SOCAT Quality Control Cookbook
- For version 2025 of the Surface Ocean CO_2 Atlas -

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Table of Contents

1 Context for the cookbook update

This is the SOCAT quality control (QC) cookbook for SOCAT version 2025. It is an update to the cookbooks for version 1 (Olsen and Metzl, 2009), version 3 (Olsen et al., 2015; Wanninkhof et al., 2013) and version 2019 (version 7) (Lauvset et al., 2018). It incorporates the data set quality control flags defined in earlier cookbooks and reflects community discussions during the 2023 Surface Ocean pCO_2 Workshop at the Flanders Marine Institute (VLIZ), Oostende, Belgium (IOCCP, 2024; Steinhoff et al., 2024). This document focuses on the quality control of a submitted dataset and does not provide information on how to upload data to SOCAT.

This revision aims to maintain the quality and integrity of the SOCAT synthesis and gridded products. The outcomes of the 2021 pCO_2 instrument intercomparison at VLIZ (Steinhoff et al., 2025) indicate that membrane-based sensors, including those with calibration gases, do not have a consistent uncertainty of less than 5 µatm, for reasons that we do not understand. This provides compelling justification for not assigning a flag of C to any membrane-based systems in SOCAT.

In general, calibration gases for membrane-based systems are deemed to be a good thing. SOCAT would support a broader discussion by the community on how to improve membrane-based systems and their performance. SOCAT would welcome the development of Standard Operating Procedures (SOP) for membrane-based systems by users of such systems. If new evidence of consistent performance of membrane-based systems becomes available, the cookbook will be revised accordingly.

SOCAT aims to make the flag E datasets more visible.

SOCAT contains surface water fCO_2 measurements made by instruments (sensors/ systems) that directly measure dissolved CO_2 (concentration, partial pressure). It does not contain subsets of measurements collected by profiling instruments. SOCAT has (semi-)continuous CO_2 measurements, not discrete CO_2 measurements (from discrete samples) except for a small number of historic data sets. SOCAT products do not include fCO_2 calculated from other carbon variables, such as pH, alkalinity, and dissolved inorganic carbon (Bakker et al., 2014, 2016).

1.1 Main changes

The major differences and updates, compared to the previous version of the SOCAT QC cookbook are:

- Flags A-C are only for systems with air – water equilibration.
- Membrane-based sensors and other sensors, making direct measurements of surface ocean CO_2, will receive a flag of E, if flag E criteria are met.
- Flag D (incomplete metadata) will not be used for new and updated submissions.
- Flag D (incomplete metadata) may still be assigned to historic equilibrator-based data sets using gas chromatography (GC), non-dispersive infrared (NDIR) detection, or

laser-technology (such as cavity ring-down spectroscopy, or CRDS), when metadata cannot be completed anymore (e.g. where the PI is no longer active), at the discretion of the SOCAT global group.

- Datasets with incomplete metadata will be suspended (flag S). Metadata of such datasets can be updated at any time and after that the dataset must be resubmitted to SOCAT for re-evaluation. If this update happens after the yearly deadline for data submission, the dataset will be assigned to next year's QC round.
- Information has been added on what constitutes a high-quality cross-over in the cross-over and on how to evaluate whether a cross-over is of high - quality.
- Terminology of accuracy has been replaced by uncertainty, as the latter characterizes the quality of the measurements better. Uncertainty does not have a mathematical definition, but according to the VIM guide (International Vocabulary of Metrology) (JCGM, 2012) it is a parameter associated with the results of a measurement, and that characterizes the dispersion of the values that could reasonably be attributed to the measured quality. In SOCAT it can be understood as a confidence interval.
- Air-water equilibrator-based systems are now systematically referred to as such.
- Alternative sensors have been renamed to membrane-based sensors, to distinguish them from air-water equilibrator-based systems.
- The table of data set quality control flags (Table 1) has been expanded to include all criteria, including those discussed later in the cookbook.
- The cookbook has been reorganized for greater clarity.

There is no intention to retrospectively, nor retroactively implement the revised quality control criteria for data sets already published in previous SOCAT versions. Consistent quality control and adequate quality control comments fully justifying all quality control steps are extremely important (SOCAT, 2014).

2 SOCAT quality control

The SOCAT quality control process leads to the following:

- A quality control flag with an estimated uncertainty is assigned to each data set
- Each (re-)calculated fCO_2 (fCO_2rec) value of each data set is given a WOCE flag 2 (good), 3 (questionable), or 4 (bad).

Only data sets with a flag of A, B, C, D or E will be included in the SOCAT data products. The synthesis and gridded data products include data sets with a flag of A to D and fCO_2rec values with a WOCE flag of 2 (Table 8 in Bakker et al., 2016).

2.1 Defining data set quality control flags

The data set quality control flags provide information on the expected quality of each data set and must be assigned to each data set in the quality control process. To assign the data set flag, it is necessary to evaluate both the data and metadata. The quality control criteria for the data set flags of A to E are in Table 1.

Table 1. Data set quality control flags for SOCAT version 2025 and later. All criteria need to be met for assigning a flag of A to E. The uncertainty takes precedence over the criteria that follow.

Flag	Criteria[a]	Section in document
A	**For direct air-water equilibrator-based NDIR, GC, CRDS, and other laser-based detector[b] systems only** (1-9) Meets all the criteria of Flag B plus (10) A high-quality cross-over[c,d] with another data set (also flagged A or B) is available.	2.2.1; 2.3.1.1; 2.4
B	**For direct air-water equilibrator-based NDIR, GC, CRDS, and other laser-based detector systems only** (1) Uncertainty of calculated fCO_2rec (at SST[e]) is less than 2 µatm (2) Followed the SOP criteria[f] for equilibrator-based systems (3) Metadata documentation complete (4) Data set QC is deemed acceptable. (5) Overall warming or cooling between in situ (SST) and measurement (Teq) is less than 1 °C. (6) The calibration included at least two non-zero gas standards which can be referenced to the WMO mole fraction scale. (7) The standard gases should cover the range of observed concentrations. However, up to 20% of the observations may be outside the standard gas range. (8) Both temperatures (SST and Teq) measured to within 0.05 °C uncertainty. (9) Absolute equilibrator pressure (via direct measurement or calculated via differential pressure) measured to within 2 hPa uncertainty.	2.2.1; 2.3.1.1
C	**For direct air-water equilibrator-based NDIR, GC, CRDS, and other laser-based detector systems only** (1) Uncertainty of fCO_2rec (at SST) is less than 5 µatm (2) Did not follow the SOP criteria for equilibrator-based systems (3) Metadata documentation complete (4) Data set QC is deemed acceptable. (5) Overall warming or cooling between in situ (SST) and measurement (Teq) is less than 3°C. (6) At least two calibration gases were used, one of which can be a zero gas (natural or artificial air with CO2 removed, N2 gas or generated from a CO2 scrubber cartridge filled with soda lime). (7) The standard gases should cover the range of observed concentrations and be referenced to the WMO mole fraction scale. However, up to 20% of the observations may be outside the standard gas range. (8) Both temperatures (SST and Teq) measured to within 0.2 °C uncertainty (9) Absolute equilibrator pressure (via direct measurement or calculated via differential pressure) measured to within 5 hPa uncertainty.	2.2.1; 2.3.1.2
D	**Closed for new and updated data sets from version 2025 onwards** (Retained for historical equilibrator-based data sets with GC, NDIR, CRDS, or other laser-based detectors and may be applied on a case-by-case basis) (1) Uncertainty of fCO_2rec (at SST) is less than 5 µatm. (2) Did or did not follow the SOP criteria for equilibrator-based systems (3) Metadata documentation incomplete. (4) Data set QC is deemed acceptable. (5) Overall warming or cooling between in situ (SST) and measurement (Teq) is less than 3 °C.	2.2.1; 2.3.1.3
E	**For membrane-based systems and sensors** (1) Uncertainty of calculated fCO_2rec (at SST) is less than 10 µatm. (2) Followed best practice for membrane-based systems. (3) Metadata documentation complete.	2.3.1.3; 2.3.2.1

