

First steps to implement SOCONET-Tier 1 measurements and data delivery

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Foreword

This document describes the first operational steps to implement the reference-quality measurements of the Surface Ocean CO₂ Observing Network (SOCONET-Tier 1). The network aims to coordinate groups making high-quality surface water fugacity¹ of CO₂ (fCO_{2w}) and marine boundary dry mole fraction (xCO₂) observations. SOCONET-Tier 1 will be the observational cornerstone for surface ocean fCO_{2w} observations to quantify sea-air CO₂ fluxes with sustained delivery of reference quality datasets in support of efforts such as the WMO Global Greenhouse Gas Watch (G3W). The requirements for SOCONET-Tier 1 are to perform high-quality observations with an accuracy of $<2 \mu$ atm in fCO_{2w} and $<0.2 \text{ ppm} (\mu \text{mol mol}^{-1})$ in mole fraction in dry air, xCO_{2a}, and implementation of these measurements in a coordinated framework with benefits outlined in Table S1. This approach and these accuracies are necessary to constrain global annual sea-air CO₂ fluxes to 0.2 Pg C (10¹⁵ g C) or uncertainties of less than 10% of the current annual global sea-air CO₂ flux (Bender et al. 2002). Here we provide the practical considerations to establish uniform presentation, documentation, and (meta)data delivery. It incorporates ideas and common practices in place by established operators with the goal of providing a unified outward-facing presence of the entities providing high-quality measurements. Therefore, adoption of the steps by established groups is envisioned to be relatively straightforward. This document is focused on Tier 1 operations, but much of the practices will likely be adapted for non-Tier 1 measurements once experience is gained in incorporating the procedures by the established groups. This document is not an implementation plan for SOCONET, which would entail a holistic view of SOCONET and its role in a surface water CO₂ observing system, including detailed network design and gap analysis of spatial and temporal coverage of measurements.

Introduction

There is a need to operationalize surface ocean and air CO_2 measurements such that they can be used to create sea-air CO_2 flux maps in a timely fashion. These maps are a first-order contribution to CO_2 monitoring of the WMO Global Greenhouse Gas Watch (WMO G3W) flagship program, which aims to create an "*infrastructure [that] will produce gridded net monthly fluxes of CO_2 and*

¹ Here we use fCO₂, which accounts for the non-ideality of CO₂ gas rather than the partial pressure of CO₂ (pCO₂). Numerically, fCO₂=0.997 pCO₂ at 25 °C, and the air-water fCO₂ difference, Δ fCO₂, is essentially the same as Δ pCO₂.

*CH*⁴ at a spatial resolution of 1° latitude by 1° longitude with a maximum delay of 1 month", [with the resolution for N₂O to be defined]. This output, in turn, responds to the societal challenge of quantifying ocean CO₂ uptake to determine atmospheric CO₂ trajectories and to follow ocean acidification trends. SOCONET focusses on sea-air CO₂ exchange and methane (CH₄) is not a priority in the Tier-1 activities. Baseline measurements will also be required to determine changes in the ocean in response to climate change and possible interventions such as large-scale marine carbon dioxide removal (m-CDR). As described at the World Meteorological Congress of 2023, "*Greenhouse gas monitoring needs to commence within an integrated Earth system framework to be able to account for natural sources and sinks, both as they currently operate and as they will change as a result of a changing climate. This will provide vital information and support for the implementation of the Paris Agreement."*

To aid the development of products and services described above, the surface ocean CO₂ network (SOCONET) was conceptualized. SOCONET was originally envisioned as a reference network (Wanninkhof *et al.*, 2019) but is currently implemented with broader engagement and serves as a coordinating entity for all surface ocean CO₂ measurements. Here we focus on what is referred to as the Tier 1 component to distinguish it from the larger SOCONET efforts, and describe the best practices required to meet the goals of SOCONET-Tier 1. These best practices should propagate through the relevant oceanographic communities and stakeholders, and elevate the quality and traceability of all surface ocean and marine boundary layer GHG measurements. The development of SOCONET-Tier 1 protocols takes advantage of recommendations regarding instrumental analysis in several established efforts. In particular, procedures described in the SOCAT Quality Control (QC) cookbook and dataset QC flags therein, will be adopted (Gkritzalis *et al.*, 2025). The procedures in the SOCAT QC cookbook were informed by recommendations in other works such as Pierrot *et al.* (2009), Wanninkhof *et al.* (2013), and Steinhoff *et al.* (2019). Metadata standards developed in other related activities such as OCADS/NCEI, GOA-ON SDG 14.3 submissions, and OceanOPS will be consulted to assure compatibility (Supplement 2).

SOCONET-Tier 1 is an operational entity. "Operationalize" is a loaded term with different interpretations for different fields and applications, but it has a common denominator in that it implies streamlining and harmonizing approaches following common and well-defined practices. This is often accomplished through full automation of observations and turnkey operations. It includes automated metadata and data flows through machine-to-machine services to designated endpoints. For reference quality fCO_{2w} measurements, automation and turn-key operation are not feasible due to the complex nature of data collection and the appreciable personnel resources required to maintain instrumentation and engage in appropriate quality control/quality assurance protocols for the reference data. As a result, only limited consolidation of operations is practical. Therefore, a distributed network design is being pursued for SOCONET-Tier 1.

Here, we outline the initial steps necessary to operate the SOCONET-Tier 1 platforms and the requirements for data quality, posting, and tracking. The procedures are set up such that SOCONET-Tier 1 data and metadata can be seamlessly incorporated into SOCAT, meet the OceanOPS metadata standards, and the WMO G3W data requirements. Many of the steps and protocols are well-established in current efforts by the major contributors, and the focus of this document is on aiding in unifying and clarifying approaches.

