SOCAT Quality Control Cookbook
-For SOCAT version 3-

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1 Context

This is the SOCAT quality control (QC) cookbook for SOCAT version 3. It is an update to the cookbook for version 1 (Olsen and Metzl, 2009). It incorporates the revision of the dataset 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) and recommendations from the SOCAT Community Event on 23 June 2014 (IOCCP, 2014).

Consistent quality control and the adequate quality control comments fully justifying all quality control steps are extremely important (IOCCP, 2014).

Datasets from alternative sensors and platforms included in SOCAT versions 1 and 2 need to be quality controlled following the revised flagging scheme (IOCCP, 2014). Otherwise there is no intention to retrospectively implement the revised quality control criteria for datasets in SOCAT versions 1 and 2 (Wanninkhof et al., 2013)

2 The SOCAT quality control process

The SOCAT quality control process leads to the following:

- A dataset quality control flag is assigned to each data file.
- 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 datasets with a flag of A, B, C, D and E will be included in the SOCAT data products for version 3. Only fCO_2rec values with a WOCE flag of 2 are included as default in the synthesis products (Table 2 in Bakker et al., 2014)

2.1 Dataset quality control flags

The dataset quality control flags provide information on the expected quality of each dataset and must be assigned to each dataset in the quality control process. To assign the dataset flag it is necessary to evaluate both the data and metadata. The flags and criteria have been revised for version 3 (Table 1) (Wanninkhof et al., 2013). One can summarize the quality control criteria for the dataset flags of A to E as follows (Table 1):

- 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.
- A high-quality cross-over with another dataset is required for a flag of A.
- SOP (Standard Operating Procedures) criteria need to be fulfilled for a flag of A or B.
- Flags of A, B, C and E require complete metadata documentation.
- Dataset quality control needs to be deemed acceptable for flags of A-E.

Table 1. Dataset quality control flags for SOCAT version 3 (Wanninkhof et al., 2013). Changes relative to SOCAT versions 1 and 2 are in bold.

Flag	Criteria[a]
A (11)	(1) Accuracy of calculated fCO_2w (at SST) is better than 2 µatm. (2) **A high-quality cross-over[b,c]** with another dataset is available. (3) Followed approved methods/SOP[d] 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) Did or did not follow 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 dataset).
X (Exclude) (15)	The dataset duplicates another 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.

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

[b]A high-quality cross-over is defined in version 3, as a cross-over between two datasets 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_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.

[c]A cross-over is defined as a distance of less than 80 km. This criterion combines distance and time as $([dx^2 + (dt*30)^2]^{0.5}) \leq 80$ km. One day of separation in time is equivalent (heuristically) to 30 km of separation in space.

[d]SOP or Standard Operating Procedure following Dickson et al. (2007).

2.1.1 A high-quality cross-over for a flag of A

A flag of A now requires the presence of a high-quality cross-over (Wanninkhof et al., 2013). This new requirement clarifies what constitutes an 'acceptable comparison with other data' (in versions 1 and 2). A cross-over between two datasets is defined as a distance of less than 80 km. The cross-over algorithm combines distance and time as ($[dx^2 + (dt*30)^2]^{0.5}$) ≤ 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 datasets 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.

Inconclusive cross-overs 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.

2.1.2 Approved methods/SOP criteria for flags of A and B

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. Cavity ring-down spectrophotometers (CRDS) should be checked daily with at least two non-zero calibration gases to meet the requirements for a flag of A or B (Wanninkhof et al., 2013).

Seven SOP criteria **all** need to be fulfilled for a flag of A or B (Wanninkhof et al., 2013):
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;
4. The calibration has included at least two non-zero gas standards, traceable to World Meteorological Organisation (WMO) standards;
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 equilibrator pressure has been measured to **within 2 hPa** accuracy.

The criterion for the accuracy of the pressure of equilibration has been relaxed from 0.5 hPa to 2 hPa in version 3 (Wanninkhof et al., 2013).

2.1.3 Flags of C and D for shipboard NDIR, gas chromatographs and CRDS systems

All datasets assigned a flag of C or D need to have an accuracy of better than 5 µatm (Wanninkhof et al., 2013). For infrared-based systems, this means at least two calibration gases, such that the sample is bracketed by both gases, one of which can be a zero gas.

