SOCAT Quality Control Cookbook
-For SOCAT version 7-

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1 Context

This is the SOCAT quality control (QC) cookbook for SOCAT version 7. It is an update to the cookbook for version 1 (Olsen and Metzl, 2009) and version 3 (Olsen et al., 2015; Wanninkhof et al., 2013). It incorporates the revision of the data set quality control flags for version 3 (Wanninkhof et al., 2013), quality control procedures defined for versions 1 and 2 (Pfeil et al., 2013; Bakker et al., 2014), recommendations from the SOCAT Community Event on 23 June 2014 (SOCAT, 2014), and updates as discussed at the SOCAT event at ICDC10 in September 2017.

There is no intention to retrospectively implement the revised quality control criteria for data sets in SOCAT versions 1-6. Consistent quality control and the adequate quality control comments fully justifying all quality control steps are extremely important (SOCAT, 2014).

Compared to the previous version of the SOCAT cookbook, the major differences in criteria are:

- For flags A and B (accuracy estimate of better than 2 µatm) the overall warming between in situ and measurement should be <1 °C.
- For flags C and D (accuracy estimate of better than 5 µatm) the non-zero standard gas should preferably cover the entire range of observations, but the observations can be up to 20% outside the certified standard gas value.

2 The SOCAT quality control

The SOCAT quality control process leads to the following:

- A data set quality control flag 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 and E will be included in the SOCAT data products. Some data products only include data sets with a flag of A to D. Only fCO_2rec values with a WOCE flag of 2 are included as default in the synthesis products (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. One can summarize the quality control criteria for the data set flags of A to E as follows (Table 1):

Table 1. Data set quality control flags for SOCAT version 3 and later. All criteria need to be met for assigning a flag of A to E.

Flag	Criteria[a]
A	(1) Accuracy of calculated fCO_2rec (at SST[b]) is better than 2 µatm. (2) A high-quality cross-over[c,d] with another data set (also flagged A or B) is available. (3) Followed approved methods/SOP[e] criteria. (4) Metadata documentation complete. (5) Data set QC was deemed acceptable.
B	(1) Accuracy of calculated fCO_2rec (at SST) is better than 2 µatm. (2) Followed approved methods/SOP criteria. (3) Metadata documentation complete. (4) Data set QC was deemed acceptable.
C	(1) Accuracy of calculated fCO_2rec (at SST) is better than 5 µatm. (2) Did not follow approved methods/SOP criteria. (3) Metadata documentation complete. (4) Data set QC was deemed acceptable.
D	(1) Accuracy of calculated fCO_2rec (at SST) is better than 5 µatm. (2) Did or did not follow approved methods/SOP criteria. (3) Metadata documentation incomplete. (4) Data set QC was deemed acceptable.
E	(Primarily for alternative sensors) (1) Accuracy of calculated fCO_2rec (at SST) is better than 10 µatm. (2) Did not follow approved methods/SOP criteria. (3) Metadata documentation complete. (4) Data set QC was deemed acceptable.
S (Suspend)	(1) More information is needed for data set before flag can be assigned (2) Data set QC revealed non-acceptable data and (3) Data are being updated (part or the entire data set).
X (Exclude)	The data set duplicates another data set in SOCAT.
N (New)	Data submitted to SOCAT that has not undergone independent data set quality control.
U (Updated)	Data re-submitted to SOCAT following updates by the data provider. Will be quality controlled as if new.
Q	A data set with conflicting flags, usually different flags in different regions.

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

[b]SST or sea surface temperature.

[c]A high-quality cross-over is defined in version 3, 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 fCO_2rec difference of 5 µatm. Inconclusive cross-overs, defined as having a temperature difference greater than 0.3°C or a fCO_2rec difference exceeding 5 µatm, will not have a flag A.

[d]A cross-over is defined as a distance of less than 80 km. This criterion combines distance and time 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]SOP or Standard Operating Procedure following Dickson et al. (2007).

2.2 Assigning data set quality control flags

2.2.1 Only Surface water fCO_2 measurements

SOCAT products do not include fCO_2 calculated from other carbon parameters, such as pH, alkalinity or dissolved inorganic carbon (Bakker et al., 2014, 2016). SOCAT contains surface water fCO_2 measurements made by surface water instruments. It does not contain subsets of measurements collected by profiling instruments.