	(4) Data set QC is deemed acceptable. (5) Overall warming or cooling between in situ (SST) and the membrane is less than 3 °C. (6) The intake seawater temperature (SST) has been measured to within 0.2 °C uncertainty. (7) The equilibration temperature (Teq) near the membrane, if available, has been measured to within 0.2 °C uncertainty. If not available, there needs to be a robust explanation on how the temperature near the equilibration membrane was estimated, and what the resulting uncertainty is. (8) The pressure at the gas side of the membrane is measured to within 5 hPa uncertainty.	
E	**For other systems** (1) Uncertainty of calculated *f*CO_2rec (at SST) is less than 10 µatm (2) Did not follow SOP criteria for equilibrator-based systems (3) Metadata documentation complete (4) Data set QC is deemed acceptable. (5) Overall warming or cooling between in situ (SST) and measurement (Teq) is less than 3 °C. (6) The intake seawater temperature (SST) has been measured to within 0.2 °C uncertainty. (7) The equilibration temperature (Teq), if available, has been measured to within 0.2 °C uncertainty. (8) The equilibration pressure is measured to within 5 hPa uncertainty.	
S (Suspend)	Some or all of the following apply: (1) More information is needed for data set before a flag can be assigned (2) Data set QC reveals non-acceptable data. (3) Metadata documentation not complete (except for some historical data sets) (4) Data set is being updated	3.5
X (Exclude)	The data set duplicates another data set in SOCAT, has no surface CO_2 data, or is considered of unacceptable quality.	
N (New)	A data set submitted to SOCAT that has not undergone independent data set quality control.	
U (Updated)	A data set re-submitted to SOCAT following updates by the data provider. The data set will be quality controlled as if new.	
Q	A data set with conflicting data set flags, usually different flags in different regions	

[a]The uncertainty takes precedence over the criteria that follow.

[b]NDIR for non-dispersive infrared detection, GC for gas chromatography and CRDS for cavity ringdown spectroscopy

[c]For a high-quality cross-over, both data sets need to have an overall uncertainty for *f*CO_2rec of less than 2 µatm (Flag of A or B). A high-quality cross-over is defined as a cross-over between two data sets with a maximum cross-over equivalent distance of 80 km, a maximum difference in sea surface temperature of 0.3°C and a maximum *f*CO_2rec difference of 5 µatm. Inconclusive cross-overs, defined as having a temperature difference greater than 0.3°C or a *f*CO_2rec difference exceeding 5 µatm, do not receive a flag of A.

[d]A cross-over between two data sets is defined as an equivalent distance of less than 80 km. This criterion combines distance (in km) and time (in days) as $([dx^2 + (30\ dt)^2]^{0.5}) \le 80$ km. One day of separation in time is equivalent (heuristically) to 30 km of separation in space.

[e]SST or sea surface temperature.

[f]SOP or Standard Operating Procedure amended from Dickson et al. (2007)

2.2 Key considerations for data set quality control flags

SOCAT contains surface water fCO_2 measurements made by instruments (sensors/ systems) that directly measure dissolved CO_2 (concentration, partial pressure). It does not contain subsets of measurements collected by profiling instruments. SOCAT has (semi-)continuous CO_2 measurements, not discrete CO_2 measurements (from discrete samples) except for a small number of historic data sets. SOCAT products do not include fCO_2 calculated from other carbon variables, such as pH, alkalinity, and dissolved inorganic carbon (Bakker et al., 2014, 2016).

The data submitter or principal investigator (PI) should deliver datasets that have been quality controlled and have been flagged according to the WOCE QC system (Swift and Diggs, 2008). It is recommended that the PI indicates the QC flag that the dataset can receive in SOCAT, however this will not dictate the assignment of the SOCAT QC flag. The SOCAT quality controller (QCer) will evaluate the data set and assign a SOCAT QC flag. The SOCAT QC flag can be better or worse than the flag indicated by the PI.

2.2.1 Direct air-water equilibrator-based systems

Direct air – water equilibrator-based systems that are well-designed, well-operated, and maintained can produce the highest quality data (Pierrot et al., 2009).

The **SOP (Standard Operating Procedure) criteria for equilibrator-based systems** follow the methodology suggested by Dickson et al. (2007), Pierrot et al. (2009), Pfeil et al. (2013), and Bakker et al. (2016). The main criteria are:

1. The data are based on xCO_2 analysis, not on fCO_2 calculated from other carbon variables, including pH, total alkalinity, and dissolved inorganic carbon.
2. Continuous CO_2 measurements have been made, not discrete CO_2 measurements.
3. The detection is based on a system using direct air – water equilibration and is measured by infrared analysis, gas chromatography, cavity ring-down spectroscopy, or another laser-based method.
4. The calibration has included at least two non-zero gas standards traceable to World Meteorological Organization standard gases (WMO scale), which bracket at least 80% of the measured data.
5. The equilibrator temperature (Teq) has been measured to the necessary uncertainty (Table 1).
6. The intake seawater temperature (SST) has been measured to necessary uncertainty (Table 1) .
7. The absolute equilibrator pressure (Peq) has been measured to the necessary uncertainty (Table 1). Many equilibrator-based instruments only have a differential sensor in the equilibrator itself, and an external pressure sensor (often the LI-COR internal pressure sensor) is used to estimate the absolute pressure:
   $$P_{eq_{ABS}} = \Delta P_{eq} + P_{Atm}$$
   If this is the case, then the absolute equilibrator pressure is a sum of two sensors, so the uncertainty of both (alternatively the combined uncertainty of both) must be

documented, as well as the estimation of the total uncertainty based on uncertainty propagation equations[1].

2.2.2 Membrane-based systems

Membrane-based systems are increasingly popular for seawater CO_2 measurements as they are relatively easy to use, affordable and fairly small. They can be used on fixed or moving platforms and can operate in continuous mode or sample periodically but frequently enough so that they can produce adequate time-series records. However, it is still difficult to fully characterize their performance and have high confidence in the quality of the final data, even if the system uses gas reference standards to check the detector and to correct the data (Steinhoff et al. 2025).

For this reason and until there is solid evidence of the quality of these data, such data should receive a flag of E, provided the criteria listed in Table 1 and discussed in sections 2.2.3.2 and 2.3.2 are met.

2.2.3 Metadata evaluation

Data set flags of A, B, C and E require **complete** metadata documentation. Metadata requirements differ between platforms and sensors. The details of the measurement system, uncertainty of sensors and the calibration of the measurements and sensors should be fully documented in the metadata, and the SOCAT QCer needs to go through them meticulously, before assigning the data set QC flag and WOCE flags.

2.2.3.1 Required metadata for direct air – water equilibrator-based systems using NDIR, GC, CRDS, or other laser-based detectors

Complete metadata, as described in Pfeil et al. (2013) have **all** the following information:

1. The investigator
2. The vessel
3. The temporal coverage
4. Detailed description of the analytical method (either in the metadata form or as a suitable reference)
5. The type(s) of reported CO_2 data (xCO_2, pCO_2, fCO_2)
6. The number of CO_2 standards used with their CO_2 molar fraction and documented traceability to WMO standards
7. For primary standard gases: calibration laboratory and bottle numbers
8. For secondary standard gases: method of calibration, calibration laboratory for primary standards used
9. A list of sensors
10. Documented uncertainty, including how this is determined, for:
    a. The CO_2 analyzer
    b. The equilibrator temperature

[1] Based on the equation z = x±y, if δx and δy are the reported uncertainties then the total uncertainty $\delta z = (\delta x^2 + \delta y^2)^{1/2}$

c. The seawater intake temperature
d. The equilibrator pressure

11. Frequency of standard gas measurements. For NDIR detectors, it is necessary to inform when the detector had a zero and span calibration.
12. Documentation that the range covered by the standard gases bracket the observed xCO_2 range. More than 80% of the data should be within the range of the standard gases.
13. Documented fulfillment of all other SOP criteria.

