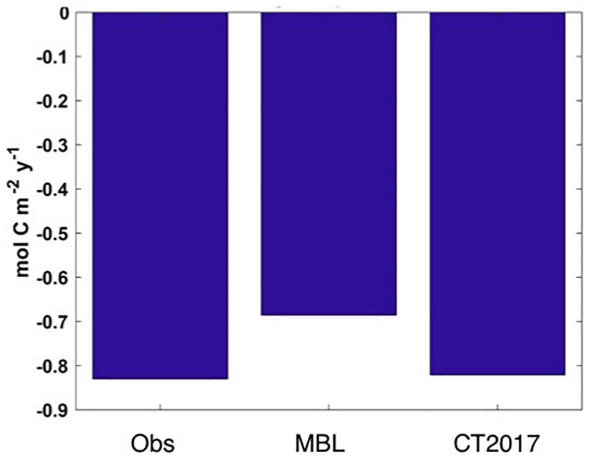


FIGURE 5 | Air-sea CO_2 fluxes at Martha's Vineyard, calculated using three different sources of atmospheric CO_2: *in situ* observations at the site (obs); the NOAA MBL reference product (MBL) and CarbonTracker 2017 (CT2017).

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_{2a} is often not considered to be significant compared to other sources of uncertainty in Eq. 1, **Figures 5**, **6** indicate that inaccurate atmospheric CO_2 values can lead to significant biases in F_{CO2} at both local and regional scales. Using the *in situ* atmospheric CO_2 data from ships and moorings will likely eliminate these F_{CO2} biases, provided that the MBL CO_2 data are sufficiently accurate and devoid of ship contamination.

Other benefits to the oceanic community from improving or validating shipboard and mooring MBL CO_2 data include increased confidence in CO_2 flux data products that include data from multiple different ships/measurement platforms, and better traceability of pCO_2 data to the Central Calibration Laboratory (CCL) of WMO/GAW currently housed at NOAA/ESRL. The process of upgrading current shipboard CO_2 measurement systems and protocols to facilitate high-accuracy atmospheric CO_2 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_2 data from ships will benefit the atmospheric research community by substantially augmenting the atmospheric CO_2 measurement network in regions that are currently undersampled. Such data will be of value to the atmospheric inverse modeling community, who estimate surface CO_2 fluxes using a "top-down" approach, an alternative methodology for the calculation of global air-sea CO_2 fluxes to the bulk flux approach (Eq. 1) that utilizes surface ocean pCO_2 measurements (e.g., Takahashi et al., 2009; Landschützer et al., 2013, 2014). The "top-down" approach combines measurements of atmospheric CO_2 (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_2 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_2 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_2 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_2 measurement platforms with the aim to maximize the scientific return of investment.

High-Accuracy Atmospheric CO_2 Measurement Approaches and Data Validation

The task of improving oceanic community MBL CO_2 measurements will be approached in two ways: by upgrading existing measurement systems that are not currently optimized for atmospheric CO_2 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_2 data are already sufficiently accurate to be used in F_{CO2} 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_2 are discussed, as well as the importance of data validation and quality control. Detailed technical information regarding atmospheric CO_2 measurement can be found in WMO/GAW Report 229 (2016) and in the ICOS atmospheric stations specifications document (Laurent, 2017).

Most existing underway pCO_2 measurements are currently made using instrumentation following ocean surface water pCO_2 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_2 measurements capabilities using a non-dispersive infrared (NDIR) analyzer (typically those manufactured by LI-COR Inc.), the traditional method for continuous atmospheric CO_2 measurement. Ocean community MBL CO_2 measurements are typically only required to be accurate to about ± 1 ppm in order to calculate air-sea CO_2 fluxes to specifications (Bender et al., 2002); hence, these measurement systems are not designed for atmospheric CO_2 measurement, with the priority instead focused upon ensuring the highest possible quality of near-continuous pCO_{2w} measurements. As such, the setups of these measurement systems are not optimized for obtaining high-accuracy MBL 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 CO_2 measurement, sample air drying might not be sufficient (insufficient drying can lead to CO_2 dilution, pressure broadening effects, and surface effects with tubing walls, all of which can bias CO_2 measurement), and there may be small undetected leaks, which can cause non-negligible CO_2 biases owing to the rigorous precision requirements of atmospheric CO_2 measurement. Furthermore, calibration protocols are currently not sufficiently rigorous to meet the compatibility standards aspired to by the atmospheric CO_2 measurement community as outlined in WMO/GAW report