2.2.2 Assessment of overall fCO_2 accuracy

- The accuracy of (re-)calculated fCO_2 is better than 2 µatm for flags of A and B, better than 5 µatm for C and D, and better than 10 µatm for E.

Overall accuracy of the fCO_2 data, including the method 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 accuracy. Use the temperature checks outlined in section 2.3 as a guide to assess the warming between *in situ* and measurement.

For an accuracy estimate of better than 2 µatm (A or B):

- The seven standard operating procedures (SOP) must all be fulfilled and properly documented.
- In addition, warming between in situ and measurement should be <1 °C.

The seven SOP criteria below all need to be met, and properly documented in the metadata, for a flag of A or B (SOP criteria updated from Wanninkhof et al., 2013; Bakker et al., 2016). Surface water fCO_2 data have an accuracy of 2 µatm or better if approved methods or SOP criteria are followed (Pfeil et al., 2013). 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) (Bakker et al., 2014).
Based on a comprehensive error analysis performed by ICOS OTC (Battisti et al., 2018), it is estimated that the correction of 1 °C warming adds an uncertainty of ~1 µatm to the final fCO_2. Therefore, the overall accuracy can only be estimated to better than 2 µatm if the warming between in situ and measurement is less than 1 °C.

<u>Seven SOP criteria</u>:

1. The data are based on xCO_2 analysis, not fCO_2 calculated from other carbon parameters, such as pH, alkalinity or dissolved inorganic carbon;
2. Continuous CO_2 measurements have been made, not discrete CO_2 measurements;
3. The detection is based on an equilibrator system and is measured by infrared analysis, or gas chromatography or cavity ring-down spectroscopy;
4. The calibration has included at least two non-zero gas standards, traceable to World Meteorological Organisation (WMO) standards, which bracket the observed range in xCO_2;
5. The equilibrator temperature has been measured to within 0.05 °C accuracy;
6. The intake seawater temperature has been measured to within 0.05 °C accuracy;

7. The absolute equilibrator pressure has been measured to within 2 hPa accuracy. Note that many equilibrator-based instruments only have a differential sensor in the equilibrator itself, and an external pressure sensor (often the LiCor pressure sensor) is used to estimate the absolute pressure (i.e., abs_equ_pressure = diff_equ_pressure + abs_lab_pressure). If this is the case then the absolute equilibrator pressure is a sum of two sensors so the accuracy of both (alternatively the combined accuracy of both) must be documented.

In addition, **warming between in situ and measurement should be <1 °C** as explained above.

For an accuracy estimate of better than 5 µatm (C or D) the criteria differ depending on type of instrumentation:

- Shipboard NDIR, gas chromatographs and CRDS systems must have:
  - Two calibration gases, one of which can be a zero gas. The non-zero gas should span nearly the entire range observed in fCO_2 (i.e. the observations cannot be >20% outside the certified standard gas value).
  - Both temperatures must be measured to within 0.2 °C accuracy, and absolute equilibrator pressure has been measured to within 5 hPa accuracy.
  - **The warming between in situ and measurement should be <3°C**.
  - In addition, all other SOP as given above are fulfilled and properly documented in the metadata.
- Alternative sensors need to have:
  - 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.
  - A clear and detailed description of the calibration (including the frequency of it) needs to be provided in the metadata.

For an accuracy estimate of better than 10 µatm (E):

- Laboratory and pre- or post-deployment tests of the alternative sensors need to provide a general estimate that an accuracy of better than 10 µatm is obtained in the (re-)calculated fCO_2 value (Wanninkhof et al., 2013).
- The metadata need to document how the accuracy of the sensor has been determined.

Alternative sensors need sufficient metadata to assess the overall accuracy (see section 2.2.4). In addition, Table 2 in Wanninkhof et al. (2013) and the IOCCP website (www.ioccp.org/index.php/instruments-and-sensors#pco2) provide information on how commonly used sensors have performed in (field and laboratory) comparison studies. Sutton et al. (2014) is a good reference for the performance of the MAPCO2 system.

Influence of temperature and pressure accuracies on overall fCO_2 accuracy

The uncertainty in seawater fCO_2 due to an uncertainty in temperature is:

$\Delta fCO_2 = fCO_2 \, e^{-(0.0423 \, \Delta T)}$

The uncertainty in fCO_{2w} due to an uncertainty in pressure is:

$\Delta fCO_2 = xCO_2 \, \Delta P$.