2.2.3.2 Required metadata for membrane-based systems and sensors

Complete metadata for membrane-based systems have **all** the following information:

1. The investigator
2. The vessel
3. The temporal coverage
4. Detailed description of the analytical method (either in the metadata form or as a suitable reference). If specific procedures exist for the use and data processing of the membrane sensor, these should be documented (as a suitable reference) and there should be a clear description how these have been followed.
5. The type(s) of reported CO_2 data (xCO_2, pCO_2, fCO_2)
6. A clear description of the calibration of the CO_2 measurements:
   Information on the calibration (where, when, frequency, how), e.g. *in situ*, pre-deployment and/or post-deployment, laboratory tests, comparison to another instrument
7. The number of CO_2 standard gases used with their approximate CO_2 molar fraction and documented traceability to WMO standards
8. For primary standard gases: calibration laboratory and bottle numbers
9. For secondary standard gases: method of calibration and calibration laboratory for primary standards used
10. A list of all the sensors that produce values that are used for the CO_2 measurements, their documented uncertainty (especially for any temperature and pressure sensors), including how this is defined and calculated and frequency of their calibration.

2.2.4 Assessment of overall fCO_2 uncertainty

Overall uncertainty of the fCO_2 data, including the method or equations used to determine this, should be documented in the metadata. Type of instrumentation, accuracy of the temperature and pressure measurements, and the difference (usually warming) between the *in situ* and measurement temperature, all affect the overall uncertainty. Use the temperature checks outlined in Section 2.5 as a guide to assess the warming between *in situ* and measurement.

Influence of the uncertainty of temperature and pressure on overall fCO_2 uncertainty

The uncertainty in seawater fCO_2 due to an uncertainty in temperature is:
$\Delta fCO_2 = fCO_2\,(1-e^{-(0.0423\,\Delta T)})$ (T in °C)

The uncertainty in fCO_2 due to an uncertainty in pressure is:

$\Delta fCO_2 = xCO_2\, \Delta P$ (P in atm)

Figure 1 (from Wanninkhof et al., 2013) below shows isopleths of uncertainty in calculated fCO_2 (ΔfCO_2) arising from uncertainty in the temperature (T_{equil}, elsewhere Teq) and pressure (P_{equil}, elsewhere Peq) of equilibration, respectively. For equilibrator-based systems, the uncertainty in the *in situ* (SST) and equilibrator (T_{eq}) temperatures and the measurement pressure (i.e. equilibration pressure, Peq) needs to be documented and evaluated to assess the overall uncertainty of fCO_2.

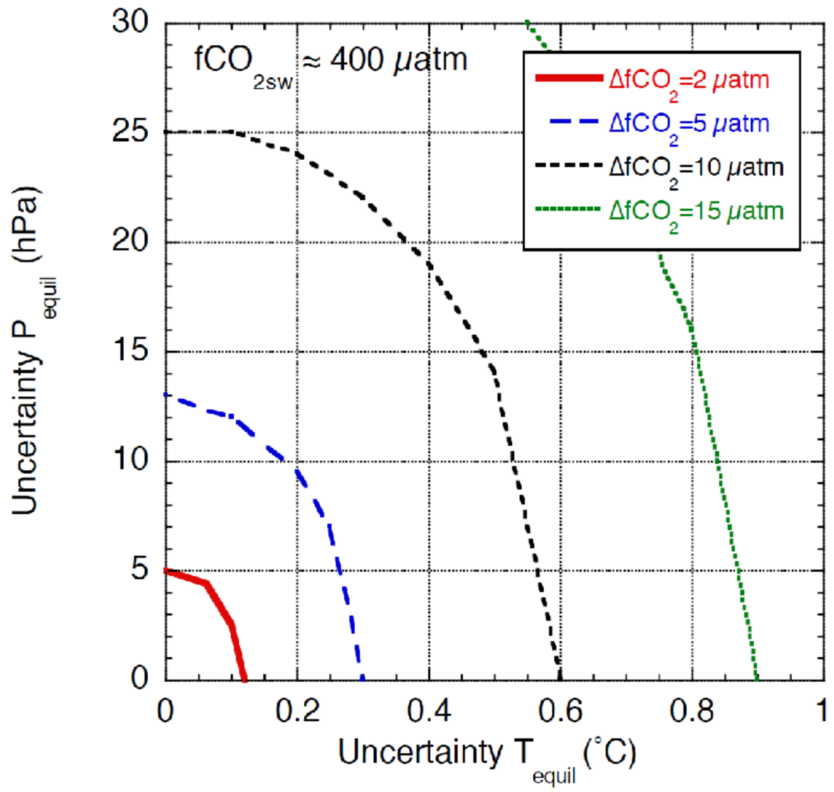

Figure 1. The impact of uncertainties in temperature and pressure on fCO_2 (from Wanninkhof et al., 2013)

2.3 Assigning data set flags using uncertainty

2.3.1 Direct air – water equilibrator-based NDIR, GC, CRDS, and laser-based detector systems only

2.3.1.1 Flags A and B

For an uncertainty estimate of less than 2 µatm (A or B):

- All the criteria in Table 1 for Flags A or B must be met, including:
- The SOP criteria for equilibrator-based systems listed in section 2.2.1 must be fulfilled and properly documented.
- Warming or cooling between in situ (SST) and equilibration temperature (Teq) should be less than 1 °C.

Surface water *fCO_2* data have an uncertainty of 2 µatm or less if approved methods and the seven SOP criteria mentioned in section 2.2.1 are followed (Pfeil et al., 2013; Wanninkhof et al., 2013; Bakker et al., 2016). These criteria were defined for continuous ship-based measurements of surface water fCO_2, using non-dispersive infrared (NDIR) analysis or gas chromatography (GC). The same criteria apply to measurements by cavity ring-down spectroscopy (CRDS) and other laser-based detection (Bakker et al., 2014).

Based on a comprehensive uncertainty and sensitivity analysis (Humphreys, 2024), it is estimated that a correction of 1 °C warming adds an uncertainty of ~1 µatm to the final fCO_{2rec} for fCO_2 of around 400 µatm.

Assigning Flag B:
Flag B is assigned to datasets that fulfill all the above criteria and where cross-over has not been detected or where the cross-over is inconclusive (ΔfCO_{2rec} > 5 µatm, ΔSST > 0.3 °C).

Assigning Flag A:
Flag A is assigned to datasets that fulfill all the above criteria and there is a conclusive high-quality cross-over.

When a high quality cross-over is found between a dataset in the new SOCAT version with a data set (with flag B) in a previous SOCAT version, the older B flag dataset is not re-QCed to receive an A flag. Only the new data set will receive an A flag.

2.3.1.2 Flag C

For an uncertainty estimate of less than 5 µatm (C):
All the criteria for a Flag of C in Table 1 must be met, including:

- Direct air-water equilibration, coupled to a NDIR, GC, CRDS, or another laser-based detector
- Two calibration gases, one of which can be a zero gas. The non-zero gas should span the entire range observed in fCO_2 for more than 80% of the data coverage.
- Both temperatures (SST and Teq) must be measured to within 0.2 °C uncertainty, and absolute equilibrator pressure (calculated via differential pressure or direct measurement) has been measured to within 5 hPa uncertainty.
- The warming or cooling between SST and Teq should be less than 3 °C.
- In addition, all other SOP as given above are fulfilled and properly documented in the metadata.
- For systems using direct air-water equilibration that are installed on autonomous platforms or moorings, the Sutton et al. (2014) reference describes the main principle of these systems and how they perform.