Surface ocean CO₂ measurements are currently loosely coordinated with several international groups providing reference-quality data. A deficiency in the current reporting framework is that the status of measurements at the international level is not known until data is submitted annually on a voluntary basis to SOCAT. The decline in open ocean observations submitted to SOCAT since 2017, partially as a result of funding shortfalls, has been of great concern. Providing a "front-end" to SOCAT with an operational focus on the measurements has been an impetus to create SOCONET. The decline in observations highlights the need for sustained observational efforts and tracking of data using a network approach (Table S1).

Operational steps to implement SOCONET-Tier 1

Operational priorities of SOCONET-Tier 1 include tracking of platforms, measurements, and data quality. Tracking of platforms will be done through OceanOPS, which is the operational network metadata service of the Global Ocean Observing System (GOOS). Quality-controlled fCO_{2w} observations will be submitted to SOCAT with augmentations listed below. Coordination and adherence to performance criteria will be overseen by a steering committee (SC) as described in the SOCONET Steering Committee (SC) Terms of Reference (ToR) (Supplement 4).

Several operational steps need to be implemented for a platform to become part of the SOCONET-Tier 1 network. These are provided below, along with an estimate of the priority for implementation and high-level requirements. All these requirements have financial and labor costs associated with them, which are largely above and beyond the current efforts of the SOCONET-Tier 1 contributors.

	Step ¹	Priority ²	Requirement ³
1	Identify current platforms and instruments meeting SOCONET-Tier 1 requirements	Ι	Personnel time and commitment
2	Confirm that instrumentation is capable of measuring fCO_{2w} to <2 µatm and xCO_{2a} measurements to <0.2 µmol mol ⁻¹ (ppm) ⁴	Ι	Resources to validate
3	Platforms are labeled, and approved by the SOCONET steering committee (SC) and metadata is submitted to OceanOPS	Ι	Establishing a SOCONET SC; resources for IOCCP
4	Determination of location and status of platforms through near-real time (NRT) tracking	М	Expertise to implement: resources to OceanOPS
5	Perform uniform rigorous QC steps per updated documentation and recommendation	М	Development of QC protocols, implementation costs
6	Implement steps to post near real-time NRT xCO_{2w} and xCO_{2a} data	L	Software development and telecommunication
7	Provide quality controlled xCO_{2a} and $\Delta fCO_{2(w-a)}$	L	Personnel time and QC protocols

Table 1. Operational steps to implement SOCONET-Tier 1

8	Provide estimated uncertainty for each observation	L	Procedures and
			personnel time
9	Overall network representativeness	L	Observing system
			analyses and
			expansion

- 1. Each step is described in more detail below.
- 2. I: (Immediate) needs to be implemented before a platform can be part of SOCONET-Tier 1; M: (Medium-term) will facilitate identity and exposure of SOCONET-Tier 1; L: (Long-term) will lead to long-term improvement of the SOCONET-Tier 1 deliverables.
- 3. These are shorthand for the key resources needed for each step.
- 4. The uncertainty requirement of xCO_{2a} measurements is tentative and will require more study

Each of the 8 steps in Table 1 is described below, including recommendations for implementation, and issues that need to be resolved. The first three steps pertain to instrumentation and infrastructure as documented in appropriate metadata; the second three steps involve posting; and the last steps pertain to quality of the observational data.

1. Identify current platforms and instruments that meet SOCONET-Tier 1 requirements

Several different platform types and instrumentation will be used in SOCONET-Tier 1. However, all analyses are based on equilibration of CO_2 in surface water with a headspace and measurement of the headspace with a well-calibrated analyzer and accurate temperature and pressure measurements in the headspace and water of the equilibrator. Sea surface temperature taken to be the temperature of water at the inlet of the ship's piping at the hull needs to be measured at the high accuracy as well.

While specific instrumentation and infrastructure are not mandated for SOCONET-Tier 1, having a set of recommended instruments and operating principles is advantageous for operational purposes to achieve measurements of known high quality. There are a limited number of commercially available instruments that meet SOCONET-Tier 1 uncertainty specifications (second row Table 1 and detailed below). The instruments listed below have been shown to meet the accuracy requirements for SOCONET-Tier 1, including side-by-side checks in intercomparison efforts. Observations obtained from other instruments need to demonstrate that they meet the standards for SOCONET-Tier 1 before inclusion, such as regular participation in instrument intercomparisons and documented assessment of total measurement uncertainty including lab and field validation. In addition to having instrumentation that meets SOCONET-Tier 1 criteria, the instruments also need to be operated and maintained to provide the high-quality data. Other criteria include data reduction and QC that need to be performed according to SOCONET-Tier 1 protocols.

Current instruments for underway CO₂ systems that meet the <2 µatm accuracy requirement are equilibrator-based systems with the non-dispersive infrared analyzer (ND-IR) (Pierrot *et al.* 2009). The requirements to meet the SOCONET-Tier 1 criteria should be updated, particularly in light of new analyzers such as the laser-based analyzers (for example, the LICOR 7815 and Picarro G2301

analyzers) that are superior to the ND-IRs conventionally used. The laser-based instruments are highly linear and stable and likely require less frequent calibration. Modifications to standard operating procedures and requirements should be done after careful and documented tests.