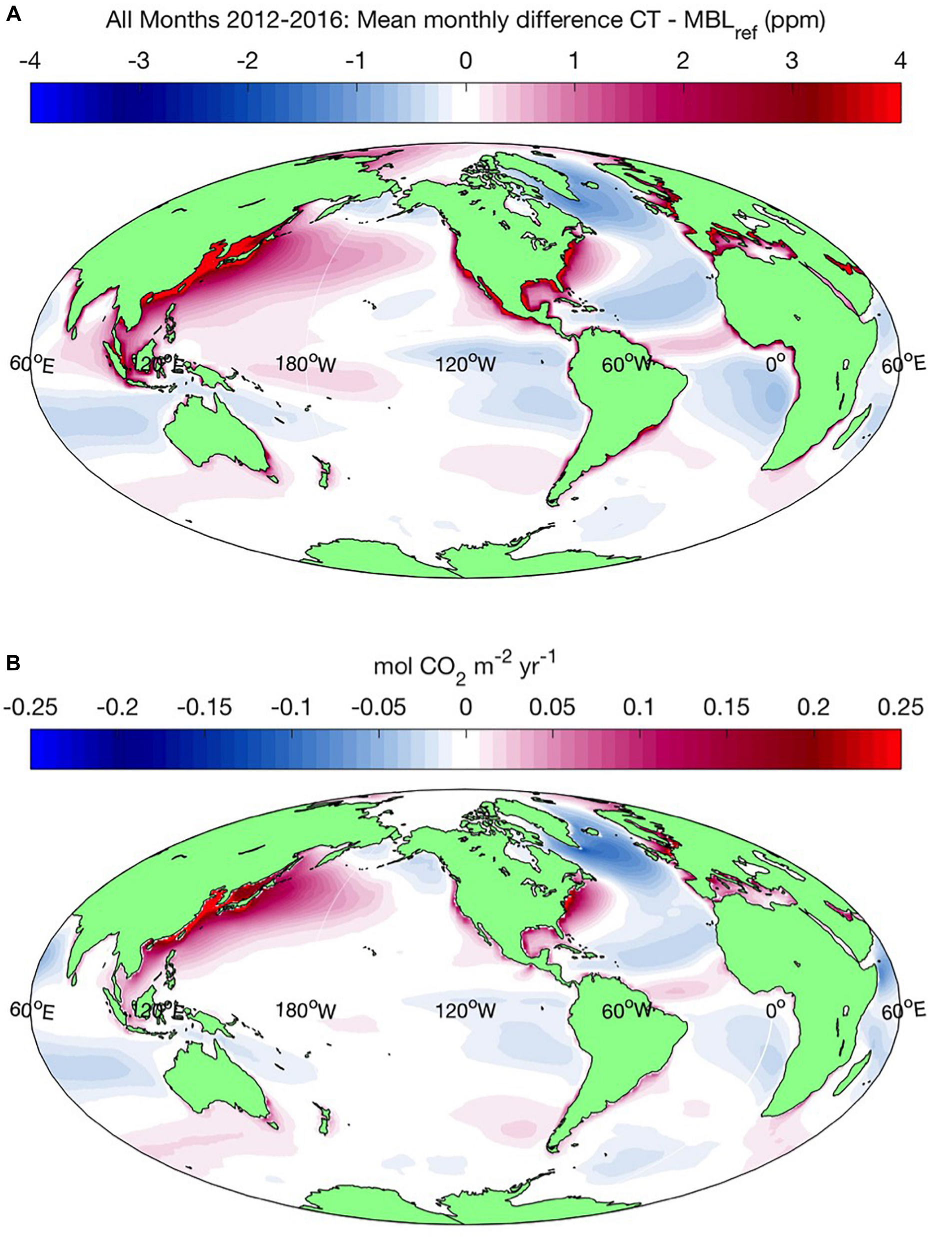


FIGURE 6 | (A) Mean monthly difference in atmospheric CO_2 over the oceans between CT2017 and the NOAA MBL CO_2 reference product, for the period 2012–2016. Note the differences downwind of the northern hemisphere continental land masses; **(B)** annual mean difference in F_{CO2} that arises from using atmospheric CO_2 from CT2017 compared to the NOAA MBL reference product.

no. 229. Nevertheless, with careful adherence to established protocols and procedures, it appears possible to obtain well-calibrated, accurate atmospheric CO_2 data using these existing systems.

Moored pCO_2 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_2 reference gas and zeroed using air stripped of CO_2, prior to every measurement. The sample air is not as completely dried as in the underway pCO_2 method (Sutton et al., 2014). Current development efforts are focused on improving accuracy through incorporation of a higher-quality NDIR or other CO_2 analyzer, further drying of air sample, and incorporation of a CO_2 reference/target gas.

The advent of commercial CO_2 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_2 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_2O, 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_2O 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_2 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_2. These newer spectroscopic analyzers are much more expensive than NDIR analyzers; they can, however, be used for pCO_{2w} measurement as well as MBL CO_2 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_2 ($^{13}C/^{12}C$) in water and air (Cheng et al., 2019).

To make an informed decision about how best to obtain high-accuracy MBL CO_2 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_2 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_2 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_2 value obtained from the shipboard measurement system matches the CCL declared value, thus enabling the compatibility of the pCO_2 system to be quantified relative to the laboratory where the TT CO_2 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_2 offsets.