2.3.1.3 Flag D

For an uncertainty estimate of less than 5 µatm (D):
A flag of D can be assigned in exceptional cases for a historic data set with incomplete metadata, where the PI is no longer active in the field. Here the quality controller contacts a

member of the global group, active in SOCAT QC, for their input. The flag D will be assigned on a case-by-case basis.

2.3.1.4 Flag E

For an uncertainty estimate of less than 10 µatm (E):
Data from direct – air water equilibration systems that have complete metadata but do not meet the criteria for a Flag of A, B, or C should be assigned with an E flag.

2.3.2 Sensors and systems with membrane-based equilibration

2.3.2.1 Flag E

For an uncertainty estimate of less than 10 µatm (E):
All the criteria for a Flag of E in Table 1 must be met, including:

- Laboratory, pre-deployment, or post-deployment tests of the membrane-based sensors need to provide an estimate that an uncertainty of less than 10 µatm is obtained in the (re-)calculated fCO_2 value (Wanninkhof et al., 2013, Arruda et al., 2020, Macovei et al., 2021).
- Well documented, best practice procedures for the use of the membrane-based system and for the processing of its data, with complete references to, for example, a peer-reviewed, published paper, and the manufacturer's manual.
- Metadata documentation is complete, including a clear and detailed description of the calibration, including the frequency of calibration. The metadata needs to document how the uncertainty of the CO_2 values has been estimated.
- Data set QC is deemed acceptable.
- The temperature difference between *in situ* (SST) and measurement (membrane) is less than 3 °C.
- The intake seawater temperature (SST) has been measured to ± 0.2 °C.
- The pressure at the gas side of the membrane is measured to ± 5 hPa.

In addition, the following is highly recommended:

- Daily or more frequent *in situ* (i.e. when the instrument is operating in its natural environment) calibration with at least two calibration gases, one of which can be a zero gas. The non-zero gas must span the range observed in fCO_2 for more than 80% of the data coverage.

Membrane-based sensors need complete metadata to assess the overall uncertainty in fCO_2rec (see section 2.2.1). Table 2 in Wanninkhof et al. (2013) and Steinhoff et al. (2025) have information on how commonly used sensors have performed in (field and laboratory) comparison studies.

2.4 Evaluation of a high-quality cross-over

- A high-quality cross-over with another data set is required for a flag of A.

The Live Access Server software identifies **potential** high-quality cross-overs, where specific criteria for temperature and *f*CO_2rec differences (see below) are met for at least one data point. However, many potential high-quality cross-overs are 'inconclusive' cross-overs, as they are not representative for the data set, occur in heterogeneous waters (e.g. coastal waters or near-sea ice) or this one point is an outlier. Therefore, **each potential high-quality cross-over must be evaluated** by the quality controller to establish whether it is a high-quality cross-over or an inconclusive cross-over.

A **cross-over** between two data sets is defined as an "equivalent" distance of less than 80 km (Table 1). The cross-over algorithm combines distance (in km) and time (in days) as $([dx^2 + (30\ dt)^2]^{0.5}) \leq 80$ km (Pfeil et al., 2013; Wanninkhof et al., 2013). One day of separation in time is equivalent (heuristically) to 30 km of separation in space.

A high-quality cross-over (after Wanninkhof et al., 2013) meets the following criteria:

- It is a cross-over between two data sets with a maximum cross-over equivalent distance of 80 km.
- Both data sets have an overall uncertainty for *f*CO_2rec of less than 2 µatm (Flag of A or B).
- It has a maximum difference in sea surface temperature of 0.3 °C.
- It has a maximum difference in *f*CO_2rec of 5 µatm.

A flag of A requires the presence of a high-quality cross-over (Wanninkhof et al., 2013). A flag of A will only be assigned if **both data sets** involved in the cross-over have an overall *f*CO_2rec uncertainty of **less than 2 µatm (Flag of A or B)**. This must be verified by the quality controller.

Inconclusive cross-overs, where one of the data sets does not have a flag of A or B, or with a sea surface temperature difference greater than 0.3 °C or a *f*CO_2rec difference exceeding 5 µatm, do not receive a flag of A. High-quality cross-overs are rare in heterogeneous coastal waters and near-sea ice.

If a conclusive high-quality cross-over is found between a new dataset and one with a B flag in a previous SOCAT version, only the new dataset will receive an A flag. The B flag of the older dataset will not be upgraded to A.

The specific method of this cross-over evaluation varies between QC operators, but most like to grab a subset of the latitude/longitude figure that first appears and then plot *f*CO_2rec versus time, before examining properties (sea surface temperature, *f*CO_2) versus latitude or longitude are examined to determine the quality of the crossover. See section 3.4 for further details.

2.5 WOCE Flags

Data set QC needs to be deemed acceptable for flags of A to E.

All (re-)calculated *f*CO_2 values receive a WOCE flag of 2 (good), 3 (questionable) or 4 (bad) with 2 as the default setting. This allows inclusion of data sets with some questionable or bad

fCO_2 values in SOCAT. Surface water fCO_2 values can be bad for several reasons (e.g. erroneous position or time, unrealistic *in situ* or measurement temperatures, large temperature difference between *in situ* and measurement, etc). Using WOCE flags enables retaining the data set, with identification of any questionable or bad data via the flags of 3 or 4 in a traceable way.

All data sets submitted to SOCAT should have passed primary QC by the data provider. Therefore, if more than 5% of the data appear to need a WOCE flag other than 2, the quality controller should pass the data set back to the data provider for additional primary QC.

SOCAT quality controllers only carry out quality control for surface water fCO_2 and only flag (re-)calculated fCO_2 values. Other variables do not receive WOCE flags. Other variables, such as salinity and sea surface temperature are checked only to the extent relevant for (re-)calculation of surface water fCO_2 (SOCAT, 2014). Of these, temperature is the most important for the (re-)calculation of fCO_2 values, so there are some defined quality control criteria for temperature to consider.

Additional temperature-based quality assessment

The following six quality control criteria should be considered for open ocean data away from sea ice and large freshwater outflows (Bakker et al., 2014). The criteria are based on the temperature change between the seawater intake and the equilibrator or membrane:

1. For data sets to receive a flag of A or B, the difference between the SST and the Teq should be less than 1 ^{o}C.
2. For data sets to receive a flag of C or E, the difference between the SST and the Teq should be less than 3 ^{o}C
3. The warming or cooling rate should be less than 1 °C h^{-1}, unless a sharp temperature front is apparent.
4. Warming and cooling outliers should be less than 0.3 °C, compared to background data.
5. Cooling between the seawater intake and the equilibrator or membrane is unlikely in high-latitude oceans for an indoor measurement system.
6. Zero or constant temperature change may indicate absence of sea surface temperature values
7. The difference between intake and equilibrator temperatures should be relatively constant in time (i.e. no discernible trend).

The above features may apply for some data points, in which case appropriate WOCE flags should be assigned to those specific points, or for a whole data set, in which case it is appropriate for the quality controller to discuss the quality concerns with the data provider.

3 Quality control in practice

3.1 Starting quality control

Regional groups carry out quality control. Discuss with your regional group which data sets you will quality control. QCers are encouraged to see the video in the SOCAT help section (also available as a YouTube link), demonstrating the main parts of the QC process.

The quality control system resides at PMEL's Live Access Server. Enter the quality control system at http://access.pmel.noaa.gov/SOCAT using your username and password. Contact Kevin O' Brien (kevin.m.o'brien@noaa.gov), if you have forgotten these.
Use the LAS tools to find the data set you will quality control (Fig. 2).