The commercial instrument for ship-based CO₂ measurements that meets the SOCONET-Tier 1 requirements is the community-designed instrument for underway CO₂ measurements assembled to specification by General Oceanics Ltd. It is described in Pierrot *et al.* (2009), and it is the default system for ship-based applications. The MAP-CO₂ system (Sutton *et al.*, 2014) is a well-tested buoy-based system that can be obtained from Sensors Systems Solutions, USA. The Hagan-GenX (Hagan Technologies, South Africa), formerly called VeGAS, and the ASVCO₂TM (NOAA PMEL and Saildrone Inc, USA) instruments (Sabine *et al.*, 2020) are equilibrator-based systems with non-dispersive infrared analyzer for uncrewed surface vehicles (USVs). While the procedures for operating the ASVCO₂TM instruments are trademarked, they are currently not commercially available. The measurements from all these systems are referenced to compressed air standards tied to the WMO scale which are defined as a dry mole fraction of CO₂ with a balance of natural air. The dry mole fraction of CO₂ from the headspace of the equilibrator, xCO_{2w} (at temperature and pressure of equilibration), is the base for all instrumental output that, with appropriate temperature, moisture, and pressure corrections, can be converted to the quantity of interest, the fugacity in air, fCO_{2a}, and water fCO_{2w}.

There are several instruments and platforms currently in operation that, in principle, meet the SOCONET-Tier 1 requirements. This identification step of potential SOCONET-Tier 1 platforms involves reaching out to the community and making a tally of these platforms. An initial list of possible SOCONET-Tier 1 contributors was created in 2019, and a questionnaire released by the International Ocean Carbon Coordination Project (IOCCP) in early 2024 has provided information on the platforms. Perusing the SOCAT database for data that meet dataset A or B criteria will be another means to seek out potential participants. An active SOCONET secretariat at the IOCCP will be very helpful in this recruitment stage.

2. Requirement setting for accuracy

A defining attribute of SOCONET-Tier 1 measurements is the quality of data with an accuracy of $< 2 \mu atm$ in fCO_{2w} and $< 0.2 \text{ ppm xCO}_{2a}$, where xCO_{2a} is the mole fraction of CO₂ in dry air). These accuracies are necessary to constrain global sea-air CO₂ fluxes to 0.2 Pg C, or $\approx <10 \%$ of the current sea-air CO₂ flux (Bender *et al.* 2002). Rigorous QC protocols need to be exercised for all observations to meet these standards. These accuracies will be achieved and maintained through the following steps:

- All components of the instruments, including materials, analyzers, pressure and temperature sensors, and standardization, need to meet documented specifications showing that these targets can be achieved.
- Pre-deployment checks need to be performed and documented to show individual instruments meet the targets.
- Installation of systems following recommendations. For SOOP-CO₂ installations these are provided in Pierrot and Steinhoff (2019).

- Participation in pCO₂ instrument intercomparison exercises organized by the SOCONET community.
- Perform vicarious checks during deployments and on campaigns where redundant measurements are made.
- Establish protocols and checks to assure that instruments are operating to specification during deployment.
- Implement rigorous QC protocols, as described in relevant SOPs, for all measurements, including ancillary measurements such as temperature and pressure.

In the Wanninkhof et al. (2019) an accuracy of shipborne MBL CO_2 measurements of 0.2 µatm was suggested as a target which meets the extended network compatibility goal of WMO /GAW (Table 1, Crotwell and Steinbacher, 2018). To meet the network compatibility goal of < 0.1 ppm in the Northern hemisphere and <0.05ppm in the Southern Hemisphere dedicated air measurement instruments will likely be required.

3. Labeling and approval of platforms

The procedures, installation, performance, and infrastructure of the surface water CO₂ observations for each platform should be detailed. This process, referred to as labeling in the European Integrated Carbon Observation System (ICOS), provides an indication that observations meet the stated requirements, assures commonality of approaches, and assures that stated accuracy can be reached with the setups. It dovetails with the platform metadata requirements of GOOS OceanOPS. A process similar to that used by the ICOS-Ocean Thematic Center (OTC) should be followed (Supplement 3). This includes a review of the labeling/metadata documents by the technical coordinators and approval by the SOCONET SC. Metadata templates need to be created to facilitate labeling and ensure all elements of the procedures, installation, performance, and infrastructure are included.

The content and narrative contained in the ICOS labeling documents (Supplement 3) are important for describing the setups and operating parameters, but a more streamlined approach with a markup language and file format for encoding documents in a format that is both human-readable and machine-readable will be implemented. Metadata templates and tools such as those used in the NCEI Ocean Carbon and Acidification Data System (OCADS) [https://www.ncei.noaa.gov/products/ocean-carbon-acidification-data-system] and SOCAT can serve as examples.

While we can draw on the ICOS-OTC labeling procedures for ships, there are no ICOS labeling examples available for mooring-based systems. Most of the mooring-based systems in the field are MAPCO₂ systems (Sutton *et al.*, 2014), but other systems such as GENx-CO2 (Hagan techn. Ltd) are commercially available. As many installations are very similar and already operate under a common framework, uniform labeling should be straightforward. ASVCO₂ sensors (Sabine *et al.*, 2020) are similar to the MAP CO₂ systems, with trademarked operating procedures facilitating the labeling process [https://github.com/NOAA-PMEL/ASVCO2/blob/main/ASVCO2%20Trademark_v1.pdf]. A separate template should be developed for autonomous platforms that includes the common criteria for all SOCONET-Tier 1

measurements. Compatibility with established metadata protocols such as with the SOCAT metadata editor and ICOS-OTC metadata requirements as much as feasible will be maintained.