2.1.4 Flags of C and D for well calibrated alternative sensors and platforms

The current generation of alternative sensors does not meet the 2 µatm accuracy required for a flag A or B (Wanninkhof et al., 2013). Some alternative sensors meet the 5 µatm accuracy required for a flag of C or D, based on well documented calibration (Wanninkhof et al., 2013). To obtain a flag of C or D alternative sensors need to have an *in situ* calibration with at least two standards, one of which can be a zero gas. An in situ calibration is a calibration, when the instrument is operating in its natural environment (on a ship, drifter or mooring). The frequency of the calibration needs to be such that the standardization can correct for drift and noise to meet an accuracy of better than 5 µatm. This would generally need to be a daily or more frequent calibration. A clear description of the calibration of alternative sensors needs to be provided in the metadata. (By consequence, a flag of D will rarely be assigned to alternative sensor data.)

2.1.5 Flag of E for alternative sensor and platforms

Some alternative sensors systems do not meet the criterion of a verifiable accuracy of better than 5 µatm for flags of C and D by *in situ* calibration (Wanninkhof et al., 2013). For a flag of E, laboratory and pre- or post-deployment tests of 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). Internal diagnostics and standardization and when possible post-deployment tests are necessary. The metadata need to document how the accuracy of the sensor has been determined.

2.1.6 Complete metadata for flags of A, B, C and E

Flags A, B, C and E require complete metadata (Table 1). This information must appear either in the metadata themselves (preferably) or in a publication cited in metadata.

Complete metadata for continuous shipboard measurement of surface water fCO_2 by NDIR, gas chromatography or CRDS contains all this information (Pfeil et al., 2013):

1. The investigator;
2. The vessel;
3. The temporal coverage;
4. The analytical method;
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 traceability;
7. A list of sensors and their accuracy, notably for:
    a. The equilibrator and seawater intake temperature;
    b. The equilibrator pressure.

Complete metadata for alternative sensors and platforms contains all the following information:

1. The investigator;
2. The vessel;
3. The temporal coverage;
4. The analytical method;
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. The number of CO_2 standards used with their approximate CO_2 mixing ratio and traceability;
    c. Accuracy obtained during the calibration;
7. A list of sensors and their accuracy, e.g. for:
    a. The equilibrator and seawater intake temperature;
    b. The equilibrator pressure.

2.2 WOCE Flags

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 us to include datasets with some questionable or bad fCO_2 values in SOCAT. Using WOCE flags enables us (in a traceable way) to retain the dataset, with easy identification of any questionable or bad data via the flags of 3 or 4. Surface water fCO_2 values can be bad for several reasons (e.g erroneous position, time, unrealistic intake or equilibrator temperatures, large temperature difference between the intake and the equilibrator, xCO_2, etc).

SOCAT carries out quality control for surface water fCO_2 only and we 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 (IOCCP, 2014).

2.3 Additional quality control criteria based on temperature change

The following five 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 rapid 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.

The above features may occur for some data points, in which case appropriate WOCE flags should be assigned, or for a whole dataset, 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 datasets 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 dataset you will quality control (Fig. 1). As a result of the automation effort, changes have been made to the quality control system (for version 3). For the quality controllers these changes will not be very visible.

Quality control the dataset either online using the LAS tools or download the whole dataset and carry out the QC offline using your favorite software. You need to ensure that you quality control the full dataset, not a sub-selection of the dataset. This applies both to online quality control and to data download. The full data files for each dataset can be accessed by pressing the "Table of Cruises" button on the main LAS interface. It is more efficient to make this choice after reducing the number of cruises shown – either by selecting a particular cruise by Expocode, or by constraining in space and/or time. Please see section 3.3 for general information on how to use the LAS interface to QC fCO2 data.