Employing at least one of the methods mentioned above to regularly validate MBL CO_2 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_2 emissions; thus, shipboard CO_2 measurement differs from land-based CO_2 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_2 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_2 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_2 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_2 dataset is to assess the $\pm 1\sigma$ standard deviation (sd) of the CO_2 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_2 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_2 maps; the global air-sea CO_2 fluxes at monthly resolution and 1° by 1° grid that will be served annually; and MBL CO_2 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_2 data.

Surface maps of ocean acidification can by created in a similar fashion as surface ocean CO_2 maps, utilizing surface ocean pCO_2 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_2 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_2 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_2 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_2 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_2 (Müller et al., 2016).

There are several efforts to create air-sea CO_2 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_{2w} climatologies to determine changes in time and space by establishing correlations between pCO_2 and SST for each $4° \times 5°$ pixel. This provided the first observation-based estimate of interannual changes in air-sea CO_2 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_2 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_2 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_2 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_{2w} 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 ¼° by ¼° for the coastal ocean are provided by SOCAT as well.

A challenge in producing accurate global surface ocean CO_2 and flux maps is that the magnitudes of longer-term trends in pCO_{2w} 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_2 fluxes are driven by increases in atmospheric CO_2 and the resulting disequilibrium between marine air and surface ocean, which is small. This small disequilibrium is difficult to discern. Atmospheric CO_2 values that are currently increasing by 2.4 ppm yr^{-1} and seasonal changes in pCO_{2w} that can be greater than 150 μatm. Regional annual mean differences are over 50 μatm (**Figure 7**). Moreover, near-surface gradients in CO_2 caused by temperature and other physical and chemical effects can influence the CO_2 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_2 measurements and biases