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}) and pressure (P_{equil}) of equilibration, respectively. For equilibrator-based systems, the uncertainty in the *in situ* and measurement temperatures and the measurement pressure needs to be evaluated in order to assess the overall accuracy of fCO_2.

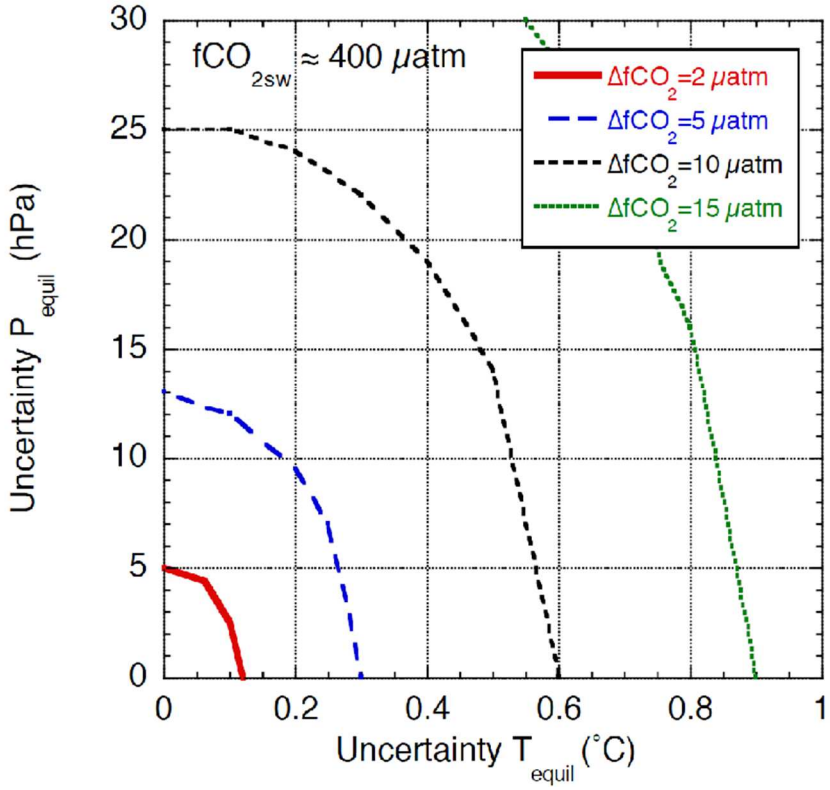

Figure 1. The impact of uncertainties in temperature and pressure on fCO_2 (from Wanninkhof et al., 2013).

2.2.3 Assessment of potential high-quality cross-overs

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

A flag of A requires the presence of a high-quality cross-over (Wanninkhof et al., 2013). A cross-over between two data sets is defined as a distance of less than 80 km. The cross-over algorithm combines distance and time 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 (Wanninkhof et al., 2013):

- Is a cross-over between two data sets, each with an overall accuracy for fCO_2rec of better than 2 µatm, with a maximum cross-over equivalent distance of 80 km,
- Has a maximum difference in sea surface temperature of 0.3°C and
- Has a maximum fCO_2rec difference of 5 µatm.

A flag of A will only be assigned if both data sets involved in the cross-over have an overall fCO_2 accuracy of better than 2 µatm. 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 fCO_2rec difference exceeding 5 µatm, will not receive a flag of A.

The LAS (Live Access Server) software automatically identifies potential high-quality cross-overs, i.e. instances where the above criteria for the temperature and fCO_2rec differences are met for at least one point. However, this one point could be an outlier, so each potential cross-over must be evaluated by the quality controller to ensure that this cross-over is representative of the data set. The specific method of this evaluation varies between QC operators, but most like to grab a subset of the latitude/longitude plot that first appears and then plot fCO_2 versus time before properties (temperature, fCO_2) versus latitude or longitude are examined to determine the quality of the crossover.

2.2.4. Metadata evaluation

- SOP criteria (see section 2.2.2) need to be met for a flag of A or B.
- Flags of A, B, C and E require complete metadata documentation. Metadata requirements differ between platforms and sensors.

Required metadata for NDIR, GC or CRDS

Complete metadata for measurements by NDIR, GC or CRDS contains all this information (Pfeil et al., 2013):

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 of reported CO_2 data (xCO_2, pCO_2, fCO_2);
6. The number of CO_2 standards used with their approximate CO_2 mixing ratio and documented traceability to WMO standards;
    a. For primary standards: calibration laboratory and bottle numbers;
    b. For secondary standards: method of calibration, calibration laboratory for primary standards used;
7. A list of sensors;
8. Documented accuracy, including how this is determined, for:
    a. The equilibrator and seawater intake temperature;
    b. The equilibrator pressure;
9. Frequency of calibration;
10. Documentation that the range covered by the standard gases bracket the observed xCO_2 range;
11. Documented fulfilment of all other SOPs.