Quality control the data set either online using the LAS tools or download the whole data set and carry out the QC offline using your favorite software. You need to **quality control the full data set, not a sub-selection of the data set**. This applies both to online quality control and to data download.

When using LAS for quality control, increase the performance and speed of the system by reducing the number of data sets shown on the main LAS user interface, for example by selecting a particular data set by Expocode, or by constraining in space and/or time.

The full data set files and History of Quality Control for each data set can be accessed by pressing the "Table of Datasets" button on the main LAS interface.

Using the LAS interface for assigning quality control flags for data sets and WOCE flags for individual fCO_2 measurements is described in sections 3.2 and 3.3. The main steps and considerations for a cross-over analysis, when a cross-over is detected by the automated cross-over check, are outlined in Section 3.4. Suspending a data set is covered in Section 3.5

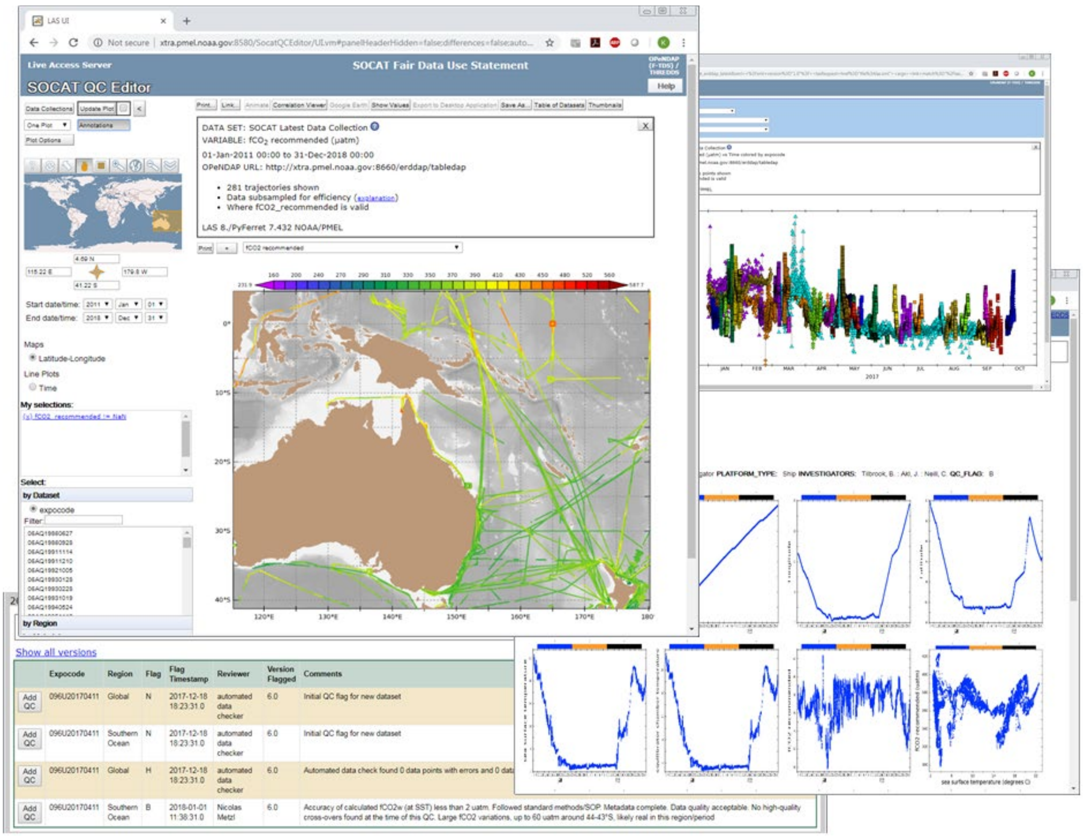

Figure 2. A selection of quality control tools in the SOCAT Live Access Server, including the main LAS user interface, the Correlation Viewer, the Thumbnail Viewer, and the History of Quality Control.

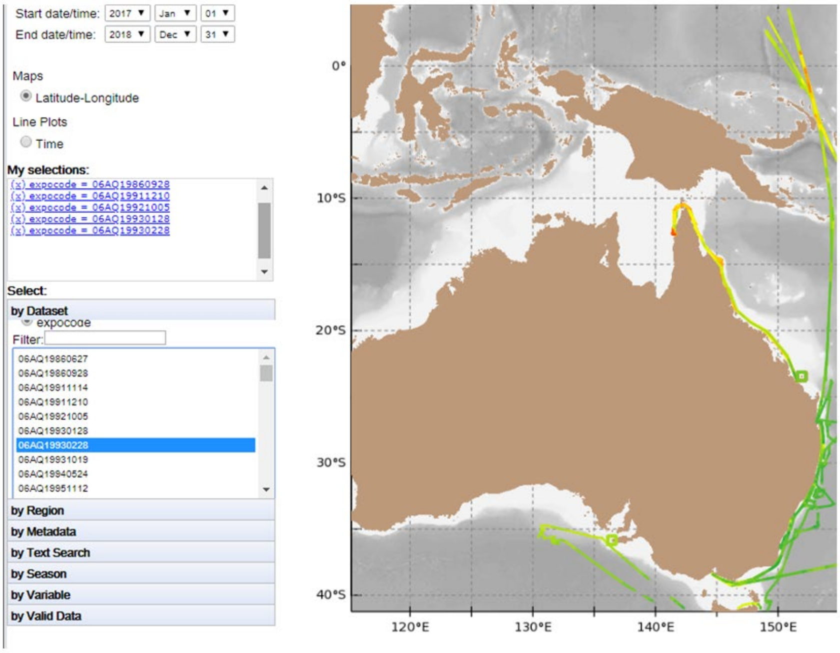

Figure 3. Selection of individual data set from the Expocode filter on the main user interface of the SOCAT LAS.

3.2 Assigning data set QC flags and adding QC comments

When you have completed quality control and you are ready to assign the data set quality control flag:

1. Find your data set in the main LAS user interface page by filtering on Expocode (Figs. 3).
2. Once you have limited the user interface to a single Expocode (Fig. 3), click the "Table of Datasets" button in the top bar.
3. Press the "Edit the QC Flag" link and you will arrive at a listing of the history of QC for this data set (Fig. 2).
4. To modify the QC flag, click the "Submit QC" button (some data sets may have several, one for each region the data set covers, remember to select your region).
5. In the pop-up window specify:
   - Region (drop down menu);
     Note: Selecting the Global region will cause all other region flags to be overridden. Only Global group members should set the Global flag.
   - Uncertainty of calculated aqueous fCO_2 (at SST);
   - Whether approved methods/SOP criteria were followed;
   - Metadata documentation completeness;
   - Data quality;
   - High-quality crossovers and associated Expocode(s);
   - QC flag (drop down menu);
   - Enter your comment for this data set. The comment should adequately justify the choice of the flag. There is a character limit, so make a copy before you submit.
6. After you have pressed the "Submit this QC evaluation" button in the pop-up window, this window can be closed.

Each of the input choices made above will result in a comment in the "Complete QC comment" box. This is to ensure a complete comment is associated with the data set QC flag. You are encouraged to enter additional comments in the "Complete QC comment" box.

Quality control comments should be adequate and fully justify a data set quality control flag (SOCAT, 2014). An adequate record of why a data set passed (or failed) certain quality control criteria is critical, so that another quality controller or the data provider can assess how the initial quality controller came to their conclusion and exactly what was checked. For example, **comments should be entered on the completeness of the metadata, on the variables that have been checked (most critical are fCO$_2$rec, SST and ΔT) and on each crossover check, regardless of whether the crossover is conclusive or inconclusive (while noting the Expocode).** Appendix 1 lists examples of adequate and poor data set quality control comments.