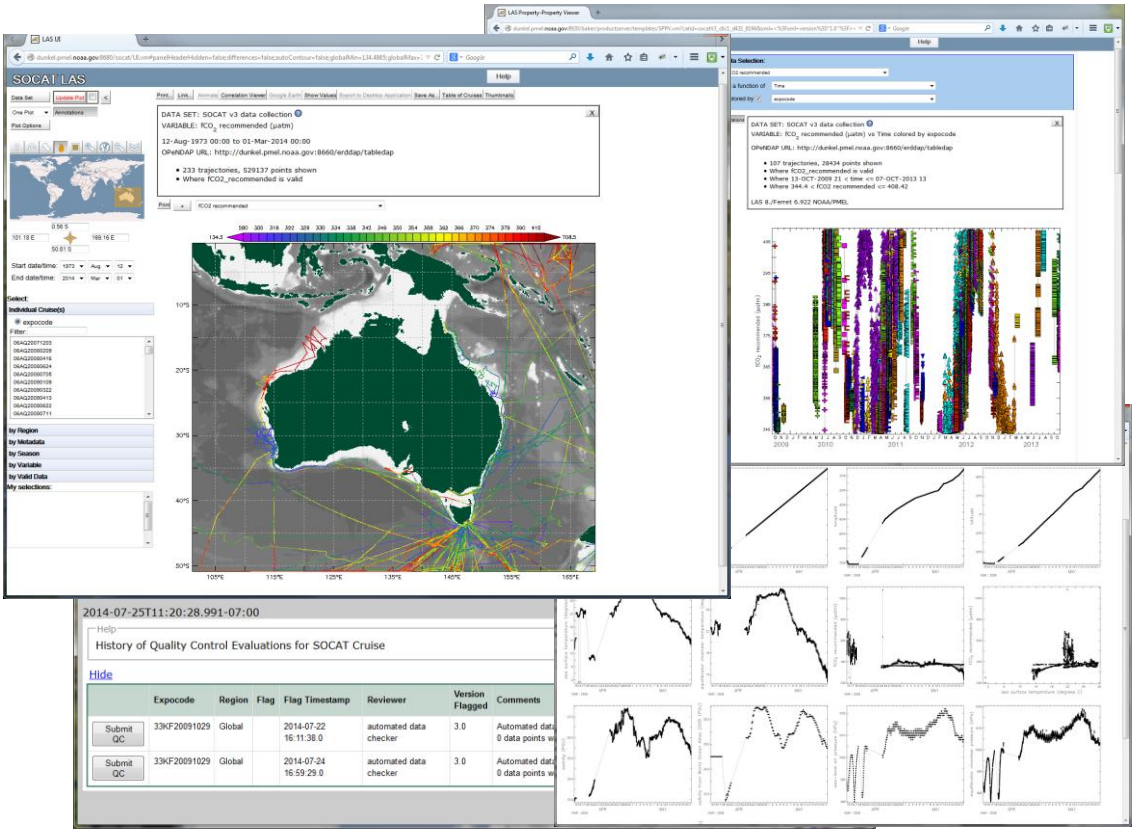

Figure 1. SOCAT version 3 quality control will be done using version 8.1 of the Live Access Server (LAS). Above is a collection of LAS version 3 quality control tools, including the main LAS user interface, the correlation viewer, the thumbnail viewer and the History of QC.

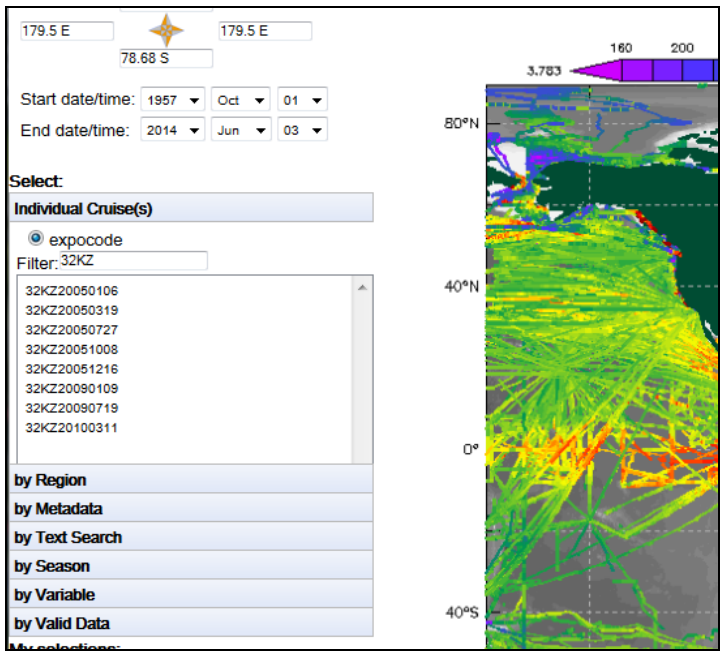

Figure 2. Selecting an individual cruise from the Expocode filter on SOCAT LAS main UI