Required metadata for alternative sensors and platforms

Complete metadata for alternative sensors and platforms contains 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 of reported CO_2 data (xCO_2, pCO_2, fCO_2);
6. A clear description of the calibration of alternative sensors:
    a. Information on the calibration (where, when, frequency, how), e.g. *in situ*, pre- and/or post-deployment, laboratory tests, comparison to another instrument;
    b. If used as a calibration method, the number of CO_2 standards used with approximate CO_2 mixing ratio and documented traceability to WMO standards;
    c. Accuracy obtained during the calibration;
7. A list of all sensors and their documented accuracy (especially any temperature and pressure sensors);
8. If SOPs exist for the alternative sensor these should be documented (as a suitable reference) and fulfilled.

2.3 WOCE Flags

- Data set quality control needs to be deemed acceptable for flags of A-E.

All (re-)calculated fCO_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. 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). 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).

All data sets submitted to SOCAT should have passed primary QC by the data provider. Therefore, if >5% of the data looks 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 parameters do not have WOCE flags. Other parameters, such as salinity and sea surface temperature are checked only in as far as this is relevant for (re-)calculation of surface water fCO_2 (SOCAT, 2014). Of these, temperature is the most important for the (re-)calculation 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:

1. Warming should be less than 3 °C;

2. The warming rate should be less than 1 °C h^{-1}, unless a sharp temperature front is apparent;
3. Warming outliers should be less than 0.3 °C, compared to background data;
4. Cooling between the seawater intake and the equilibrator is unlikely in high-latitude oceans for an indoor measurement system;
5. Zero or constant temperature change may indicate absence of sea surface temperature values;
6. 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 lead which data sets you will quality control.

The quality control system resides at PMEL's Live Access Server (LAS). Enter the quality control system at http://access.pmel.noaa.gov/SOCAT using your username and password. Contact Karl Smith (karl.smith@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 ensure that you 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.

For quality control on the LAS:
Increase the performance of the system by reducing the number of cruises shown on the main LAS user interface, for example by selecting a particular cruise by Expocode, or by constraining in space and/or time.

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

Sections 3.2 and 3.3 describe using the LAS interface for assigning quality control flags for data sets and WOCE flags for individual fCO_2 measurements.

