Incorporation of Alternative Sensors in the SOCAT Database and Adjustments to Dataset Quality Control Flags

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Abstract

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With the advent of new sensors and platforms to measure surface water carbon dioxide (CO_2) levels, the dataset quality control (QC) criteria are updated in the Surface Ocean CO_2 Atlas (SOCAT) to accommodate surface water fugacity of CO_2 (fCO_{2w}) data from these sensors. The current dataset QC flags and their rationale are described. The new sensors and platforms are briefly presented. Some changes in the criteria for assigning dataset QC flags and a new data quality flag are introduced. The term "dataset QC flag" replaces "cruise QC flag" to reflect the alternate platforms that are included in SOCAT. All dataset QC flags will incorporate a specified accuracy[1] of the data. For equilibrator based systems the criteria for equilibrator pressure measurements are relaxed as they are unnecessary stringent for the accuracy of fCO_2 in surface seawater. The acceptable comparison with other in situ data, defined as a high quality cross-over, will meet specific criteria of maximum distance, differences in fCO_{2w} and sea surface temperature (SST) between two datasets. The scientist submitting the dataset will enter a preliminary dataset flag. Platform type including alternative platforms, such as buoys and self-propelled surface vehicles, will be provided in the metadata and will be available as a selectable option in the Live Access Server (LAS) for SOCAT. These updates facilitate better separation of

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[1] Since there is no absolute standard for pCO_2 in seawater, the term accuracy throughout refers to agreement with accepted values obtained from conventional state-of-the art systems such as described in Pierrot et al. (2009).

data of differing origin and quality, and enable incorporation of fCO_{2w} data from alternative platforms and sensors in SOCAT. The revised criteria will be implemented during quality control for all new and updated datasets in version 3 onwards, but not to datasets already in versions 1 or 2. To view recommendations the reader should peruse section 6. The updated criteria for dataset QC flags are in Table 3.

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1. **Introduction**

The Surface Ocean CO_2 Atlas (SOCAT) is a global surface ocean CO_2 data collection that incorporates fugacity or partial pressure of CO_2 (fCO_2, pCO_2)[2] data for the open oceans and coastal seas into a uniform dataset. The first release, version 1.5, occurred in 2011 and was comprised of 6.3 million observations. The second release was in 2013 (Bakker et al., 2013). These datasets are iterations upon which the international marine carbon research community continues to build using agreed data and metadata formats, and standard quality-control procedures. The effort is endorsed and partially supported by several international ocean science programs[3].

The version 1.5 and 2.0 releases mostly contain data acquired from automated underway pCO_2 systems based on infrared analysis (IR) of CO_2 in the headspace of equilibrators operated on research and commercial vessels, largely following the standard operating procedures (SOP) as outlined in SOP 5 of Dickson et al. (2007). Some older data (prior to ~1995) were measured by gas chromatographic (GC) analysis of the CO_2 content in the headspace. During the assembly and quality control of an updated SOCAT release, observations were submitted from alternative platforms and alternative sensors whose data did not fit well in the current quality assessment scheme. It is anticipated that in the future there will be significantly more data arising from alternate approaches. This requires a reassessment of dataset quality control flags, as used for version 1.5 (Table 6 from Pfeil et al. 2012; also shown in Appendix A as Table A1).

Here we provide recommendations regarding fCO_{2w} measurements made from platforms other than ships, and instruments that differ from conventional IR headspace analysis from flowing equilibrators. The assessment includes:

- Whether the data should be included in version 3 of SOCAT,
- What metadata is necessary to perform the secondary quality control, and,
- What added information should be provided in the SOCAT output files such that queries can easily distinguish the data obtained from different approaches.

To place the recommendations in context, we will first provide an overview of select current sensors and dataset quality control procedures. This is followed by a brief description of the

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[2] The chemical potential of CO_2 gas in water is either expressed as a partial pressure (pCO_2) or, when accounting for the non-ideality of CO_2, fugacity (fCO_2) with a conversion utilizing virial coefficients as described in Weiss (1974). The $fCO_2 \approx 0.993\ pCO_2$. Here we generally use the term fCO_2 as this is the reported quantity in the SOCAT dataset.

[3] Including: the International Ocean Carbon Coordination Project (IOCCP) which is a joint project of the International Oceanographic Commission (IOC) of the United National Educational, Scientific and Cultural Organization (UNESCO) and the Scientific Committee on Ocean Research (SCOR); the Surface Ocean-Lower Atmosphere Study (SOLAS); and the Integrated Marine Biogeochemistry and Ecosystem Research (IMBER).

sensors and platforms that are under consideration. The final section provides the recommendations. The recommendations are based on deliberations of the authors of this white paper and communications with the manufacturers. A draft was sent to the SOCAT list server for additional comments and the suggestions have been taken into consideration in this submission.

We recognize that this is a living document in that recommendations on quality control and flagging will change with time as sesnors are improved, other sensors and approaches are put in place, and as the needs of users of SOCAT information evolves.

2. SOCAT Quality Control (QC) Criteria for Version 1

A comprehensive description of the history of SOCAT, and procedures of assembly and quality control can be found in Pfeil et al. (2012). As stated in the paper, the primary goals of the SOCAT effort are:

- To assemble all available surface water fCO_2 data.
- To encourage application of best practices including recommendations on instruments and standardization.
- To encourage submission of quality controlled and appropriately documented data.
- To provide a dataset quality control[4] focused on the regional consistency of data and adequacy of the metadata information.
- To provide a user-friendly interface to obtain data, metadata and data visualization and products.

This effort to provide an integrated and quality controlled dataset does not enjoy a single or sustained funding source. Much of the required post-submission quality control is performed by "volunteers", most of who have submitted data to SOCAT and are familiar with surface water fCO_2 data. To facilitate an objective and consistent dataset quality control, prescribed procedures are followed ("a cookbook"), using the SOCAT LAS server (www.socat.info) for retrieval of data and metadata, and for visualization.

The dataset quality control includes a quick check of individual outliers in the data but it is primarily focused on the integrity and quality of the submitted data that usually consists of a single cruise or deployment. Emphasis is placed on inclusion of sufficient metadata to evaluate data quality. The cruises are assigned a dataset quality control flag based on the accuracy of the sensors used, the completeness of the metadata and an assessment of accuracy.

High-quality submissions are those with an accuracy of fCO_2 in surface water of 2 μatm or better. This requires documented instrumental accuracies of CO_2 analysis, pressure of CO_2 analysis, temperatures of CO_2 analysis, and temperature of surface seawater. A ship-based system that meets these requirements, given that all sensors (temperature, pressure, etc.) are within factory specifications, was developed based on community input and is extensively used (Pierrot et al., 2009). It is referred to as the GO system and manufactured by General Oceanics

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[4] Dataset quality control (QC) focuses on the overall quality of the submitted datasets. The datasets usually cover a single cruise or deployment. The dataset is viewed in context of other datasets with a brief visual assessment of outliers in position, sea surface temperature salinity, fCO_{2w} and cross-over, if available. It is not meant to supplant the quality control and metadata submissions by the individual investigators. The dataset quality control is also referred to as cruise QC, secondary QC, extended QC, or contextual QC.

(http://www.generaloceanics.com). A second system, the Kimoto Air /Marine CO_2 Automatic Monitoring System with tandem type gas-liquid equilibrator (www.kimoto-electric.co.jp/english/product/ocean/co2.html) has shown equal or better performance in shore-based intercomparison exercises.