The Global Ocean Observing System (GOOS) operational center, OceanOPS, will serve the platform metadata for SOCONET. The details of the incorporation of SOCONET platforms into the GOOS OceanOPS framework as part of becoming a Global Ocean Observing System emerging network are under discussion and deliberation in the SOCONET SC and OceanOPS. SOCONET is based around the concept of essential ocean variables (EOV) rather than the platform-based approach of current GOOS networks. It is envisioned that SOCONET ship-based systems, including those on research ships, cruise ships, cargo ships, and icebreakers, will also be part of the GOOS SOOP (Ship of Opportunity Network) of the Ship Observations Team (SOT). Coordination and liaising will occur through the SOOP Implementation Panel (SOOP-IP) and OceanOPS. Buoy- and USV-based systems will be closely aligned with the GOOS USV and OceanSITES networks and some may be implemented, in part, on buoys under the Data Buoy Cooperation Panel (DBCP). However, not all moorings with MAPCO2 or similar sensors are part of OceanSITES. In particular, those in coastal sites and near the shelf edge are currently not registered in OceanSITES. The SOCONET SC, in consultation with operators, IOCCP, and OceanOPS, will need to determine the ideal coordination of SOCONET mooring-based CO2 systems.

4. Determination of the locations and status of platforms through near real-time tracking

A basic requirement for operational networks, including SOCONET-Tier 1, is that assets and data delivery are tracked. All SOCONET-Tier 1 platforms will be tracked in near real-time (NRT), that is within a day, through GOOS OceanOPS.

Several tracking options are available, and it is likely that different approaches will be used depending on the platform. Options include:

- Tracking by using the WMO VOS and OceanSITES platform codes
- Tracking through NRT transmission of data from the platforms
- Tracking through the Automatic Identification System (AIS) system

Tracking of SOCONET platforms by using data flows, standards, and identifiers of other, already implemented, observing systems that use the same vehicle, such as VOS in the WIS structure, will be investigated. Through the integrated GOOS implementation support via OceanOPS, the aim is to have all vessels that host a SOCONET platform also become a VOS, if not the case already. However, not all fixed stations and VOS platforms have the necessary transmission capacity such that the other options listed above will likely be implemented. Using AIS will require a license and certain restrictions on posting locations on public sites that will need to be investigated. A first-step tracking protocol will include information if the platform has a CO₂ system on board and if the system is operating.

As noted, the options depend on the facilities on the platform, but the GOOS OceanOPS vision is to be the single tracking source that covers all sensors on the platform and serving as the integrated network service following GOOS-OSG network criteria (Table S2). In addition to tracking

platforms, we will work with OceanOPS to investigate the options of coordinated transfer of observational data.

5. Rigorous QC steps using documented automated approaches

A significant number of data reduction steps are required to obtain the fCO_{2w} from the surface water CO_2 measurements. The basic measured parameter is xCO_2 referenced to known CO_2 mol fractions in compressed gas standards. The is converted, through well-established formulations involving ambient pressure and water temperature, to fCO_{2w} which is the reported parameter.

Appreciable advances have been made to streamline and automate data QC with software provided with GO systems (available on request from D. Pierrot, NOAA/AOML) and the QuinCe software (Jones et al., https://github.com/quince-science/QuinCe). The routines to date have not been fully documented, and they lack straightforward instructions of use, which would facilitate greater adoption. The software products have several visualization options and the ability to output property-property plots and on-screen tagging that aid in contextual QC, which is a necessary step to determine outliers and offsets that should be flagged prior to submission to SOCAT. Uniform data reduction and QC software will ensure that all data undergo similar and rigorous quality checks and assure uniform high-quality of all data submissions under the SOCONET-Tier 1 umbrella.

An ongoing effort is to enhance contextual QC through providing a graphical interface to superimpose observations over agreed-upon climatological fields such as sea surface height, temperature, salinity, oxygen, and chlorophyll-*a* (Chl-*a*). Climatological fCO₂ fields with subsetting capabilities at platforms and along cruise tracks are envisioned as enhancements to facilitate the QC of SOCONET-Tier 1 data. A NRT-mapped field of fCO_{2w} using machine learning approaches will be introduced. These capabilities, once shown robust, will be shared with the SOCONET community at large to facilitate improved data quality within the overall SOCONET framework.

6. Implement steps to deliver NRT xCO_{2w} and xCO_{2a} data

Near real-time (NRT) data transmission (that is, transmission of data within 24 hours) is desirable for status checks of instruments, validation of low-latency products such as monthly G3W surface flux maps, and a first look at data. The latter can be particularly useful from a communication standpoint, such as discerning changing CO₂ levels during extreme events. Currently, several groups obtain NRT data from platforms. We envision collating this data at a central hub, which will be combined with ancillary data for visualization and semi-automated QC. The hub will serve preliminary xCO₂ data corrected to SST. Automated QC/range checking to screen preliminary data will be implemented as the next step once the NRT data system is fully operational.

7. Provide quality-controlled xCO_{2a} and ΔfCO_2

For estimating sea-air CO₂ fluxes, the sea-air fugacity difference, ΔfCO_2 , needs to be determined, which requires accurate xCO_{2a} data. Most reference-quality surface water CO₂ instruments perform routine measurements of air. For those platforms that make air measurements, procedures

will be established to quality control xCO_{2a} taken as part of the fCO_{2w} measurements with the aim to obtain accuracies <0.2 ppm. A value-added component will be the provision of NRT regional estimates of marine boundary layer xCO_{2a} that can be provided for contextual QC. Independent, high-quality measurements from dedicated instruments that meet Global Atmosphere Watch (GAW) standards will be obtained on select ships, and a movable ship-based instrument for air measurements will be used to spot check different instruments. Currently, buoy and USV-based instruments do not meet the xCO_{2a} goals of <0.2 ppm due to instrumental limitations (Sutton et al. 2014). Potential advancements in instrumentation to improve accuracy for these platforms should be investigated.

The ΔfCO_2 information from the same instrument will improve local sea-air CO₂ flux estimates as these observations account for deviations of xCO_{2a} from marine boundary layer (MBL) background values, particularly near the coast influenced by continental air masses. Moreover, as xCO_{2w} and xCO_{2a} are measured with the same instrument and same standards, any wholesale instrument biases caused by, for instance, assigning incorrect concentrations in standard gases could be better tracked.