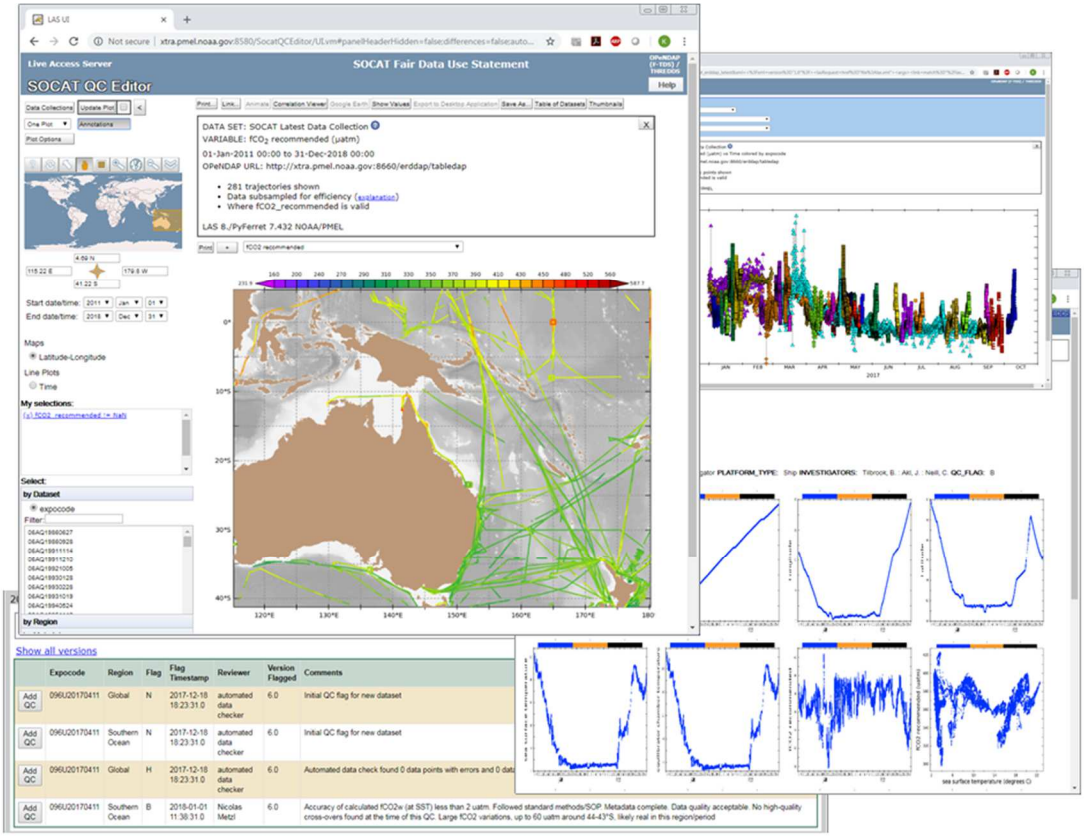

Figure 2. A selection of quality control tools in the LAS for SOCAT version 3, including the main LAS user interface, the Correlation Viewer, the Thumbnail Viewer and the History of Quality Control.

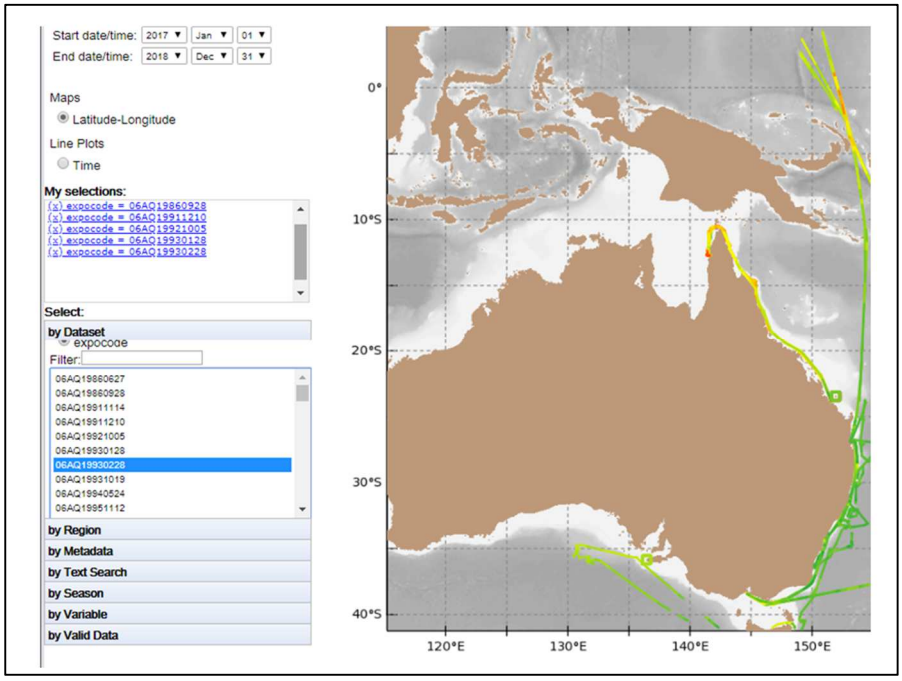

Figure 3. Selection of individual cruises from the Expocode filter on the main user interface of the SOCAT LAS.

3.2 Assigning data set quality control flags and quality control 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. 2, 3).
2. Once you have limited the user interface to only a single Expocode (Fig. 3), click the "Table of Cruises" button.
3. Press the "Edit the QC Flag" link and you will arrive at a listing of the history of QC for this cruise (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.
    - Accuracy of calculated aqueous fCO_2 (at SST);
    - Whether approved methods/SOP criteria were followed;
    - Metadata Documentation completeness;
    - Data Quality;
    - High value crossovers and associated Expocode(s);
    - QC flag (drop down menu);
    - Enter your comment for this data set. The comment should adequately justify choice of the flag.
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 each property check, on each crossover check (while noting the Expocode) and on the adequacy of the metadata.** Appendix 1 lists examples of adequate and poor data set quality control comments.