An important aspect of these systems is that they have a gas-liquid showerhead equilibrator and the quantity measured is a dry mole fraction of CO_2 (XCO_2) in the equilibrated headspace. The detector response can be standardized with traceable compressed gas standards of CO_2 in air. The fCO_2 can be calculated knowing the pressure in equilibrator and detector, and temperature of water in equilibrator and sea surface temperature. This approach has been used over 50 years (Takahashi, 1961), and calibration and calculation procedures are well described (e.g. Dickson et al., 2007). The novel sensors described here have differences ranging from subtle to dramatic compared to the equilibrator NDIR based systems. In several cases the calibration routines are not well worked out challenging the assessment of accuracy.

The dataset QC criteria are focused on underway measurement of surface seawater fCO_2 from ships. The flags and criteria for checking dataset for SOCAT version 1.5 and 2 are provided in Appendix A, Table A1. The flagging system is set up such that cruises with an A or B flag have documented procedures and measurements in place such that surface water measurements have an accuracy of fCO_2 of better than 2 μatm. The instrumental requirements to meet these criteria are listed in Table 1. The impact of uncertainty in pressure and temperature of equilibration is shown in Figure 1, and the impact of uncertainty in water vapor pressure on the calculation of fCO_{2w} is given in Appendix B.

The current recommendations for quality control and dataset QC flags are aimed to provide a broad qualification of data quality of a particular cruise. It is a guide of the necessary sensor accuracy and documentation for data submitted to SOCAT, as well as an assessment of data quality of a particular cruise in SOCAT. In previous releases of SOCAT a flag of C or D was deemed acceptable, but no quantification of accuracy of 'acceptable' data was provided.

Table 1. Instrumental requirements for accuracy of fCO_2 in surface water of better than 2 μatm (Pfeil et al. 2012)

Instrument	Accuracy or procedure
Infrared analyzer	Data are based on XCO_2 analysis, not fCO_{2w} calculated from other carbon parameters, such as pH, alkalinity or dissolved inorganic carbon; Continuous CO_2 measurements are made, not discrete CO_2 measurements; 2 non-zero compressed gas standards spanning range with certified mole fraction to within 1 ppm[a].
(Analysis of moist gas)[b]	Measurement of water vapor pressure to within 0.5 hPa (≈ 2 % @ 20 ˚C)
Temperature equilibrator	0.05 ˚C
Temperature sea surface	0.05 ˚C
Pressure equilibrator	0.5 hPa (=mBar)

[a] Required based on the typical non-linearity of a LI-COR 6262 sensor.

[b] Pfeil et al. (2012) do not mention measurement of vapor pressure as measurement of dry mole fraction was assumed. The specified accuracy in water vapor measurement is what is needed to determine the fCO_{2w} to within 2 μatm if the humidity of analysis is 100 %. Measurement of dried gas eliminates this uncertainty and is preferred. See Appendix B for detail.

For some applications, e.g. for constraining global sea-air CO_2 flux estimates, only data of the highest quality are acceptable. For other applications data quality can be relaxed and even insufficiently documented data can be useful. These include datasets in regions where there is little or no data, or for purposes such as determining temporal and spatial scales of variability. Moreover, several applications such of study of surface water CO_2 variability in coastal regions often have lower accuracy requirement than utilization of fCO_{2w} to constrain global sea-air flux estimates.

The SOCAT database was conceived as data holdings from ships measuring surface water fCO_2. Surface water fCO_2 is determined by analysis of the equilibrator headspace using non-dispersive infrared (NDIR) analysis or gas chromatography. Gas chromatographs have been used extensively in the past (Weiss, 1981) but because of cost, size and need for considerable extra equipment, these types of systems are infrequently used nowadays. New types of sensors are substituting the IR sensors. They are based on cavity ring-down spectrophotometers (CRDS) which are used for very accurate atmospheric measurements of CO_2 and other trace gases, and their isotopes. The CRDS based sensors experience no water vapor interference and the units require minimal calibration. Their cost is much higher than most infrared analyzers and they are significantly bigger. They have been used successfully in conventional underway pCO_2 systems with showerhead equilibrators on ships (Becker et al., 2012). Initial tests suggest they hold rock-steady calibration at sea for weeks. However, until more experience is gained with these analyzers they should be checked daily with at least two non-zero standard gases to meet A or B requirements (listed in Table 1). The CRDS most often used are instruments produced by Picarro (www.picarro.com) and Los Gatos Research Inc. (www.lgrinc.com).

3. Brief description of alternative sensors

Several novel sensors and platforms have been developed for fCO_{2w} determination. These include the sensors and platforms listed in Table 3 and which are described below. We limit the discussion to sensors that are predominantly used to determine near surface fCO_2 levels. A cursory overview of instrumental performance based on exchanges with manufacturers, company literature, and intercomparisons in the field is provided in Appendix C. A comprehensive listing of sensors and manufacturers can be found at http://www.ioccp.org/Sensors.html#pCO2.

Table 2. Examples of alternative sensors used for measurement of surface water pCO_2

Sensor	Principle	Platform	Website
CARIOCA	Spec/dye	Mooring/Drifter	www.dt.insu.cnrs.fr/carioca/carioca.php
SAMI CO_2	Spec/dye	Ship/buoy	www.sunburstsensors.com
PSI CO_2-pro	Sealed IR	Ship / Mooring	www.pro-oceanus.com
Contros HydroC	Sealed IR	Buoy/ Wave Glider	www.contros.eu
Seaology	IR	Buoy	battelle.org/our-work/national-security/

SubCtech OceanPack IR	Ship	undersea-systems subctech.eu

3.1 *CARIOCA*

Details of the CARIOCA *(Carbon Interface Ocean Atmosphere)* have been described in several papers (e.g., Lefèvre et al. 1993; Merlivat and Brault, 1995; Copin-Montégut et al. 2004;Boutin et al., 2008). In short, in original form the CARIOCA is an integrated sensor system built into a float, specifically to determine sea-air CO_2 fluxes. It contains an anemometer, a salinometer, a fluorometer, air and surface water temperature sensors, and a spectrophotometric fCO_2 sensor. It usually is deployed as a free drifting float with a drogue in a Lagrangian mode with an endurance of up to 18 months, although it has been tethered to a mooring in some deployments. The CARIOCA has been adapted such that they can be installed on moorings such as the PIRATA array. Data is telemetered daily via Service ARGOS to shore. CARIOCAs have been successfully used since 1995 (Hood et al. 1999; Bakker et al. 2001; Lefèvre et al. 2008). The measurement principle for CO_2 is to flow seawater across a gas permeable membrane filled with pH sensitive dye. The CO_2 will diffuse across the membrane until the fugacity of CO_2 in the dye reaches that of the seawater. The fugacity of CO_2 is deduced from the pH of the dye solution. The pH is determined by the change in ratio of optical absorbances at two wavelengths corresponding to the maximum absorbance of the acid and conjugate base of the dye and are measured with a spectrophotometer (Copin-Montégut et al. 2004).

The calibration is done in the laboratory by comparing the response of the spectrophotometer in the CARIOCA to the fCO_2 of a seawater solution determined with an infrared analyzer. The CARIOCA response is determined over the anticipated range of fCO_{2w}. There is no independent calibration procedure when the unit is deployed, and post-deployment calibration is not routinely done. The first CARIOCA buoys used only 2 wavelengths. A third wavelength channel was added in the CARIOCA system in 1998, where the dye does not absorb to correct from drift (Lefèvre et al., 1993), which lead to improved stability of values (Copin-Montégut et al. 2004; Boutin et al., 2008).