3.2 Assigning dataset quality control flags and quality control comments

When the QC is done and you are ready to assign the dataset quality control flag,

1. Find your dataset in the main LAS UI page by filtering on Expocode
2. Once you have limited the UI to only a single Expocode, 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.
4. To modify the QC flag, click the "Submit QC" button (some datasets may have several, one for each region the dataset covers, remember to use 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 over ridden. 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 dataset. The comment should adequately justify choice of the flag.

Each of the input choices made above will result in a comment being placed into the "Complete QC comment" box. This is to help ensure a complete comment is associated with the QC flag set.

6. After you have pressed "Submit this QC evaluation" button in the pop-up window, this window can be closed.

Quality control comments should be adequate and fully justify a dataset quality control flag (IOCCP, 2014). An adequate record of why a dataset 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 his/her 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 dataset quality control comments.

The version 3 quality control system has these new features (IOCCP, 2014), as discussed above:

- Check-boxes corresponding to the criteria for dataset quality control flags;
- A dataset quality control flag can only be submitted, if the corresponding check-boxes have been ticked and a text comment has been entered.
- The Expocode of the cross-over dataset must be specified for a flag of A.
- Adding a quality control comment without submitting a dataset flag will be possible.

3.3 Assigning WOCE Flags

In addition to the dataset quality control flags we also assign WOCE flags for individual (re-)calculated fCO_2 values in each data file. Initially we assume that all fCO_2 values are 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.

WOCE flags are set in the SOCAT QC Live Access Server through the Correlation Viewer tool. There are several ways to launch the correlation tool:

1. Using the "Correlation Viewer" on the LAS main page
2. Clicking on an individual plot window in the "Thumbnails" tool
3. Clicking on a potential crossover cruise Expocode in the "Table of Cruises"

It is recommended that the user reduce the number of cruises being drawn in the main UI, as mentioned in QC flag editing above, in order to improve performance of the system. Another added benefit to reducing the subset of selected Expocodes is that the correlation viewer will be able to create a unique icon for each Expocode display on the plot. This will make it much easier to identify data by their Expocode.

Once in the correlation viewer, to set the WOCE flag for fCO2 recomputed, the user should select the values they wish to edit on the plot by dragging a rectangle over the desired data points, and then clicking the "Edit Flags" button in the upper left corner. See figure 3.