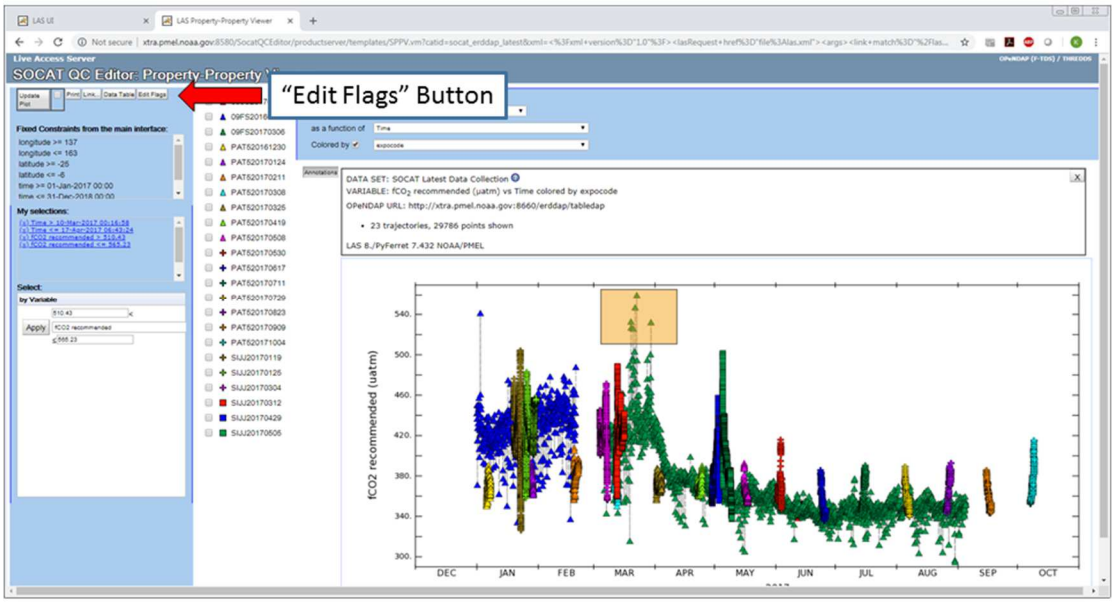

Figure 4. The SOCAT LAS Correlation Viewer with selected data sets and values, while demonstrating location of "Edit Flags" button in upper left corner.

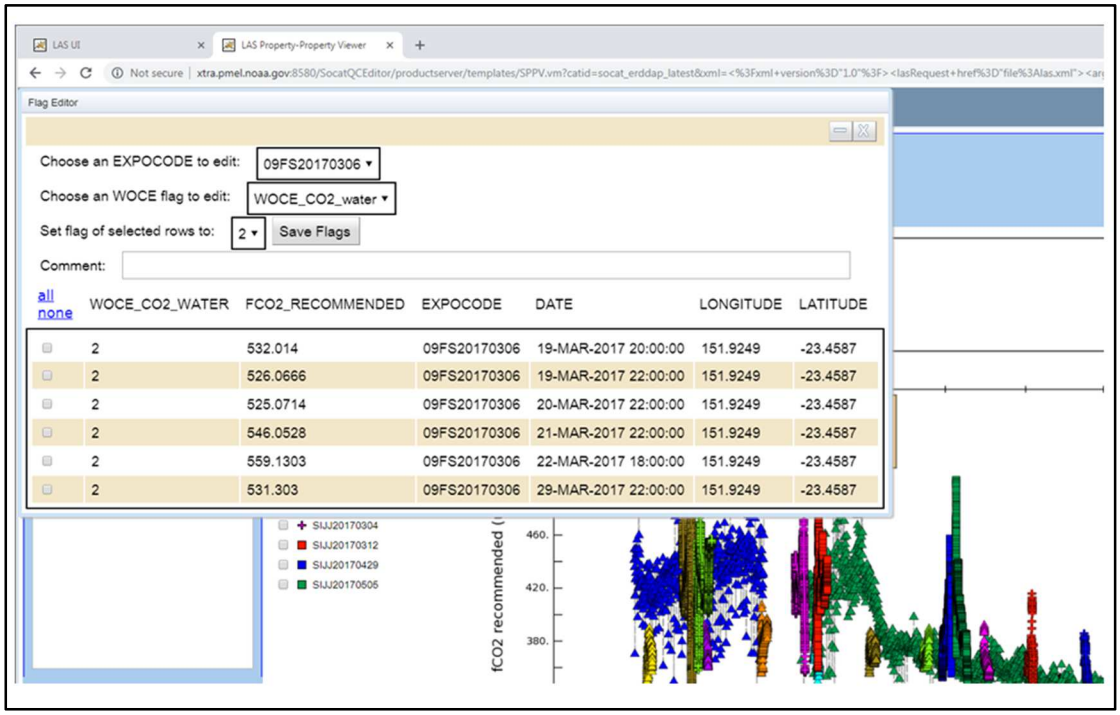

Figure 5. The WOCE flag editing tool in the SOCAT LAS.