8. Provide estimated uncertainty for each observation

An important enhancement of submitted SOCONET-Tier 1 data is that every value will include an estimate of uncertainty. These estimates are critical for determining overall uncertainty in mapped products and have been requested by modeling and assessment communities (Andrews et al., 2014). Guidelines will be developed for the uncertainty estimates and interpretation thereof. As a default, the stated uncertainty for SOCONET-Tier 1 of $<2 \mu atm$ in fCO_{2w} and 0.2 ppm in atmospheric xCO₂ data are used where the uncertainty could be random and/or systematic. Systematic errors will cause bias in the results and are thus particularly detrimental for interpretation. For example, a global bias of 1 µatm in Δ fCO₂ causes a 0.2 Pg C bias in global net flux. Improvements in data quality will thus be focused on decreasing systematic errors.

SOCAT will be the primary depository of SOCONET-Tier 1 data. Adjustments to reporting requirements and SOCAT database format will be discussed with the SOCAT global group. They will be made as necessary to accommodate the added information provided with SOCONET-Tier 1 data. SOCONET-Tier 1 data will be tagged as such in the SOCAT holdings.

9. Network representativeness

Observing system analyses should be an ongoing component of SOCONET to assess uncertainties resulting from incomplete coverage of the global surface ocean. These analyses will be very useful to determine the impact of improving coverage in undersampled regions. They will also serve to justify needed resources for network maintenance and enhancement through a cost-benefit approach. This aspect will be expanded upon in the SOCONET implementation plan.

Concluding remarks: coordination and sustainability

SOCONET-Tier 1 participants will initially be a group of established operators who have agreed to follow the protocols and procedures established to produce Tier 1 quality data and metadata

with timely dissemination. This is a priority within the SOCONET work plan, focusing on the sustainability of high-quality measurements and data management in an operational framework. It will be facilitated by working as a coordinated entity with mutual interests in sustainability of the measurements and capacity building in an operational framework. The SOCONET-Tier 1 groups will interact closely with other SOCONET, SOCAT, GOOS OceanOPS, and WMO G3W partners to develop strategies to build a sustainable observation network and to entrain more observational platforms within the SOCONET-Tier 1 framework.

The steps outlined above will require significant additional resources for many operators to implement. Once implemented, modest augmentation over and above the current efforts is envisioned. Aside from the need for augmentation of resources to implement SOCONET-Tier 1, a fundamental issue that SOCONET aims to address is to place surface water CO₂ observations on sustainable footing. Many of the current operators of surface ocean CO₂ assets operate with short-duration research funds, and more operational resources need to be sought. We expect that SOCONET will operate using traditional sources of funding as well as seek new means to secure resources to sustain the efforts. For alternative means to secure resources to support SOCONET as a global effort, we plan to work with intergovernmental organizations and their resource forums to determine a more equitable distribution of resources.

This current document provides the first practical implementation steps with the recognition that several other critical activities need to take place to implement SOCONET, including network design, establishing formal cooperation agreements; industry, academic, and (multi)-government partnerships; and technology development. That is, these requirements outlined here and SOCONET-Tier 1, in general, are a subset of much broader requirements setting that will be overseen by SOCONET under the coordination of IOCCP.

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Table 2. Acronyms and relevant websites

Organizations:

DBCP	Data Buoy Cooperation Panel; https://www.ocean-ops.org/dbcp/
G3W	Global Greenhouse gas Watch; https://wmo.int/activities/global-
	greenhouse-gas-watch-g3w
GAW	Global Atmosphere Watch (https://community.wmo.int/en/activity-
	areas/gaw)
GOA-ON SDG 14.3	Global Ocean Acidification Observing Network Sustainable Development
	Goal 14.3; https://sdgs.un.org/partnerships
GOOS	Global Ocean Observing System; https://goosocean.org/who-we-are/
ICOS	Integrated Carbon Observing System; https://www.icos-cp.eu/
ICOS OTC	ICOS-Ocean Thematic Center; https://www.icos-
	cp.eu/observations/ocean/otc
IOCCP	International Ocean Carbon Coordination Project; https://www.ioccp.org/
OCADS/NCEI	Ocean Carbon and Acidification Data System/National Centers for
	Enivronmental Information; https://www.ncei.noaa.gov/products/ocean-
	carbon-acidification-data-system
OceanOPS	Ocean operations center; https://www.ocean-ops.org/
OceanOPS	
metadata standard	https://www.ocean-ops.org/metadata/
OceanSITES	Observations at fixed locations; http://www.oceansites.org/
SOCAT	Surface Ocean CO ₂ Atlas; https://www.socat.info/)
SOCONET	Surface Ocean CO ₂ network; https://www.aoml.noaa.gov/ocd/ gcc/
	SOCONET/
SOCONET-Tier 1	Reference quality CO2 measurements under the aegis of SOCONET
SOOP	Ship of Opportunity Program; https://www.ocean-ops.org/sot/soop/
SOOP-CO2	Surface water CO2 measurements on SOOP
SOOP-IP	SOOP Implementation Panel
SOT-SOOP	ship of opportunity network of the Ship Observations Team, (SOT)
TOR	Terms of Reference
WIS	WMO Information System; https://community.wmo.int/en/activity-
	areas/wis
WMO	World Meteorological Organization; https://wmo.int/
Scientific:	
AIS	Automatic Identification System; https://www.navcen.uscg.gov/automatic
mo	-identification-system-overview
USV	uncrewed surface vehicles
EOV	essential ocean variables ; https://goosocean.org/what-we-
LOV	do/framework/essential-ocean-variables/
fCO _{2w}	surface water fugacity of CO ₂
MAPCO ₂	Moored Autonomous pCO2 system
	https://www.pmel.noaa.gov/co2/story/Buoys and Autonomous Systems
MBL	marine atmospheric boundary layer
MDL	marme aunospherie boundary layer

ND-IR	non-dispersive infrared analyzer
NRT	near real-time
pCO ₂	partial pressure of CO ₂
QC	quality control
WMO-scale	Refence gas scale; https://gml.noaa.gov/ccl/scales.html
xCO ₂	mole fraction of CO ₂ in dry air

Supplementary Materials

Supplement 1. SOCONET Network Criteria

Table S1. Benefits of the SOCONET Network

The following is paraphrased from the SOCONET Terms of Reference (see, Supplement 4), OceanOPS, and GOOS Observation Coordination Group materials.