3.2 *SAMI CO_2*

The SAMI (Submersible Autonomous Moored Instrument) pCO_2 system was developed in the early 1990's (Degrandpre et al., 1995; 2000). It is a spectrophotometric system like the CARIOCA and it was the first spectrophotometric based pCO_2 system that monitored three wavelengths, including a "null value" to determine dye degradation and drift. An upgraded version, SAMI2 CO_2, replaced the original SAMI in 2009 but the operating principle remained unchanged. It is a stand-alone unit that can be incorporated in moorings and structures, including sub-surface applications (Körtzinger et al. 2008) as it can be deployed at depth. Data is logged internally and retrieved after deployment that can last up to a year. However, the SAMIs are generally recovered after one- to three-months. Pre-deployment calibration is similar to that of the CARIOCA.

Other than the different form factor, the CO_2 sensors on the CARIOCA and SAMI are very similar, both relying on gas permeable membranes and spectrophotometric dye detection. A system with similar operating principles for shipboard applications is referred to as the AFT (autonomous flow-thru instrument).

3.3 *Pro-Oceanus Systems Incorporated (PSI) CO_2-Pro line of sensors*

The Pro-Oceanus CO_2-Pro sensor is a submersible standalone instrument that can be deployed on ships of opportunity or on moorings. The PSI CO_2-Pro uses a patented tubular gas permeable membrane through which CO_2 in the water equilibrates with a headspace gas that is pumped through an infrared analyzer in a closed circulation loop. The infrared analyzer is periodically calibrated for zero CO_2 concentration by rerouting the headspace gas through a CO_2 scrubber. It is ranged and calibrated by the manufacturer using 8-10 calibration gases traceable to NOAA standards. Recalibration is recommended annually and is offered as a service by PSI. Several ships have the Pro-Oceanus CO_2 sensor installed and side-by-side comparisons with the conventional shipboard pCO_2 sensors have been performed. (Appendix C).

In addition to the CO_2-Pro, PSI offers a compact version of the sensor that employs a flat advanced matrix interface with the same accurate and stable infrared analyzer. In 2008, Pro-Oceanus began offering the CO_2-Pro Atmosphere as a stand-alone instrument for measuring both atmospheric and sea surface pCO_2. The use of a single detector for measuring both eliminates the error associated with the use of two separate detectors for determining air-sea CO_2 fluxes.

3.4 *Contros HydroC*

The Contros HydroC sensor is a compact submersible standalone sensor that can be deployed on ships of opportunity (in flow-through mode) or on moorings/surface floats. It is capable of taking measurements at depths of up to 1000 m. The measurement principle is similar to that of the Pro-Oceanus as it is based on membrane equilibration and NDIR spectrometry. To account for sensor drift it has an auto-zeroing feature. Contros offers calibration service where the sensor is calibrated against a standard pCO_2 system at different pCO_2 levels. Two Contros sensors were compared against a GO pCO_2 system during two research cruises and procedures for drift corrections were developed that was very successful (Fietzek et al. (2013); Appendix C).

3.5 *Seaology/MAPCO$_2$ sensor*

This is an IR based system for buoy deployments and utilizes an air-water equilibrator at the sea surface. The $MAPCO_2$ system's development started at MBARI in the mid-1990s (Friederich et al., 1995). It was subsequently improved at NOAA/PMEL, and in 2009 was transitioned to a commercial vendor, Battelle Memorial Institute, and named Seaology. In current form it comes equipped with a low cost oxygen sensor, a humidity sensor, and a LI-COR 820 IR analyzer. The Seaology/$MAPCO_2$ system's default configuration takes a surface seawater and marine boundary air measurement every 3-hours for up to a year deployment, and the data is telemetered to shore daily. Each measurement cycle includes a span and zero calibration. Strong attributes compared to the other systems described above is that it is set up to measure mixing ratios of CO_2 in air, XCO_{2a} and that it is spanned *in situ* using standard reference gas during each measurement cycle. Currently about three dozen moorings are deployed worldwide and they have proven to be reliable. Some of this mooring data has been quality controlled and is available at CDIAC (cdiac.ornl.gov/oceans/Moorings/).

3.6 *SubCtech OceanPack*

The SubCtech OceanPack sensors are based on membrane equilibration with subsequent IR based determination of CO_2. They use an IR analyzers are built by LI-COR (model 840). They offer the sensor for both, ship based underway and underwater measurements. A side-by-side evaluation with a GO system was performed on the Polarstern in late 2012 and described in the document referenced at the website provided in Table C2.

4. Sensor intercomparisons and evaluations

The studies with alternative sensors generally have different purposes than the ship of opportunity work focused on sea-air CO_2 fluxes, and often the objectives do not require the same accuracy. The accuracy of the alternate sensors in the field is difficult to establish as they frequently lack calibration routines and have poorly described corrections for pressure, salinity temperature and water vapor interference. Several evaluation and comparison exercises have been performed with the sensors that provide some insight as to their performance. Some, but not all the sensors described above, were used in intercomparison and evaluations exercises. An intercomparison of systems used on shipboard took place in Japan in 2007 that included some alternate sensors. A comprehensive report has not been released for the experiment. During February-March 2009 a second international ocean pCO_2 instrument inter-comparison including underway and autonomous buoy systems was held at National Research Institute of Fishery Engineering in Kamisu City, Ibaraki, Japan using an indoor seawater pool. SAMI, $MAPCO_2$, underway GO systems, and underway Tandem equilibrators by Kimoto Electric Co. were deployed during the study. While no report has been released, a general summary can be found at http://www.ioccp.org/FinalRpts/WR221_eo.pdf (pages 10 and 11). The Seaology/MAPCO2 showed good agreement (within 2 µatm) with the GO and Kimoto Electric Co. IR based systems with equilibrators during these tank studies. The SAMI sensor showed some offsets and drifts compared to the systems commonly used on ships. In 2009, an evaluation of mooring based pCO_2 systems as part of the Alliance for Coastal technology (ACT) effort included the Seaology/$MAPCO_2$, Contros and Pro-Oceanus sensors. This study was designed as an evaluation rather than an intercomparison. The sensors were deployed at two field sites, one in Hood canal, Oregon, and one in Kaneohe Bay, Hawaii. Both sites experienced extreme and rapid daily fCO_{2w} variations of over 400 µatm.

Of the 3 systems the Seaology/$MAPCO_2$ sensor had the smallest offsets and differed by 3 ± 9 µatm and 12 ± 30 µatm from the reference system for the two deployments. The Pro-Oceanus sensor differed by 9 ± 14 µatm from the reference sensor during the Hawaii evaluation. The Contros prototype differed by 7 ± 20 µatm, 16 ± 26 µatm, 55 ± 117 µatm, 96 ± 25 µatm from the reference measurements for different time periods. However, the frequency of measurement differed for the systems with the reference system not always providing accurate data as the environment changed so rapidly and drastically. The accuracy of the reference system and reference approaches was not constrained in the study. The evaluation reports of the ACT deployments can be found at:
http://www.act-us.info/sensor_list.php?cat=Dissolved%20Gases&type=Chemical;
http://www.act-us.info/Download/Evaluations/pCO2/PMEL_MAPCO2_Battelle_Seaology/files/act_ds10-02_pmel_pco2.pdf ;
http://www.act-us.info/Download/Evaluations/pCO2/Pro_Oceanus_Systems_PSI_CO2_Pro/;
http://www.act-us.info/Download/Evaluations/pCO2/Contros%20HydroCTM_CO2/.