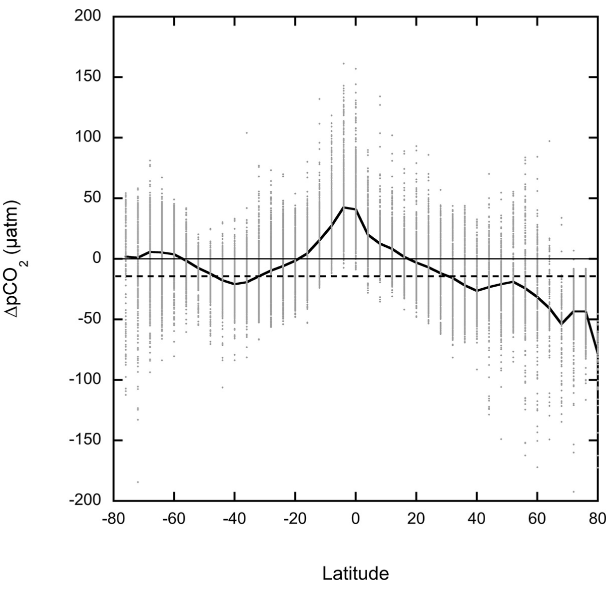


FIGURE 7 | Meridional cross section of the ΔpCO_2 (=$pCO_{2w} - pCO_{2a}$) climatology of Takahashi et al. (2014). The black line is the annual mean ΔpCO_2 per 4° interval and the gray squares are the monthly averages for the 4° by 5° circumglobal grid boxes for the particular interval. Points above the solid horizontal line ($\Delta pCO_2 = 0$) mean that the area is a CO_2 source to the atmosphere. The dashed line is the average disequilibrium needed for the global ocean to sequester 2.5 Pg C yr^{-1}.

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 CO_2 maps and 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 CO_2 fields and 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 CO_2 mapping efforts rely on interpolation and/or creating algorithms of pCO_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 pCO_2 data available, its timeliness, and, because the fluxes are greatly influenced by bias, on the accuracy of pCO_{2w} and pCO_{2a} values. The MBL and surface ocean CO_2 values are systematically changing with time due to emission of anthropogenic CO_2 into the atmosphere, such that obtaining values in a timely fashion is critical.

The need for up-to-date CO_2 values for accurate and timely products is emphasized as current approaches rely on creating relationships of pCO_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 CO_2, such that continued updates using recent pCO_{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 pCO_{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 pCO_{2w} and independent variables is invariant. If pCO_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 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 pCO_2 network, whose data are largely captured by SOCAT, and contains pCO_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 CO_2 values can be used to constrain CO_2 fluxes in a similar fashion as heat and momentum fluxes (Edson et al., 2004). The MBL 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 pCO_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_2 observations and interpretation, and are often critical for their transformation to OA parameters. All underway and mooring CO_2 systems have TSGs but these data do not undergo quality control as part of the pCO_2 data reduction. While TSG data are captured in the pCO_2 files, it is at lower temporal resolution congruent with the pCO_2 measurements. Interactions with JCOMM/SOT/SOOP should facilitate that the TSG data on SOOP-CO2 and Mooring-CO2 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_2 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_2 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_{2a} from SOCONET platforms can be used to improve the NOAA/GMD MBL CO_2 reference product; to validate of MBL CO_2 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_2 based on the OCO2 mission values on global scales is provided in **Figure 8**.

The value of underway pCO_2 system MBL CO_2 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 $+/-$ 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_2 data from pCO_2 systems on ships could potentially contribute to. The atmospheric inverse modeling community as potential users of MBL CO_2, for example, those involved in the TransCom and IG3IS initiatives, is another way the underway pCO_2 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_2 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_2. The current estimated accuracy for pCO_{2w} values derived from pH is about 7 μatm (Williams et al., 2017; Gray et al., 2018). However, the pH sensors cannot be calibrated once deployed, and pCO_{2w} 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_2 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_2 is a key component of the inorganic carbon system. Monitoring pCO_2 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_2 NETwork is a partnership of many investigators that have as major goal measuring surface ocean CO_2 and MBL CO_2 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. 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