The establishment of an organized, international surface ocean CO₂ network will provide the following anticipated outcomes:

- Increase the visibility and identity of participants and their efforts, and reinforce the importance of sustained observations.
- Work towards a common set of standards and best practices.
- Provide training, education, and capacity-building efforts, encourage developing countries to start measuring fCO₂.
- Build a coherent vision of the need for sustained surface ocean CO₂ measurements as part of a global integrated carbon observing system.
- Common data management, QC, and data products (streamline the output of data releases, etc.).
- Connectivity to other networks (e.g., help in recruitment of ships and other platforms where our systems can be installed).
- Target data gaps and determine where and how gaps can be best filled.
- Improve network usability, such as atmospheric CO₂ measurements from ships.

Table S2. Attributes of a GOOS-OCG Network.

Network criteria as developed through the GOOS Observation Coordination Group (From Wanninkhof et al. 2019).

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. Follows FAIR principles.
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.

Supplement 2. Details of SOCONET-Tier 1 metadata

Documentation of procedures, instruments, and data handling assures that SOCONET-Tier 1 operations meet the specified criteria. These steps are commonly referred to as metadata and labeling. Labeling is a term used in ICOS that describes the rigorous procedures to become an ICOS station, including the commitment of funding. The steps in the ICOS station labeling process are described, in short, in Supplement 3.

The metadata for SOCONET-Tier 1 will be in template form including fields for freeform entry. The template format will facilitate machine-to-machine interactions and harvesting of information on the network. Three types of metadata will be of relevance for SOCONET-Tier 1 platforms.

Platform metadata

The term platform has different connotations. Here we use it as the vehicle upon which the CO_2 system is placed. Currently, these include ships of opportunity (SOOP), uncrewed surface vehicles (USVs), and moorings. Within OceanOPS, the term platform refers to the specific system taking the measurements. The system in turn can have several instruments or sensors. For instance, an underway pCO₂ system is comprised of an air-water equilibrator, a CO₂ analyzer, temperature and pressure sensors, and a computer for automated instrument operation, data storage, and transmission.

The platform metadata for SOCONET provides a description of the installation, including all auxiliary sensors and manufacturers claims of stability, accuracy, and precision. Any pre-cruise tests by the manufacturer or operator will be included. The metadata will include the needed information for the platform to be part of the OceanOPS network. This metadata is focused on measurements meeting specified quality.

Observational metadata

This metadata pertains to the measurement campaigns of surface water fCO_2 observations. This includes documentation on measurement quality, issues in obtaining the data, data reduction procedures, and quality control steps executed. This metadata is directly linked to the data that is submitted to SOCAT and would be directly connected to the observations. It would be part of the data submission package to SOCAT and include a reference/link to the platform metadata.

Metadata documenting the dataset.

Data will be submitted to SOCAT in common format, including metadata describing the data reduction and particular attributes of the datasets. All data entries will be described with descriptions of column headers and units. The dates of submission and revisions will be included to facilitate version control.

The metadata templates will be in compliance with the metadata requirements of the entity receiving the information. For example, the platform metadata will meet the requirements set forth in OceanOPS. The observational and dataset metadata will be created in coordination with SOCAT and would largely follow the current metadata format of SOCAT (see, https://socat.info/index.php/data-upload-and-quality-control/). Efforts will be made to streamline and simplify metadata requirements for SOCONET.

Supplement 3. ICOS labelling

Adapted from: https://www.icos-otc.org/labelling

ICOS Station Labelling

ICOS aims to have a high-quality standardized station network across Europe, and therefore all the stations entering into the ICOS network must go through a station labeling process. This process includes a testing period and training to become familiar with the ICOS methodology.

The three-step labeling process takes several months and is as follows for ocean stations:

Step 1 - Formal application

Before an application can be submitted to ICOS, it must be approved by the national government funding the station. Once approval has been received, it will be submitted to the ICOS European Research Infrastructure Consortium (ICOS ERIC) and added to the list of proposed stations. The Principal Investigator (PI), or the station owner, of each station must provide all required application documents to the Ocean Thematic Centre (OTC).

The OTC will evaluate the station applications and propose acceptance to the Director General (DG). The DG will consult with the ICOS Research Infrastructure Committee (RI Committee) and inform the applicant of the decision.

Step 2 - Evaluation period

The stations accepted under Step 1 must pass through an evaluation period that shall facilitate their compliance with the defined protocols for measurements. The aim of this period is to familiarize the station staff and PI with the ICOS standard methodologies, with the quality of the systems, and of the rights and responsibilities of networks and OTC as part of the ICOS RI and commit the station staff and PI to them.

The station will submit metadata and measured data to the OTC for evaluation. The OTC will ensure that it meets the requirements of either a Class 1 or Class 2 marine station. Required parameters, frequency of measurements, and criteria to become a Class 1 or Class 2 marine station are defined in https://www.icos-otc.org/measurements. Read more about labeling step 2 in the Station Labeling Step 2 document.