3.3 Assigning WOCE flags in practice

In addition to the data set quality control flags, assign WOCE flags for individual re-calculated fCO$_2$ values in each data file. Initially all fCO$_2$ values are assumed to be of good quality (WOCE flag of 2). Assign flags of 3 or 4 to any questionable or bad fCO$_2$ values and provide adequate comments on why WOCE flags of 3 or 4 were selected. If more than 5% of the data need to be assigned flags 3 or 4, the entire data set should be passed back to the data provider for additional primary QC.

WOCE flags are set in the SOCAT QC Live Access Server through the Correlation Viewer tool. There are several ways to launch the Correlation Viewer tool:
1. Select the "Correlation Viewer" on the LAS main user interface;
2. Click on an individual plot window in the "Thumbnails" tool;
3. Click on the Expocode of a potential crossover cruise in the "Table of Cruises".

It is recommended to limit the number of cruises selected in the main LAS user interface to improve performance of the system. An added benefit to reducing the subset of selected Expocodes is that the Correlation Viewer will create a unique icon for each Expocode display on the figure (Fig. 4). This will make it easier to identify data by their Expocode.

Once in the Correlation Viewer, to set the WOCE flag for individual fCO$_2$rec values, the user should select the values they wish to alter the WOCE flag on the plot by dragging a rectangle over the desired data points, and then clicking the "Edit Flags" button in the upper left corner (Fig. 4).

In "Edit Flags" mode, it is possible to assign new WOCE flags to one or many fCO$_2$rec values (Fig. 5). Before saving the modified WOCE flags, the quality controller should submit a detailed and clear comment to explain the reason for the WOCE value assignment. Entry of a comment is a prerequisite for saving the new WOCE flags.

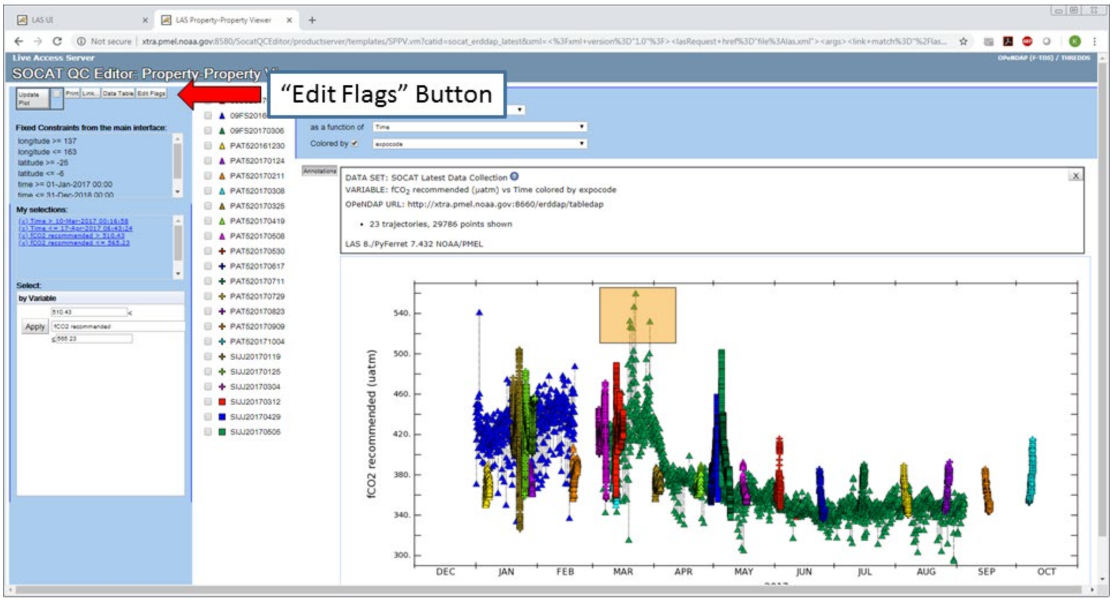

Figure 4. The SOCAT LAS Correlation Viewer with selected data sets and values, with the “Edit Flags” button in the upper left corner.

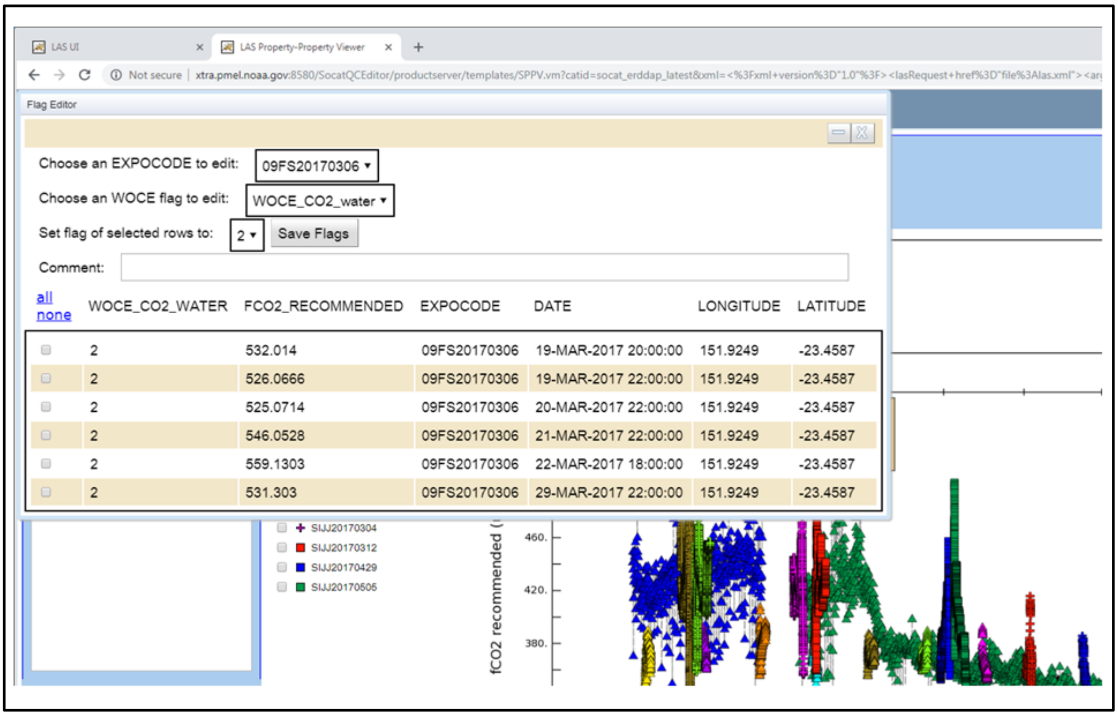

Figure 5. The WOCE flag editing tool in the SOCAT LAS.

3.4 Evaluation of a cross-over in practice

All data sets submitted to SOCAT will be checked for a cross-over with any dataset from any SOCAT version. The selection algorithm is described in previous sections (Footnote to Table 1 and Section 2.4). This algorithm is based only on a time - space separation between the datasets, and it does not include checks of any variables relevant for the

quality of the cross-over (e.g. *f*CO_2rec, Teq, SST, data set flag). The evaluation of whether a conclusive high-quality cross-over is present is up to the QCer!
The current cross-over selection criteria are selected based on open ocean physical characteristics and dynamics. Cross-overs in very dynamic environments like coastal regions or close to sea ice can be challenging and are in most cases inconclusive. The QCer needs to evaluate this.

The basic steps are described below.

- Select the area of interest and click on the "Table of Datasets" button (Fig. 6).
- A table (Table 2) will come up.
- Click on the 'Check for crossovers' link.
- Any cross-overs will appear as expocodes underlined, which when clicked will bring up a longitude - latitude map with the positions of the two datasets (one in blue the other in red) (Fig. 7). The cyan encircled star shows the position of the cross-over.
- The QCer can now start looking at various plots of fCO_2rec as a function of time, SST, latitude and longitude to assess the quality of the cross-over.
- Select an area that can be zoomed in to better identify the cross-over (Fig. 8).
- Only data sets that meet the criteria for a high-quality crossover (a maximum difference in sea surface temperature of 0.3 °C and a maximum difference in *f*CO_2rec of 5 µatm), should be assigned a flag of A (Section 2.4).