Several of the instruments were improved since then, partly because of issues discovered during the evaluations. This points to the importance of such exercises. The performance of the current Contros sensor is better than that of the model used in the 2009 ACT evaluation (Steinhoff, personal communication; Fietzek et al. (2013). The PSI CO_2-Pro sensors have been improved through better temperature regulation of the detector, advances in the automatic zeroing function, and the use of NOAA traceable gases for calibrations (Johnson, personal communication).

There is limited information about the accuracy and drift of the alternative sensors in the field in large part because the sensors have no *in situ* standardization (or spanning) routine, except for the Seaology/$MAPCO_2$. The Seaology/MAPCO2 sensor is spanned prior to each measurement and showed good agreement (< 2 µatm) with the GO and Kimoto Electric Co. IR based systems with equilibrators during the tank studies in Japan. The current Contros and Pro-Oceanus sensors have an auto-zeroing feature but no in situ spanning capability. However, new Pro-Oceanus and SubCtech OceanPack units will offer an option of including calibration standards.

While the studies were not set up as robust intercomparisons, the alternative sensors other than the Seaology/$MAPCO_2$ showed appreciable offsets and drifts compared to the systems commonly used on ships. Drifts in these sensors have also been shown in opportunistic field comparisons (see e.g. Bates et al, 2000). Recent comparisons show improved results for the Contros sensor in large part because of use of an algorithm that corrects for drift based on the auto zeroing feature and post-deployment calibration (Fietzek et al., 2013). The CARIOCA has shown better results as well in more recent studies (Copin-Montégut et al. 2004; Boutin et al., 2008). Improvements in other sensors are being made as well, in part due to requests from the SOCAT community.

5. Alternative platforms

Most of the SOCAT data to date comes from ships. Ships have the advantage of large carrying capacity such that space and weight of instrumentation and calibration gases are not a major factor. The largest operational issues with systems on ships are access to surface seawater, measurement of the sea surface temperature, and disposal of water after it passes through the gravity drain of the equilibrator.

Alternative platforms generally do not suffer from these issues but have their own unique limitations. Data from three types of alternative platforms are considered here, fixed position buoys/moorings, drifting buoys, and autonomous propelled surface platforms. Most of these platforms have significant payload restrictions limiting the size and weight of the instruments, auxiliary equipment, batteries, and standards. The platforms have the advantage that the temperature and pressure of analysis is generally the same as that at or right above the surface seawater, minimizing corrections and adjustments of measured values to *in situ* conditions. The sensor intakes on the alternative platforms are often within 1.5 m of the surface, considerably shallower than seawater intakes of ships. Because of near-surface thermal and density stratification such as diurnal warm layer and fresh water lenses, the alternative sensors will sometimes be sampling other water properties than ship-based sensors (McNeil and Merlivat, 1996). Thus, greater [diurnal] variability can be expected with observations from these platforms. Comparison with ship-based systems, measuring water at 3-10 m depth, should be done with caution bearing these differences in mind as shown in Bates et al. (2000). These alternative platforms are important means of expanding the SOCAT data holding but the differences with ship-based measurements must be recognized and incorporated in analyses. They can augment ship-based measurements by getting time series data at a fixed location, measurements at shallow depth, and measurements in remote areas and seasons when no ship-based observations are available.

6. Recommendations

The alternative sensors challenge the dataset QC criteria as the rating criteria in SOCAT were developed for IR (and GC) ship-based systems with a general focus to constrain sea-air CO_2 fluxes. With new purposes for the data, new sensors and new platforms, adaptations are necessary. Our recommendations are several. The dataset QC evaluation criteria need to be fine-tuned and an additional QC flag should be instituted for some of the novel sensors. The LAS system used in SOCAT needs to provide the capability to screen fixed platform and alternative platform setups. The metadata forms should be adapted.

A uniform metadata structure is adopted in SOCAT as provided by the Carbon Data Information and Analysis Center (CDIAC) (see http://mercury.ornl.gov/OceanOME/newForm.htm). The general structure of this form is appropriate for the alternate platforms but some of the information requested is not pertinent. It would be useful if either a dedicated form for alternate platforms would be available or if the current forms are adapted to include specific entries for alternate platforms and sensors. At very least, some of the nomenclature should be changed including referring to surface water data as opposed to underway data; substitute platform for ship; and project for cruise.

A general need is that a knowledge base needs to be developed for these sensors and that their behavior in the field is fully characterized and documented. Side-by-side comparison with established units used for shipboard work such as the GO underway systems, and underway Tandem equilibrators by Kimoto Electric Co. are very useful in this respect. Several of such comparisons have been performed (e.g. Bates et al., 2000; Fiedler, 2013; Fietzek et al., 2013) but several others have not appeared in accessible literature. A compilation of the unreported comparisons would be useful.

The operating principles of many of the sensors are fundamentally different from those of the underway system currently used and their behavior in response to changes in temperature, salinity, ambient pressure, water vapor pressure are not well known which could impact their accuracy at sea. There is a strong need for continued intercomparison exercises and dissemination of results of previous studies.

For current and alternative sensors, fouling can be a significant problem that is difficult to discern in the quality control process (Juranek et al., 2010). Cleaning and anti-fouling procedures, and tests to detect impacts of biofouling are strongly recommended for all operations. Utilization of oxygen sensors can be useful in detecting biofouling issues. Anti-fouling measures should be included in the standard operating procedures (SOP).

Several of the alternative sensors use gas permeable membranes that can undergo fouling. This can effect the response time of the instruments but in case of biofouling there can be significant microbial oxidation and respiration on the membrane. This can cause biases that are very difficult to detect.

The specific recommendations regarding data and metadata for the SOCAT 3 release are listed below. These are focused on the alternative sensors but also include fine-tuning of the current dataset flags. A key aspect of the SOCAT data holdings is that the quality criteria should be unambiguous, and data of specified accuracy are easily selectable. Currently, the A and B flags are clearly defined, but flags C and D do not have a specified accuracy. The recommendations for the SOCAT quality control and release are below. The updated criteria are shown in Table 3 and can be compared with the SOCAT versions 1 and 2 cruise flag criteria in Table A1.

These recommendations will be implemented for all new and updated datasets in SOCAT. No effort is envisaged to retrospectively implement the relevant recommendations for cruises in SOCAT versions 1 and 2.

I. Flag A will be restricted to datasets with a high quality cross-over.

No clear definition has been given to what constitutes an acceptable comparison with other data (cross-over) in versions 1 and 2. In version 3 a high-quality cross-over is defined as a cross-over between two datasets with a maximum cross-over equivalent distance of 80 km[5] (Figure 2), a maximum difference in SST of 0.3°C and a maximum fCO_{2w} difference of 5 µatm. Inconclusive cross-overs, defined as having a temperature difference greater than 0.3°C or a fCO_{2w} difference exceeding 5 µatm, will not have a flag A.

II. The accuracy of the pressure measurement in the equilibrator for a dataset flag of A or B is relaxed to 2 hPa (from 0.5 hPa).