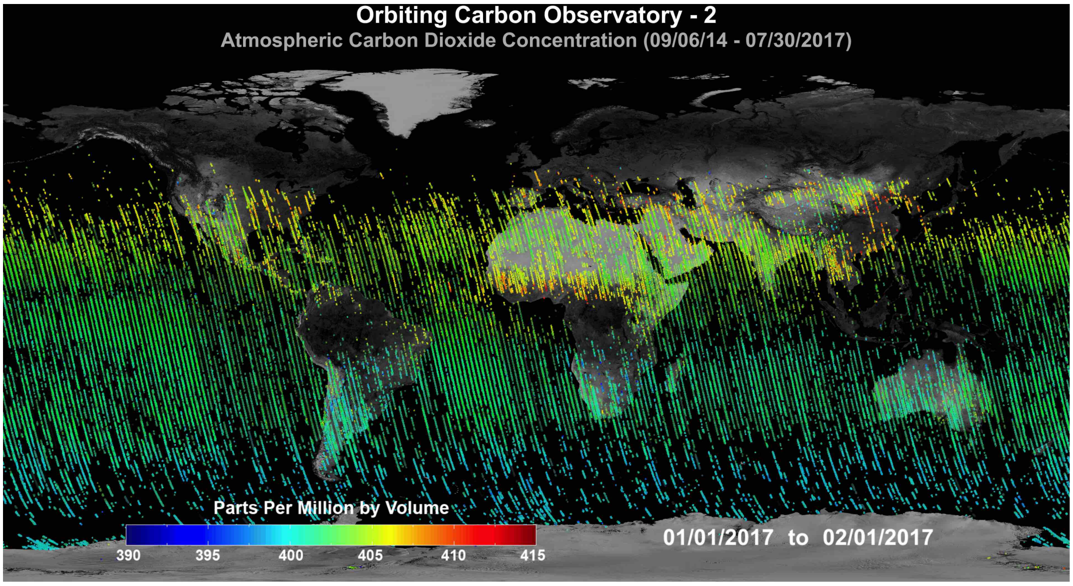


FIGURE 8 | Column xCO_2 measurement from the Observations from the Orbiting Carbon Observatory-2 (OCO-2) for January 2017. These data were produced by the OCO-2 project at the Jet Propulsion Laboratory, California Institute of Technology, and obtained from the OCO-2 data archive maintained at the NASA Goddard Earth Science Data and Information Services Center.

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

The recommendations evolve around the establishment of the network for accurate pCO_{2w} and MBL 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 CO_2 NETwork instruments should be operated with a means to verify quality though 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 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 CO_2 NETwork and associated MBL 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 CO_2 fluxes, trends and variability in MBL and surface ocean pCO_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.

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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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APPENDIX A: OCEAN ACIDIFICATION AND PCO$_2$

A direct impact of increasing pCO$_2$ 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$_2$) 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$_2$ NETwork thus addresses the key forcing components of OA involving the uptake of anthropogenic CO$_2$ and changing surface ocean CO$_2$. There is a strong correlation between pCO$_2$ and pH as can be seen from the hydration reaction and dissociation of CO$_2$ summarized by the chemical equation:

$$\mathrm{CO_2 + H_2O = H_2CO_3 = H^+ + HCO_3^- = 2H^+ + CO_3^{2-}} \quad \text{(A1)}$$

The changes in inorganic carbon speciation can impact the biogeochemical and biological responses. In particular, increasing CO$_2$ concentrations lower carbonate ion concentrations through the major net buffering reaction in the oceanic inorganic carbon system that can be summarized as:

$$\mathrm{CO_2 + CO_3^{2-} + H_2O = 2\ HCO_3^-} \quad \text{(A2)}$$

An example of the correlation between pCO$_2$ 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$_2$ 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 $\mathrm{CO_3}^{2-}$ in seawater.

Ocean acidification also impacts organisms that do not fix calcium carbonate. Increasing seawater CO$_2$ 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$_2$ 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$_2$ levels and associated acidification. SOCONET data will provide critical input on the trends of the major factors influencing OA and air-sea CO$_2$ fluxes, and resulting decreases in pH and carbonate levels.