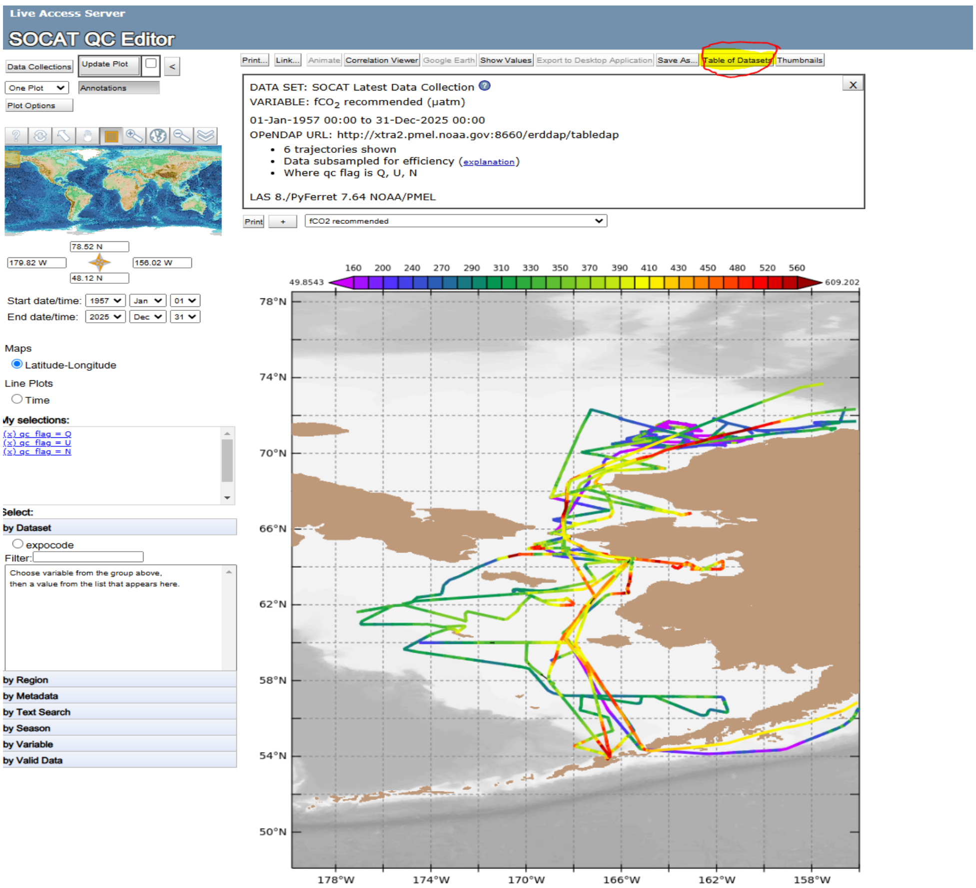

Figure 6. Area where quality control is being carried out with selection of the Table of Datasets button (yellow highlight) in the top bar.

Table 2. Table of data sets for the area where quality control is being carried out. The 'Check for crossovers' link is highlighted. If this is clicked on, any cross-overs will appear as expocodes underlined.

expocode	platform_name	platform_type	investigators	qc_flag	socat_version	documentation	download	crossovers	qc flags	thumbnails
32DB20160709	Waveglider0004_Bering	Autonomous Surface Vehicle	Monacci N.M. : Battisti R. : Cross J.N. : Maenner-Jones S. : Sutton A.	N	2025.0N	Documentation	Save As...	33BI20160827 33HO20160630	Examine QC Flags	Thumbnails
33BI20230606	R/V Sikuliaq	Ship	Sweeney C. : Newberger T. : Munro D.R.	N	2025.0N	Documentation	Save As...	none	Examine QC Flags	Thumbnails
33BI20230616	R/V Sikuliaq	Ship	Sweeney C. : Newberger T. : Munro D.R.	N	2025.0N	Documentation	Save As...	none	Examine QC Flags	Thumbnails
33BI20230807	R/V Sikuliaq	Ship	Sweeney C. : Newberger T. : Munro D.R.	N	2025.0N	Documentation	Save As...	none	Examine QC Flags	Thumbnails
33BI20230910	R/V Sikuliaq	Ship	Sweeney C. : Newberger T. : Munro D.R.	N	2025.0N	Documentation	Save As...	Check for crossovers	Examine QC Flags	Thumbnails
33BI20231023	R/V Sikuliaq	Ship	Sweeney C. : Newberger T. : Munro D.R.	N	2025.0N	Documentation	Save As...	Check for crossovers	Examine QC Flags	Thumbnails

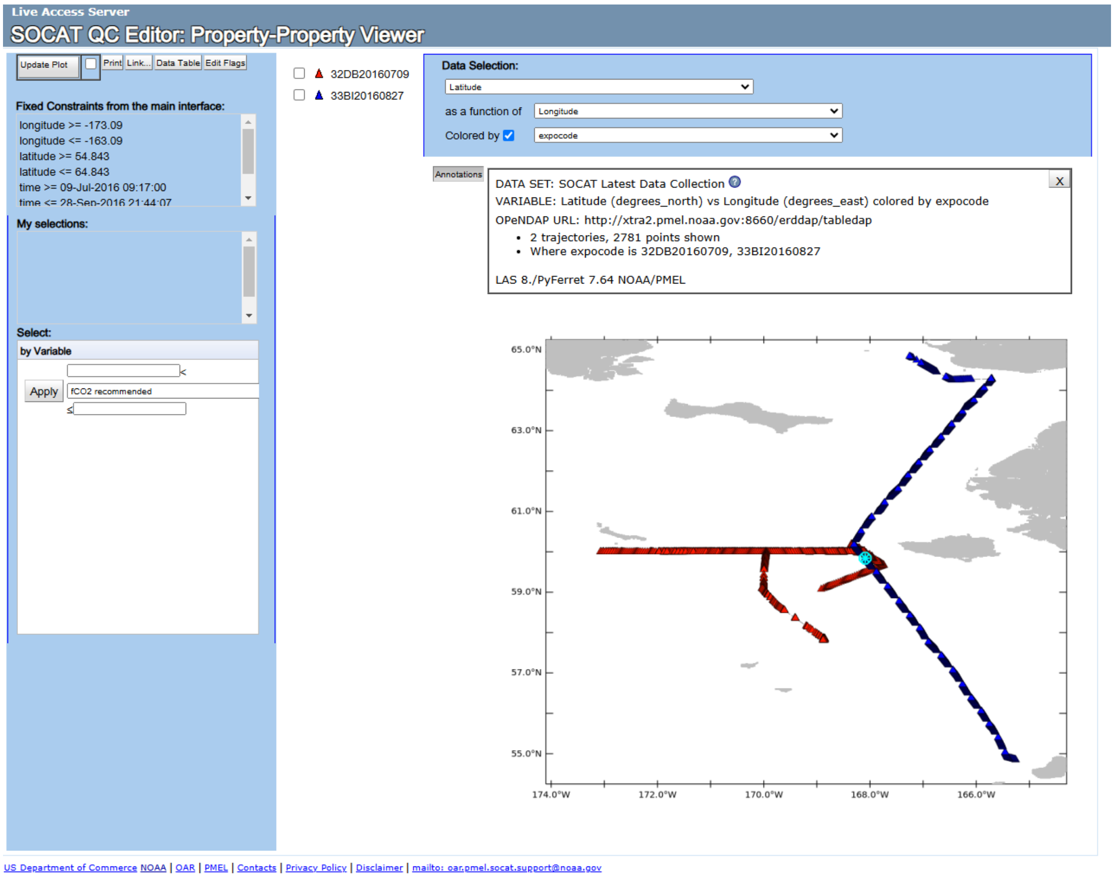

Figure 7. A map with the two data sets and the location of the cross-over (cyan encircled star).