An uncertainty in the equilibrator pressure of 2 hPa yields a corresponding uncertainty in fCO_{2w} of 0.8 µatm (for a fCO_{2w} of 400 µatm). The recommendation of accuracy of temperature of 0.05 ˚C remains unchanged, as this corresponds to an uncertainty of about 0.9 µatm. These accuracy requirements will meet the calculated fCO_{2w} accuracy limit of 2 µatm for water values for these flags (Figure 1). The relaxation of the pressure of equilibration criterion is appropriate as the criterion was originally instated for the higher accuracy needs of atmospheric CO_2 measurements that are not part of SOCAT.

III. Flagging of alternative sensor data holdings with C or D flags.

The alternative sensors described currently do not meet the verifiable high accuracy requirements to warrant a QC flag of A or B. Dataset flags of A or B require an accuracy of fCO_{2w} of 2 µatm and must have documented accuracies and standardization routines (Table 1). Based on intercomparisons and methodology the Seaology/MAPCO$_2$ sensor will be close to meeting the

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[5] The algorithm treats 1 day of separation in time as equivalent (heuristically) to 30km of separation in space, that is, if d*x* is the distance between points from two cruises in km, and d*t* is the separation between the same two points in days, then the separation between these two points would be given as $[dx^2 + (dt*30)^2]^{1/2}$). Thus, a crossing of tracks within 2.7 days (80 km/ 30 km) will qualify as a cross-over if a sample was obtained at the same location. Figure 2 provides the time space criteria for a cross-over.

threshold, but lack of sufficient number of standards used results in a C (provided appropriate metadata is supplied) or D (if metadata is not comprehensive) rating. To obtain a C or D flag the systems must have an in situ calibration comprised of two standards, one of which can be a zero. The accuracy of the Seaology/MAPCO$_2$ is estimated at 4 µatm (Appendix C); the CARIOCA2 (3 wavelengths) is estimated at 3 µatm (Appendix C). Recent studies (Fietzek et al. 2013) suggest that Contros HydroC sensors with appropriate pre- and post-deployment calibration can meet the requirements. However it is deemed impractical to trace post-deployment calibrations by the SOCAT QC groups who are dealing with thousands of cruses. Determining the accuracy without the appropriate meta data will be challenging, such that the “D” rating” will be assigned infrequently.

IV. For a dataset (ship or alternative platform) to receive a flag of C and D it should meet an accuracy estimate of 5 µatm or better based on reasonable knowledge of sensor behavior and support sensors and in situ calibration.

Alternative sensors that have in situ calibration, and meet the accuracy requirements of 5 µatm based on these calibration checks, can be assigned these C or D values. For IR based systems this means that at least one calibration standard (“span gas”) should have a concentration greater than the samples such that the sample is bracketed by the standard and the zero gas. In case of a single span gas, the linearity of the detector must be confirmed. The span gas should be calibrated to traceable standards ≈ 2 ppm. Alternatively, the accuracy of better than 5 µatm should be verified from pre- and post-deployment checks. The temperature of measurement and SST should be accurate to within 0.2 ˚C and pressure to within 10 hPa (mBar) to meet the accuracy criteria (see Figure 1).

V. A flag of “E” will be created for alternative sensor designs that are accurate to within 10 µatm

Some of the spectrophotometric and sealed IR systems currently do not meet the criteria set out by SOCAT for a dataset rating of A-D as their accuracy cannot be verified independently, unless pre- and post- deployments calibrations are performed that are difficult to track. However, the data can have significant utility as they are obtained in remote environments, or provide high-resolution sub- and multi-annual time series. Moreover, such sensors and platforms will be deployed more often in the future. As called out above more [in situ] comparisons with established instruments are warranted. The requirements for pressure and temperature are modest to obtain fCO_{2w} values of better than 10 µatm, and data from most of the sensors described likely meet this target (Figure 1). While the accuracy of many of the sensors cannot be independently verified when deployed, pre-deployment and laboratory tests can provide a general estimate if accuracies of better than 10 µatm are attained. When deployed on a buoy, the main concern for the data quality is the drift of the instruments. Internal diagnostics and standardization and when possible post-deployment tests are necessary. Some of the uncertainty in the sensor response is in the conversion of instrument output to fCO_{2w}.

VI. A preliminary dataset quality criterion will be assigned during data submission by the investigator submitting data

It is recommended that the submitting PI provide a preliminary dataset quality flag based on the criteria in the supplied metadata. When the dataset is entered in the database the flag will have the prefix “N” (e.g. NB, NC etc.). This should encourage submitting investigators to check their metadata and data during submission to assure they meet the appropriate SOCAT dataset QC flag criteria. The metadata form needs to be adjusted to accommodate such an entry.

VII. Platform type becomes an additional variable in the SOCAT data holdings.

The alternative platforms provide a critical means to extend our observations to remote locales, frequently repeated transects and time series. Most of the alternative platforms carry sensors of the types described above. Aside from the unique nature of the sensors, the sensors on the alternative platforms often measure the fCO_2 of water at a different depth than ships that commonly have their uncontaminated seawater intake between 3-6 meters depth. The Seaology/$MAPCO_2$ sensors have their equilibrator right at the air-sea interface. The CARIOCA is about 1.5 m below the sea surface, while many other sensors on alternative platforms are deployed within a meter of the surface or are mounted on moving platforms measuring at different depths. Thermal stratification can cause differences in fCO_{2w} depending at what depth the measurement is performed (McNeil and Merlivat, 1996; Bates et al., 2000). Most of the alternative platforms are either stationary or slower moving than ships of opportunity and will yield a different spatial and temporal sampling density. Depth of measurement is currently one of the metadata requirements. However there are other unique differences between the alternate platforms and ships and it is recommended that platform type is easily recognized and screened in SOCAT data holdings with a separate column or by a unique EXPOCODE. In addition to ships, which is the default, moorings (fixed platforms) and autonomous surface vehicles should be able to be easily selected separately. Table 5 provides an outline of screening criteria. It is noted that only data measured within the surface mixed layer, or at a depth shallower than 15 m, whichever is shallower, should be submitted to SOCAT.