Once the evaluation is complete, the OTC will forward a final recommendation to the DG regarding acceptance of the station and confirm its Class 1 or Class 2 status. The DG will consult with the RI Committee and submit the decision to the General Assembly (GA).

Step 3 - Formal decision by the General Assembly (GA)

The GA will formally decide whether to include the station in the Monitoring Station Assemblies (MSA) based on recommendations from the OTC and statements from the RI Committee. If accepted, the site will become an official ICOS site. In case a station is not accepted, the GA will return the station to the OTC for continued evaluation.

Ongoing evaluation

All ICOS marine stations will be re-evaluated on a regular basis, and the OTC will work with the PIs to attain and maintain the best possible data quality.

Definitions relevant to ICOS

ICOS Research Infrastructure (ICOS RI): A distributed research infrastructure which will provide data that enables analyses of emissions and sinks of greenhouse gases, ecosystem function, and related research.

ICOS European Research Infrastructure Consortium (ICOS ERIC): The legal entity of ICOS RI established to coordinate the operations and the data of ICOS distributed research infrastructure and to develop, monitor and integrate the activities and the data of ICOS RI.

Director General (DG): Responsible for the management of the ICOS ERIC and for the implementation of the decisions by the General Assembly.

ICOS RI Committee: Is consulted by the Director General for all general matters. Consists of representatives from the Head Office, Carbon Portal, the Central Facilities, and each Monitoring Station Assembly.

General Assembly (GA): The highest decision making body of ICOS ERIC, and is responsible for the overall direction and supervision of ICOS ERIC.

Monitoring Station Assemblies (MSA): Monitor, develop, and improve the scientific and technical basis of the ICOS RI and work closely with ICOS Central Facilities.

Supplement 4. SOCONET Terms of Reference



SOCONET Steering Committee - Terms of Reference

OCG Emerging Network March 2025

Purpose

In 2024, the Surface Ocean CO2 Observing Network (SOCONET) was formally recognized as an emerging network by the Global Ocean Observing System Observations Coordination Group (GOOS-OCG). SOCONET aims to develop a coordinated network of national, regional, and private sector operators to constrain the air-sea flux of CO2 and deliver surface ocean CO2 products. Annual reporting of progress to the OCG committee is expected until relevant network attributes will be fully developed.

The SOCONET Steering Committee (SC) provides scientific leadership and oversight for the development and implementation of the network. The SC is committed to working towards the OCG data, metadata and best practices requirements through following activities:

- The SOCONET SC will develop and provide oversight for execution of the SOCONET Implementation Plan including a clear strategy to secure the network coordination function.
- The SOCONET SC shall oversee the coordination of surface ocean CO₂ observations with the primary objective of delivering sustained, high-quality, and accessible observations for constraining CO₂ fluxes between the ocean and the atmosphere.
- The SOCONET SC will establish surface ocean CO₂ measurement requirements, including reference-level measurements. Different data qualities will be assigned different Tier levels. This will include developing and disseminating standard operating procedures and best practices and updating those as needed.
- The SOCONET SC will encourage, facilitate, and coordinate the recruitment of greater and global representation in SOCONET, including determination of minimum requirements for SOCONET participants and coordination of training and capacity building activities as needed.
- The SOCONET SC will facilitate collection and timely submission of data from SOCONET platforms to the Surface Ocean CO₂ Atlas (SOCAT) data repository and platform metadata through the Joint WMO-IOC in- situ Observations Program Support (OceanOPS). The SOCONET SC in

coordination with SOCAT and GOOS-OCG shall provide advice on the contents, quality, and timeliness of the SOCONET data streams to ensure that guidelines regarding measurements and data submission are met.

- The SOCONET SC will coordinate with other relevant global observing networks, including those for atmospheric greenhouse gases, other ocean greenhouse gases (N₂O and CH₄) and satellite-based measurements.
- The SOCONET SC will interact with OceanOPS through GOOS-OCG, International Ocean Coordination Project (IOCCP / GOOS Biogeochemistry Panel) and relevant panels and working groups (e.g. WMO Greenhouse Gas Watch G3W) and solicit funding from national agencies and multi-national entities for OceanOPS services.
- The SOCONET SC will facilitate interactions between nations and stakeholders to ensure surface ocean CO₂ observations that meet SOCONET quality requirements are made on research vessels, ships of opportunity, surface buoys and other emerging surface ocean observing platforms.
- The SOCONET SC will advocate for routine surface ocean CO₂ instrument intercomparison exercises, including for emerging technologies.
- To address specific tasks, SOCONET SC will convene specialized Task Teams (TT). These TTs can include relevant experts that are not part of the SOCONET SC. The TTs will report back to the SOCONET SC and be disbanded following their fixed-term.

Membership

The SOCONET SC shall be made up of scientists and technical experts from groups contributing to SOCONET and involved in the production of its data products as needed. SC members will be recruited with effort to represent as wide as possible geographic distribution, career stage and to maintain gender balance. SC members should represent expertise in fields of ocean observing, chemical oceanography, sensors and instruments, modeling, or data management. The SOCONET SC will be composed of 2 co-Chairs plus up to 18 additional SC members.

The SOCONET SC shall be led by two co-Chairs selected from within SOCONET SC. The co-Chairs should represent the diversity of the SC. Co-Chairs will be nominated by SC members or self-nominated, and appointed following the approval of more than half of the total number of SC members.

The SOCONET SC shall form a SOCONET Executive (Exec) consisting of:

- Two SOCONET SC co-Chairs
- The SOCONET Coordinator (IOCCP)
- The SOCONET Technical Coordinator (OceanOPS)

The SOCONET Executive will take care of the day-to-day operations of SOCONET such as preparing, moderating and reporting from SOCONET SC meetings and conference calls; providing recommendations and endorsements for national programs and coordination with other programs, actively engaging in bi-directional communication with GOOS-OCG and its parent organizations (IOC-UNESCO, WMO, UNEP, ISC) on matters related to SOCONET.