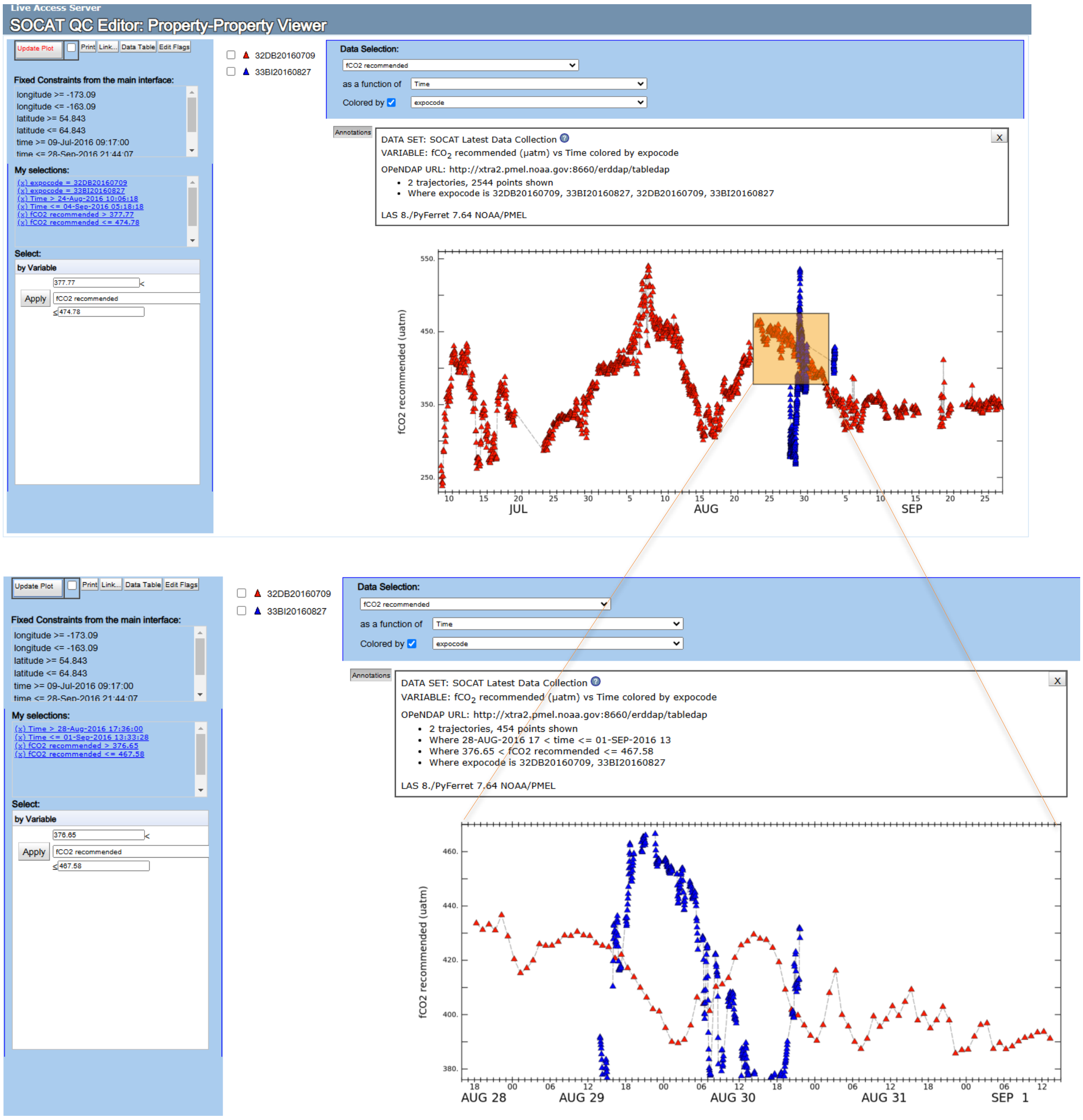

Figure 8. A diagram of fCO₂rec over time for the two data sets with a cross-over.

3.5 Suspending data sets in practice

If the data quality of a data set is not deemed acceptable, set the data set quality control flag to suspend ('S) and add a clear comment why the data set has been suspended. It is good practice to politely discuss the likely suspension of a data set with the data provider. In many cases the data provider has insights on suspected quality control issues (e.g. the absence of sea surface temperature). The data provider should always be encouraged to resubmit updated data and metadata.

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Appendix 1: Examples of quality control comments

The examples (adapted from SOCAT, 2014) below of adequate and poor quality control comments in SOCAT version 3 have been inspired by quality control comments in the Table of Cruises on the Data Set Viewer and have been adjusted to the revision of data set quality control flags in version 3. All relevant quality control comments should be entered on the quality control system. Abbreviations are: Peq – equilibrator pressure, SST – sea surface temperature, Teq – equilibrator temperature, SOP – standard operating procedures.

Examples of adequate quality control comments in version 3.

1) Flag A. The system follows SOP criteria. Metadata is complete, includes information on calibration and uncertainty of SST, Teq and Peq. The data quality looks good. The 55 km crossover with 49UU20201010 (Flag B) is high-quality with a SST difference of 0.2°C and a fCO_2rec difference of 4 µatm between both cruises.
2) Flag B. The system follows SOP criteria. The metadata is complete. The data quality looks good. The 55 km cross-over with 58XX2021212 (Flag B) is inconclusive with different SST (2°C) and fCO_2rec (50 µatm) on both data sets.
3) Flag C. Metadata complete. A flag C was given because 1) the uncertainty of pCO_2/fCO_2 (3 µatm) did not meet the SOP criteria (2 µatm) and the 2) Equilibrator temperature was not within 0.05°C. The data quality was deemed acceptable.
4) Flag D. The metadata do not state the uncertainty of Peq and Teq. Data quality looks good. Inconclusive 55 km cross-over with 06AA20200202 (Flag A) in Channel: Very different SST (6°C) and fCO_2rec (50 µatm) on 2 cruises.
5) Flag E. The measurements have been made with a spectrophotometric sensor with no in situ calibration gases but having pre-deployment calibration with documented uncertainty better than 10 µatm. The system does not follow SOP criteria. The metadata is complete and includes adequate information on pre-deployment calibration. The data quality was deemed acceptable.
6) Flag S. File lacks surface water CO_2 measurements. The data provider has been consulted.
7) Flag S. SST has not been reported, such that Teq was used in calculation of fCO_2rec. Data set suspended in consultation with data provider.
8) Flag X. This data set overlaps with data set 11FF20200808. This is an older version of the same data set. The data provider has been consulted.

Examples of poor, inadequate quality control comments:

1) Flag A. No comment.
   (*Lacks comments on high-quality cross-over, SOP criteria and metadata.*)
2) Flag B. Data looks good.
   (*Lacks comments on SOP criteria and metadata*.)
3) Flag C. Discrepancy in intake temperature and salinity of actual intake and ship sensors may lead to offsets.
   (*Lacks a comment on data quality deemed acceptable and metadata complete*).
4) Flag D. Metadata incomplete.
   (*Lacks a comment on data quality deemed acceptable, what is missing in metadata.*)
5) Flag E. A spectrophotometric sensor has been used.
   (*Lacks a comment on uncertainty of pre-deployment calibration, metadata complete, data quality.*)
6) Flag S. Data quality not good.
   (*Lacks an explanation of the nature of the problem. Has the data provider been consulted?*)
7) Flag X. This data set overlaps with another data set.
   (Which other data set? Has the data provider been consulted?)