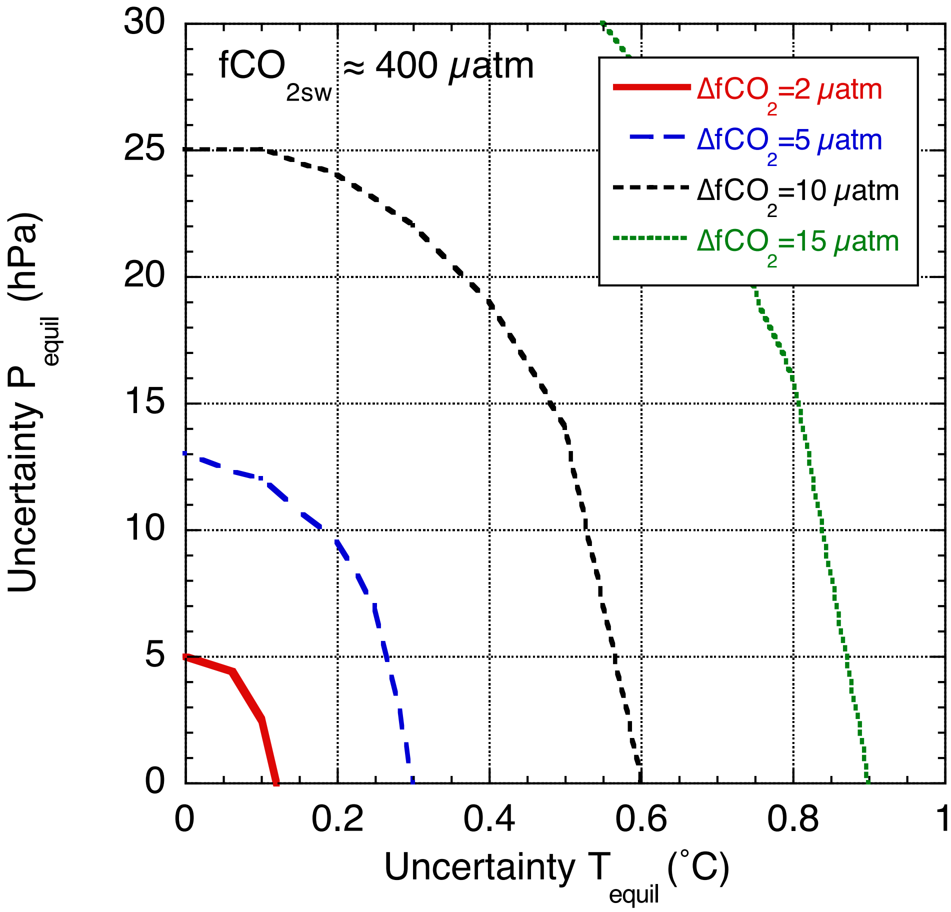

Figure 1. Isopleths of uncertainty in calculated fCO_{2w} (ΔfCO_2) arising from uncertainty in temperature and pressure of equilibration, T_{equil} and P_{equil}, respectively. The uncertainty in seawater fCO_2 due to an uncertainty in temperature is $\Delta fCO_{2w} = fCO_{2w}\, e^{-(0.0423\, \Delta T)}$; the uncertainty in fCO_{2w} due to an uncertainty in pressure is $\Delta fCO_2 = XCO_2\, \Delta P$. For example, to have an uncertainty in fCO_{2w} of less than 5 µatm, the combined uncertainty in sea surface temperature, equilibrator temperature and measurement pressure has to fall below the dashed blue line. In this example, only uncertainty T_{equil} is used but for fCO_{2w} the uncertainty in SST measurement must be included. This applies to equilibrator-based systems.

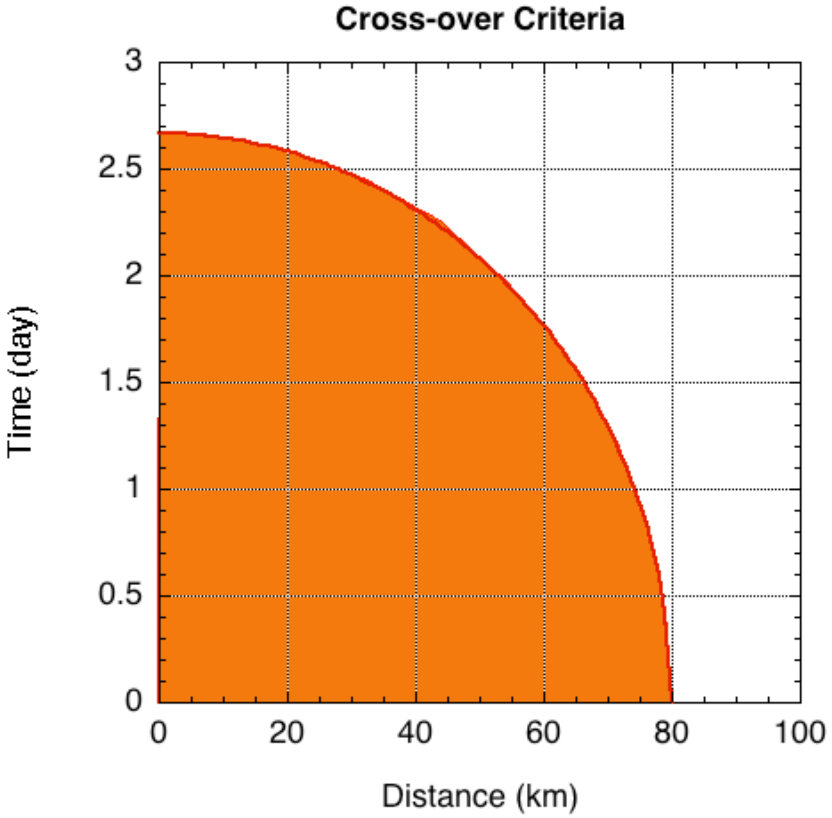

Figure 2. Distance and time criteria for a cross-over. The area in red provides the time–space relationship that defines a high-quality cross-over. One day of separation in time is equivalent (heuristically) to 30 km of separation in space. A distance of less than 80 km is considered a cross-over. The area is thus defined as $([\mathrm{d}x^2 + (\mathrm{d}t{*}30)^2]^{1/2}) \le 80$ km.

Table 3. Proposed criteria for dataset quality control flags of the SOCAT database version 3.0

Flag	*Criteria*[a]
A (11)	(1) Accuracy of calculated fCO_{2w} (at SST) is better than 2 μatm (2) A high-quality cross-over with another dataset is available (3) Followed approved methods/SOP[b] criteria (4) Metadata documentation complete (5) Dataset QC was deemed acceptable
B (12)	(1) Accuracy of calculated fCO_{2w} (at SST) is better than 2 μatm (2) Followed approved methods/SOP criteria (3) Metadata documentation complete (4) Dataset QC was deemed acceptable
C (13)	(1) Accuracy of calculated fCO_{2w} (at SST) is better than 5 μatm (2) Followed approved methods/SOP criteria (3) Metadata documentation complete (4) Dataset QC was deemed acceptable
D (14)	(1) Accuracy of calculated fCO_{2w} (at SST) is better than 5 μatm (2) Did or did not follow approved methods/SOP criteria (3) Metadata documentation incomplete (4) Dataset QC was deemed acceptable
E (17)	(Primarily for alternative sensors) (1) Accuracy of calculated fCO_{2w} (at SST) is better than 10 μatm (2) Did not follow approved methods/SOP criteria (3) Metadata documentation complete (4) Dataset QC was deemed acceptable
F (15)	(1) Does not meet A through E criteria listed above
S (Suspend) (15)	(1) More information is needed for dataset before flag can be assigned (2) Dataset QC revealed non-acceptable data and (3) Data are being updated (part or the entire cruise)
X (15)	(Exclude) The cruise (dataset) duplicates another cruise (dataset) in SOCAT
NA…NF	Submitted data to SOCAT that has not undergone independent dataset quality control as indicated by the “N”. The NA though NF are the flags provided by the submitting group

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[a] the accuracy takes precedent over the criteria that follow

[b] SOP or Standard Operating Procedure following Dickson et al. 2007

Table 4. Recommendations for dataset flags for alternative sensors

Type	Flag
Data with an accuracy of better than 5 µatm[a, b]	C or D
Sensors using spectrophotometric, GC or IR with no <u>*in situ*</u> calibration gases but having pre-deployment calibration with documented accuracy better than 10 µatm[b]	E
Sensors with no documented or verifiable accuracy, or worse than 10 µatm	F

[a] All alternative sensors currently in operation have at most one non-zero calibration gas such that it does not meet A or B criteria. Sensors with no *in situ* calibration (span gas) but undergo pre- and post-deployment calibration checks appear to meet the 5 µatm criteria cannot be assigned a C or D flag as the interpretation of the post-cruise calibration will be beyond the means of the SOCAT database QC group.