3.3 Assigning WOCE Flags

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 >5% of the

data needs 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_2rec 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_2rec 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.

3.4 Suspending data sets

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.

References

Bakker, D. C. E., Pfeil, B., Smith, K., Hankin, S., Olsen, A., Alin, S. R., Cosca, C., Harasawa, S., Kozyr, A., Nojiri, Y., O'Brien, K. M., Schuster, U., Telszewski, M., Tilbrook, B., Wada, C., Akl, J., Barbero, L., Bates, N. R., Boutin, J., Bozec, Y., Cai, W.-J., Castle, R. D., Chavez, F. P., Chen, L., Chierici, M., Currie, K., De Baar, H. J. W., Evans, W., Feely, R. A., Fransson, A., Gao, Z., Hales, B., Hardman-Mountford, N. J., Hoppema, M., Huang, W.-J., Hunt, C. W., Huss, B., Ichikawa, T., Johannessen, T., Jones, E. M., Jones, S., Jutterstrøm, S., Kitidis, V., Körtzinger, A., Landschützer, P., Lauvset, S. K., Lefèvre, N., Manke, A. B., Mathis, J. T., Merlivat, L., Metzl, N., Murata, A., Newberger, T., Omar, A. M., Ono, T., Park, G.-H., Paterson, K., Pierrot, D., Ríos, A. F., Sabine, C. L., Saito, S., Salisbury, J., Sarma, V. V. S. S., Schlitzer, R., Sieger, R., Skjelvan, I., Steinhoff, T., Sullivan, K. F., Sun, H., Sutton, A. J., Suzuki, T., Sweeney, C., Takahashi, T., Tjiputra, J., Tsurushima, N., Van Heuven, S. M. A. C., Vandemark, D., Vlahos, P., Wallace, D. W. R., Wanninkhof, R. and Watson, A. J. (2014) An update to the Surface Ocean CO_2 Atlas (SOCAT version 2). Earth System Science Data 6: 69-90. doi:10.5194/essd-6-69-2014.

Bakker, D. C. E., Pfeil, B. Landa, C. S., Metzl, N., O'Brien, K. M., Olsen, A., Smith, K., Cosca, C., Harasawa, S., Jones, S. D., Nakaoka, S., Nojiri, Y., Schuster, U., Steinhoff, T., Sweeney, C., Takahashi, T., Tilbrook, B., Wada, C., Wanninkhof, R., Alin, S. R., Balestrini, C. F., Barbero, L., Bates, N. R., Bianchi, A. A., Bonou, F., Boutin, J., Bozec, Y., Burger, E. F., Cai, W.-J., Castle, R. D., Chen, L., Chierici, M., Currie, K., Evans, W., Featherstone, C., Feely, R. A., Fransson, A., Goyet, C., Greenwood, N., Gregor, L., Hankin, S., Hardman-Mountford, N. J., Harlay, J., Hauck, J., Hoppema, M., Humphreys, M. P., Hunt, C. W., Huss, B., Ibánhez, J. S. P., Johannessen, T., Keeling, R., Kitidis, V., Körtzinger, A., Kozyr, A., Krasakopoulou, E., Kuwata, A., Landschützer, P., Lauvset, S. K., Lefèvre, N., Lo Monaco, C., Manke, A., Mathis, J. T., Merlivat, L., Millero, F. J., Monteiro, P. M. S., Munro, D. R., Murata, A., Newberger, T., Omar, A. M., Ono, T., Paterson, K., Pearce, D., Pierrot, D., Robbins, L. L., Saito, S., Salisbury, J., Schlitzer, R., Schneider, B., Schweitzer, R., Sieger, R., Skjelvan, I., Sullivan, K. F., Sutherland, S. C., Sutton, A. J., Tadokoro, K., Telszewski, M., Tuma, M., Van Heuven, S. M. A. C., Vandemark, D., Ward, B., Watson, A. J., Xu, S. (2016) A multi-decade record of high quality fCO_2 data in version 3 of the Surface Ocean CO_2 Atlas (SOCAT). Earth System Science Data 8: 383-413. doi:10.5194/essd-8-383-2016.