Appointments

In order to assure the required expertise in the SOCONET SC, a call for new members is prepared by the SOCONET Executive, approved by more than half of the total number of SC members and distributed to the community via relevant communication channels. The call is usually issued when (i) a current SC member is within 3 months of finishing their term or needs to rotate off the SC before their term finishes, or (ii) when a need for additional expertise on the SC arises. Following the application deadline (usually 4-6 weeks), the Executive Committee assesses all applicants based on the criteria listed in the call, additional information included in the application documents, and additional knowledge of applicants' involvement in relevant activities. The Exec presents the SOCONET SC with individual nominations, including justification for each proposed new SC members. A nominated applicant becomes an SC member following the approval of more than half of the total number of active SC members.

SC members are appointed for one 4-year term with the possibility to extend service for a maximum of 2 terms, pending mutual agreement after the first term. For an SC member who subsequently becomes a co-Chair, the maximum period of service may be extended up to 12 years, with a maximum period of 8 years as co-Chair. Appointments usually begin at the start of the calendar year.

The initial SOCONET SC (2025 onwards) will be composed of all the members of the SOCONET interim Steering Committee (iSC) who will agree to transition, plus additional members appointed in 2025 following the procedure above. The iSC chose not to select their co-Chairs and the Technical Coordinator is not yet appointed. The nomination and selection process will be coordinated by the SOCONET Coordinator and executed by the full iSC.

Members of iSC in 2025 are:

Adrienne Sutton, NOAA, USA Bronte Tilbrook, CSIRO, Australia Dorothee Bakker, UEA, UK Kathy Tedesco, UCAR/NOAA, USA Kevin O'Brien, CICOES/NOAA, USA Maciej Telszewski, IOCCP, Poland Martin Kramp, OceanOPS, France Mathieu Belbeoch, OceanOPS, France Richard Sanders, NORCE, Norway Rik Wanninkhof, NOAA, USA Shin-ichiro Nakaoka, NIES, Japan Steve Jones, VLIZ, Belgium Thanos Gkritzalis, VLIZ, Belgium Tobias Steinhoff, GEOMAR, Germany

Ex-officio Expert Advisors

SOCONET SC co-Chairs, following consultation with the SC members, may invite ex-officio Expert Advisors from government agencies, relevant intergovernmental and international bodies as well as national scientific programs to support the work of the SOCONET SC with their specific expertise. They will be expected to attend the SOCONET SC meetings when appointed. Ex-officio Expert Advisors are appointed for a 4-year term with the possibility to extend service for consecutive terms, pending mutual agreement after each term. Ex-officio Expert Advisors do not count as SC members, and are not formally included in any decision-taking process.

Specific roles and responsibilities of SOCONET SC members

SOCONET SC members shall be actively engaged in activities described in the "Purpose" section of this document, including outreach activities and tracking progress of SOCONET implementation and data submission by SOCONET members. SOCONET SC members are considered hubs for national and/or regional networks. They are expected to help track observations made under the auspices of their nation/region, and help facilitate timely submission of data to the SOCONET data centers. They will specifically:

- Meet at least 4 times a year via teleconference, and at least every 2 years in person. Formal and informal meetings of the SOCONET SC, in conjunction with international meetings are encouraged;
- Report at SOCONET meetings and in writing to the SOCONET Executive and SC: the views, challenges and successes of their national/regional network;
- Ensure that decisions of the SOCONET Executive and SC are relayed to the relevant national/regional networks and that appropriate actions are recommended;
- Take necessary steps to ensure that their national/regional network contributes appropriately to the SOCONET program;
- Advise the SOCONET Technical Coordinator, and SOCONET SC in a timely manner of proposed occupations of SOCONET platforms;
- Encourage scientific use of SOCONET data and publicize achievements;
- Provide guidance in execution of measurements' requirements, standard operating procedures and best practices of these measurements on all platforms.

Specific roles and responsibilities of SOCONET Coordinator(s)

SOCONET Steering Committee Coordination (IOCCP)

- Coordinate the establishment of the SOCONET Steering Committee and keep their ToR up to date.
- Coordinate the SC efforts towards identification of key science and policy stakeholders for a SOCONET to allow for efficient co-design of an ocean carbon observing system.
- Coordinate/Participate in monthly conference calls with the SOCONET SC focusing on progress of work regarding the Implementation Plan.
- Organize and co-moderate in-person SOCONET Steering Committee Meetings.

Development of SOCONET Implementation Plan (IOCCP)

• Coordinate and provide oversight for the drafting, preparation, and updating (as needed) of the SOCONET implementation plan, which should include an observing network

design.

• Coordinate the development, operation and governance of the SOCONET Task Teams as needed.

Daily Coordination Activities (IOCCP)

- Provide inter-sessional oversight for SOCONET activities.
- Oversee development of project planning documentation and schedules.
- Develop and/or review SOCONET presentations as necessary (e.g., for annual IOC-UNESCO General Assembly, annual GOOS SC Meeting, etc.).
- Maintain SOCONET website.

Network level Technical Coordination (OceanOPS)

Technical coordination at the network level will be provided by OceanOPS which will fulfill the responsibilities outlined in the Service Level Agreement between SOCONET and OceanOPS including: network monitoring, reporting, metadata management, data monitoring and work with SOCONET data providers to ensure data is submitted to SOCAT and to defined global data nodes in a timely manner, maintain visibility of SOCONET-related statistics and performance indicators through the OceanOPS website, bibliography and other fora, liaise with other OceanOPS and GOOS-OCG activities, including cross-linking of metadata ensuring SOCONET is an integral part of the GOOS vision.