[b] Metadata must include description of calibration procedure and estimate accuracy of measurement.

Table 5. Recommendations for selection of platform types in the SOCAT LAS data query system and in metadata of individual datasets

Ships of opportunity	Default
Moorings	Selectable
Drifters	Selectable
Autonomous propelled surface vehicles	Selectable
Autonomous underwater vehicles	Not in SOCAT data holdings
Data from below 15 m depth	Not in SOCAT data holding

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Appendix A. SOCAT dataset flags for Versions 1 and 2

Table A1 provides the cruise quality control flags of the SOCAT database version 1.5 and version 2.0 (Pfeil et al., 2012). This serves as a reference for the proposed updates in flags as shown in Table 3.

Table A1. Criteria for cruise quality control flags of the SOCAT database version 1.5 and version 2.

Flag	Criteria
A (11)	(1) Followed approved methods/SOP[a] criteria (2) Metadata documentation complete (3) Extended[b] QC was deemed acceptable (4) A comparison with other data (cross-over) was deemed acceptable.
B (12)	(1) Followed approved methods/SOP criteria (2) Metadata documentation complete (3) Extended QC was deemed acceptable.
C (13)	(1) Did not follow approved methods/SOP criteria (2) Metadata documentation complete (3) Extended QC was deemed acceptable (including if possible comparison with other data).
D (14)	(1) Did or did not follow approved methods/SOP criteria (2) Metadata documentation incomplete (3) Extended QC was deemed acceptable (including if possible comparison with other data).
F (15)[c]	(1) Did or did not follow approved methods/SOP criteria and (2) Metadata documentation complete or incomplete and **(3)** Extended QC revealed non-acceptable data.
S (Suspend)[c]	(1) Did or did not follow methods/SOP criteria and (2) Metadata documentation complete or incomplete and (3) Extended QC revealed non-acceptable data and (4) Data are being updated (part or the entire cruise).
X (15)[c]	(Exclude) The cruise (dataset) duplicates another cruise (dataset) in SOCAT.
N (No flag)	Original submission, no cruise flag has yet been given to this cruise.
U (Update)	The cruise data have been updated by submitter. No cruise flag has yet been given to the revised data.

[a] SOP or Standard Operating Procedures following Dickson et al. 2007

[b] Listed as dataset QC in Table 3. It is also referred to as secondary QC or second level QC

[c] Not included in the release

Appendix B. Uncertainty in calculated fCO_{2w} based on uncertainties in equilibrator temperature, pressure and water vapor pressure.

The recommended approach for obtaining quality data is to measure the dried mole fraction (XCO_2) and use the pressure and temperature of equilibration along with sea surface temperature (SST) to determine the fCO_{2w} at SST. The fCO_{2w} is the primary variable in the SOCAT holdings. The sensor response to XCO_2 is calibrated with standard gases of CO_2 in air. The measurements from alternative sensors deviate from this approach, at minimum by measuring partially dried or moist air, or by determining the fCO_{2w} levels by different means (Table C1). An overall idea of sensitivity of the results to the temperature and pressure of equilibration, and to uncertainty in water vapor pressure (in case the measurement is not done dried) is provided in Figures 1 and B1. In case of the water vapor pressure, the interference of water vapor on the sensor is not taken into account.

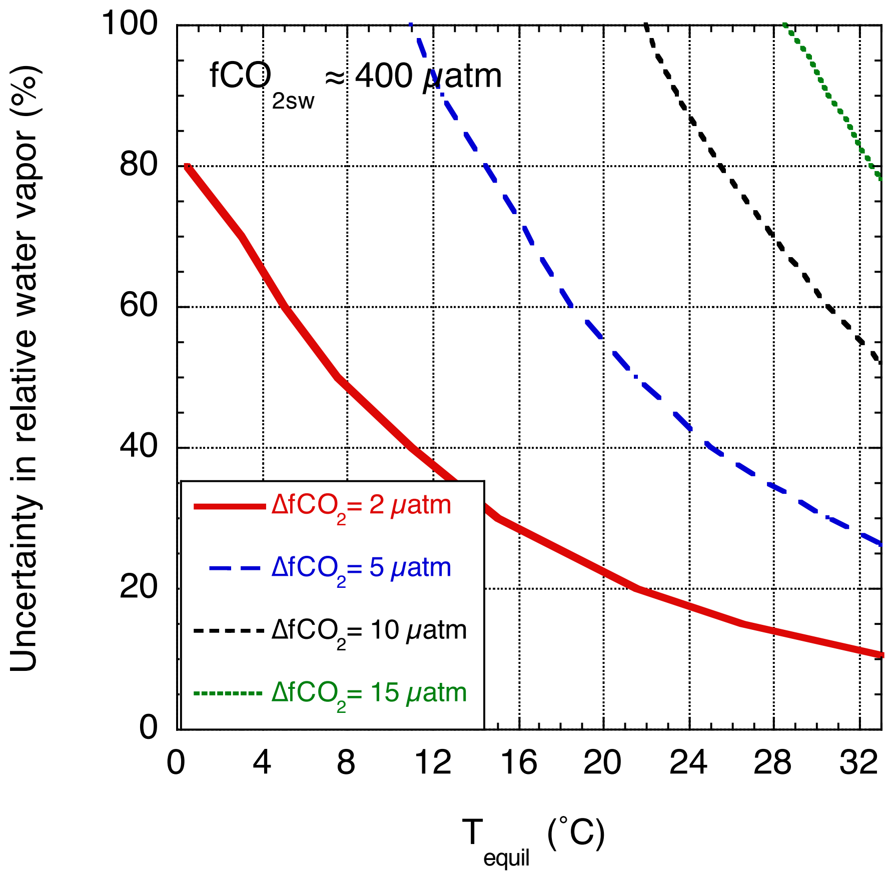

Figure B1. Uncertainty in calculated fCO_{2w} (ΔfCO_2) introduced by an uncertainty in water vapor content in headspace gas for fCO_{2w} levels of ≈ 400 µatm. Here is it assumed that the fCO_{2w} is calculated from the dried mole fraction of CO_2, XCO_2. For example, a 20% uncertainty in water vapor content at 20 ˚C will introduce a 2 µatm uncertainty in calculated fCO_2, while a 40 % uncertainty in water vapor content at 24 ˚C will introduce a 5 µatm uncertainty in ΔfCO_2.

Appendix C. Instrument specifications from company literature and other sources

The specifications of the sensors are often provided in sales literature of the manufacturers. The information from manufacturers as provided Table C1 has not been independently verified. Moreover, there often are upgrades and changes to instrumentation with time that change their accuracy and precisions. The method in which the accuracy is assessed is generally not specified. As noted in the footnotes of Table C1 sometimes the specification of individual components and/or XCO_2 is provided and we have estimated the overall accuracy of the calculated fCO_{2w} based on the manufacturers specification of the sub-components. The reported units vary and we infer that the specified mole fraction units (ppm) refer to dry gas and do not include uncertainties in pressure of equilibration, and water vapor correction in the accuracy estimate, where applicable. The values listed in Table C1 should not be used as the sole criteria of expected instrument performance at sea and these specified accuracies should not be used as sole criteria in assessing data quality flags. Table C2 provides an estimate of the accuracies based on a field studies and intercomparison exercises. Again they are provided for illustrative purposes and cannot be used for data QC purposes. Note that generally, but not always, the manufacturers specifications exceed the accuracies obtained in the field.