Battisti, C. R., Olsen, A., et al. (2018) Presentation at the ICOS OTC 2018 workshop: *fCO_2 Statistical Uncertainty Analysis and Offset Estimation*. https://otc.icos-cp.eu/sites/default/files/2018-04/2018%20ICOS%20OTC%20Workshop%20Presentations.pdf

Dickson, A. G., Sabine, C. L. and Christian, J. R. (2007) Guide to best practices for ocean CO_2 measurements. PICES Special Publication 3: 191 pp, available at:https://www.nodc.noaa.gov/ocads/oceans/Handbook_2007.html (last access: 18 December 2018).

Olsen, A. and Metzl, N. (2009) SOCAT QC cookbook for SOCAT participants, available at: https://www.socat.info/index.php/publications-on-socat/ (last access: 18 December 2018).

Olsen, A., Metzl, N., Bakker, D. C. E., O'Brien, K. (2015) SOCAT Quality Control Cookbook - for SOCAT Version 3, available at: https://www.socat.info/index.php/publications-on-socat/ (last access: 18 December 2018).

Pfeil, B., Olsen, A., Bakker, D. C. E., Hankin, S., Koyuk, H., Kozyr, A., Malczyk, J., Manke, A., Metzl, N., Sabine, C. L., Akl, J., Alin, S. R., Bates, N., Bellerby, R. G. J., Borges, A., Boutin, J., Brown, P. J., Cai, W.-J., Chavez, F. P., Chen, A., Cosca, C., Fassbender, A. J., Feely, R. A., González-Dávila, M., Goyet, C., Hales, B., Hardman-Mountford, N., Heinze, C., Hood, M., Hoppema, M., Hunt, C. W., Hydes, D., Ishii, M., Johannessen, T., Jones, S. D., Key, R. M., Körtzinger, A., Landschützer, P., Lauvset, S. K., Lefèvre, N., Lenton, A., Lourantou, A., Merlivat, L., Midorikawa, T., Mintrop, L., Miyazaki, C., Murata, A., Nakadate, A., Nakano, Y., Nakaoka, S., Nojiri, Y., Omar, A. M., Padin, X. A., Park, G.-H., Paterson, K., Perez, F. F., Pierrot, D., Poisson, A., Ríos, A. F., Santana-Casiano, J. M., Salisbury, J., Sarma, V. V. S. S., Schlitzer, R., Schneider, B., Schuster, U., Sieger, R., Skjelvan, I., Steinhoff, T., Suzuki, T., Takahashi, T., Tedesco, K., Telszewski, M., Thomas, H., Tilbrook, B., Tjiputra, J., Vandemark, D., Veness, T., Wanninkhof, R., Watson, A. J., Weiss, R., Wong, C. S. and Yoshikawa-Inoue, H. (2013) A uniform, quality controlled Surface Ocean CO_2 Atlas (SOCAT), Earth Syst. Sci. Data 5: 125-143, doi:10.5194/essd-5-125-2013.

SOCAT (2014) The Surface Ocean CO_2 Atlas (SOCAT) Community Event. Workshop 10 of the IMBER Open Science Conference, Bergen, Norway on 23 June 2014. https://www.socat.info/index.php/publications-on-socat/ (last access: 18 December 2018).

Sutton, A. J., et al. (2014) A high-frequency atmospheric and seawater pCO_2 data set from 14 open-ocean sites using a moored autonomous system, Earth Syst. Sci. Data 6(2): 353-366, doi:10.5194/essd-6-353-2014.

Wanninkhof, R., Bakker, D. C. E., Bates, N., Olsen, A., Steinhoff, T. and Sutton, A. J. (2013) Incorporation of alternative sensors in the SOCAT database and adjustments to dataset Quality Control flags. doi:10.3334/CDIAC/OTG.SOCAT_ADQCF. https://www.nodc.noaa.gov/ocads/oceans/ (last access: 18 December 2018).

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: Pequ – equilibrator pressure, SST – sea surface temperature, Tequ – 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 accuracy of SST, Tequ and Pequ. 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 accuracy 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 accuracy of Pequ and Tequ. 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 accuracy 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 Tequ 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 accuracy 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?)