An overall conclusion is that the sensors do not meet the highest accuracy standards of ship-based infrared (IR) and gas chromatographic (GC) systems of 2 µatm.

Table C1. Specified or inferred accuracies of alternative sensors[a] based on manufacturer specifications.

Sensor	Accuracy	Resolution	Sensor measurement
CARIOCA[b]	3 µatm	1 µatm	pH
SAMI2 CO_2[c]	4 µatm	< 1 ppm	pH
Pro-Oceanus Incorporated CO_2-Pro[d]	2 µatm	< 0.01 ppm	xCO_2_wet[f]
Contros HydroC CO_2[e]	4 µatm	< 1 ppm	xCO_2_wet[f]
Seaology/MAPCO$_2$ sensor	2 µatm	< 0.01 ppm	xCO_2_partial dried[g]
SubCtech OceanPack[h]	<1.5%	0.01 ppm	xCO_2_wet

[a] The impact of changing atmospheric pressure on these sensors is not well determined.
[b] http://www.dt.insu.cnrs.fr/carioca/carioca.php and http://www.dt.insu.cnrs.fr/pco2/caract_capteur.php
[c] From website www.sunburstsensors.com: Range 150-700 ppm; precision < 1 ppm, response time 5 minutes, thermistor accuracy 0.1 ˚C.
[d] From website www.pro-oceanus.com: Accuracy: CO_2 concentration ±~ 2 ppm; Gas stream humidity ± 1 hPa; Gas stream pressure ± 2 hPa; Precision: CO_2 concentration 0.01 ppm; Calibration range 0-600 ppm (other ranges available by special order). Temperature range -2-35°C.
[e] From http://www.contros.eu/download/UserReportAndReferences.pdf. Accuracy is listed as ±1 % reading
[f] xCO_2 at 100 % relative humidity of the equilibration temperature
[g] Air passes through a Nafion dryer submerged in silica gel drying agent. Relative humidity ≈ 25 %. All cycles, including the gas standard run, pass through the Nafion dryer as well and will have similar relative humidity, thereby partially cancelling a humidity correction.
[h] From website subctech.eu.

Table C2. Comparison of alternative sensors with NDIR based equilibrator systems in field and laboratory studies.

Sensor	Agreement	Precision	Source
CARIOCA[a]	2-15 µatm		Bates et al. 2000[a]
CARIOCA2[b]	0- 3 µatm	0.5 µatm	Boutin et al 2008[b]
SAMI2 CO_2[c]	3 ppm	< 1 ppm	www.sunburstsensors.com/fs3.html
Pro-Oceanus Incorporated CO_2-Pro	5 µatm	< 0.01 ppm	[d]
Contros HydroC[e]	0.7 µatm		Fietzek 2013 et al.
Seaology/MAPCO2 sensor[f]	4 µatm	< 0.1 ppm	VanderMark et al. 2011
SubCtech OceanPack[g]	4 ppm	3.5 ppm	www.subctech.eu

Agreement: difference between sensor and a proven NDIR calibrated equilibrator system
Precision: RMSE between sensor and calibrated system
The units are those provided in the documentation

[a] This paper gives a comparison of CARIOCA and ship-based pCO_2 data that suggest offsets of up to 15 µatm that change over the two months summer and winter comparison periods. This CARIOCA did not have a third reference wavelength

[b] CARIOCA with a spectrophotometer reading a third (reference) wavelength

[c] http://www.sunburstsensors.com/fs3.html Ocean CO_2measurement system intercomparison (Tsukuba, Japan; March 2003)

[d] See the ACT evaluation report at http://www.act-us.info/Download/Evaluations/pCO2/Pro_Oceanus_Systems_PSI_CO2_Pro/).

[e] Fietzek et al. 2013.Three Contros sensors were [compared] tested against a GO pCO2 system during two research cruises and procedures for drift correction were developed. Along with in situ calibrations the average difference between sensor and reference was found to be -0.7 ± 3 µatm with a root mean square error of 3.7 µatm.

[f] Based on instrument LI-COR 820 specification; PMEL pre- and post-deployment calibrations; field validations of VandeMark et al. 2011; the 2009 Japan intercomparison; and the ACT evaluation report (http://www.act-us.info/Download/Evaluations/pCO2/PMEL_MAPCO2_Battelle_Seaology/).

[g] http://www.oceanoscientific.org/wp-content/uploads/2013/01/reportberichte-pco2-polarstern.pdf

Appendix D. A brief history of SOCAT

The following is a description of the SOCAT activities as provided at www.socat.info/about.html (IOCCP, 2007; Pfeil et al., 2012). SOCAT was initiated at the "Surface Ocean CO_2 Variability and Vulnerability" (SOCOVV) workshop at UNESCO (United Nations Educational, Scientific and Cultural Organization), Paris, in April 2007, co-sponsored by IOCCP (International Ocean Carbon Coordination Project), SOLAS (Surface Ocean Lower Atmosphere Study), IMBER (Integrated Marine Biogeochemistry and Ecosystem Research), and the Global Carbon Project. The meeting participants agreed to establish a global surface CO_2 dataset that would bring together all publicly available fCO_{2w} data for the surface oceans in a common format. The fugacity of carbon dioxide, or fCO_2, is the partial pressure of CO_2 (pCO_2) corrected for non-ideal behavior of the gas. This is an activity that has been called for by several international groups, and has now become a priority activity for the marine carbon community. The dataset will serve as a foundation upon which the community will continue to build in the future, based on agreed data and metadata formats and standard quality-control procedures, building on earlier agreements established at the 2004 Tsukuba workshop on "Ocean Surface pCO_2 Data Integration and Database Development". This activity also supports the SOLAS and IMBER science plans and their joint carbon implementation plan.

This dataset is meant to serve a wide range of user communities and two distinct data products are available in this Surface Ocean CO_2 Atlas (SOCAT):

- A second level quality controlled global surface ocean fCO_{2w} dataset following agreed procedures and regional review (Pfeil et al. 2012).
- A gridded SOCAT product of monthly surface water fCO_{2w} means on a 1° x 1° grid with no temporal or spatial interpolation (Sabine et al. 2012).

The extended first level quality-controlled dataset builds on the work started in 2001 as part of the EU ORFOIS project and continues as part of the EU CarboOcean and CarboChange projects, where Benjamin Pfeil and Are Olsen (Bjerknes Centre for Climate research, University of Bergen, Norway), have compiled the publicly-available surface CO_2 data held at CDIAC (Carbon Dioxide Information Analysis Center), WDC-MARE (World Data Center for Marine Environmental Sciences) and from individual investigators into a common format database based on the IOCCP recommended formats for metadata and data reporting. The first SOCAT compilation (version 1.5) includes data from more than 10 countries, producing an initial database composed of 1851 cruises from 1968 to 2007 with approximately 6.3 million surface ocean CO_2 measurements, available in a common format, quality-controlled dataset. This dataset (version 1.5) was published in September 2011. Release of version 2 containing over 10 million data points occurred in June 2013.