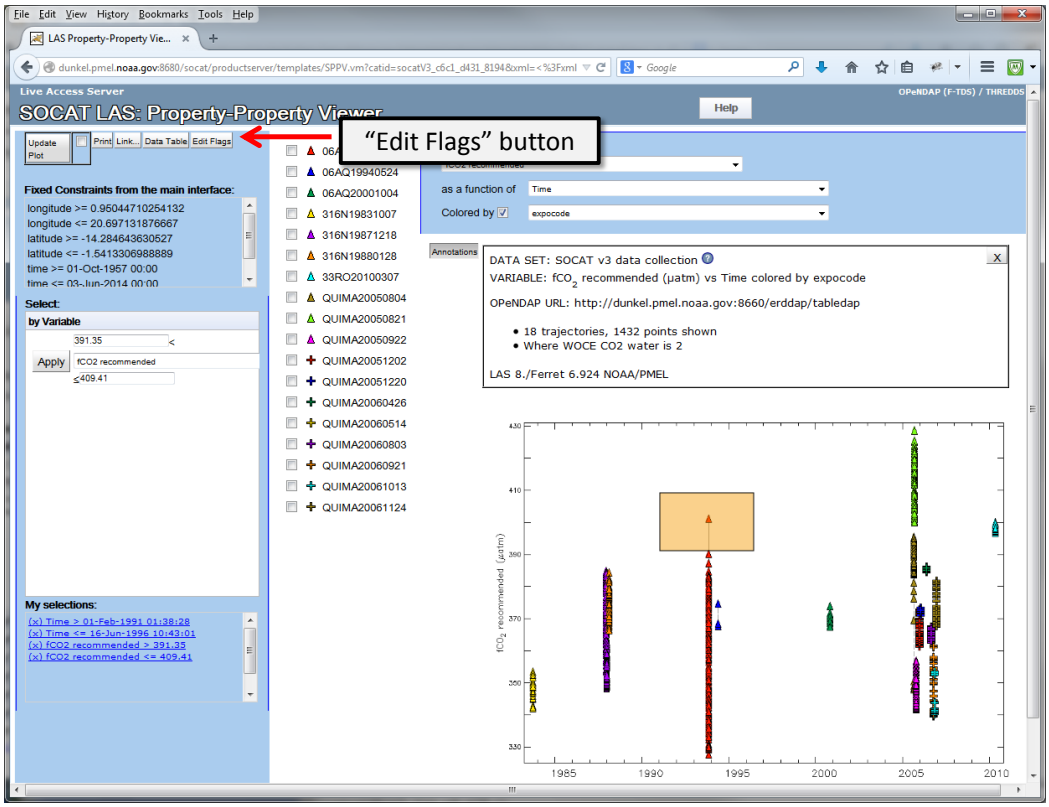

Figure 3. The SOCAT LAS correlation viewer with selected values and demonstrating location of "Edit Flags" button in upper left corner.

In "Edit Flags" mode, it is possible to assign one or many data values new WOCE flags (see figure 4). Before saving the modified WOCE flags, the reviewer should submit a detailed and clear comment to explain the reason for the WOCE value assignment. In fact, if a comment is not entered, the user will not be able to save the new values.

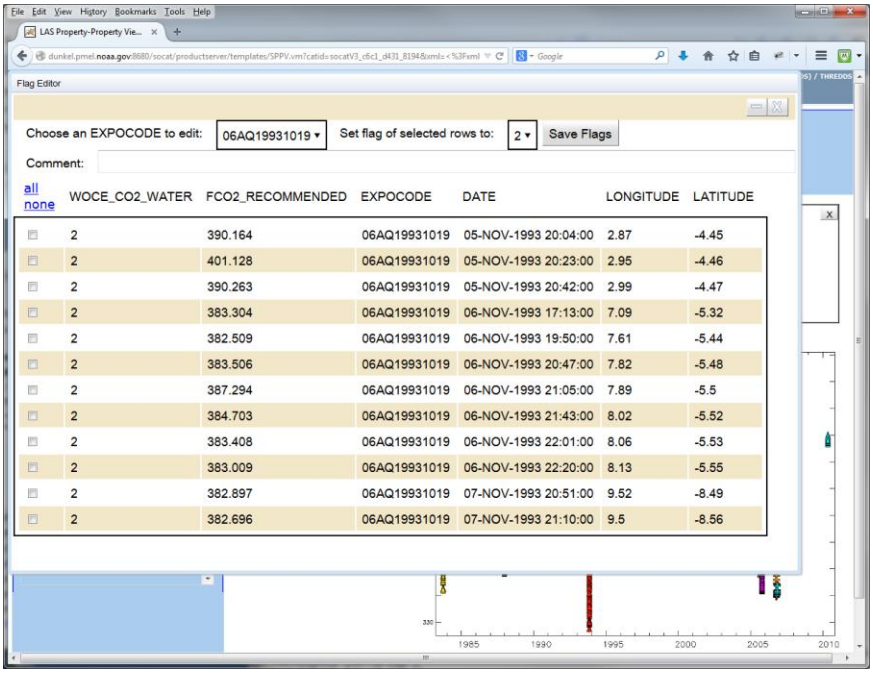

Figure 4. WOCE flag editing tool in SOCAT LAS .

3.4 Suspending data

If the dataset data quality is not deemed acceptable, set the dataset quality control flag to suspend ('S) and add a clear comment why the dataset 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).

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Appendix 1: Examples of quality control comments

The examples (IOCCP, 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 Cruise Data Viewer and adjusted to the revision of dataset quality control flags in version 3. All relevant quality control comments should be entered on the quality control system. Abbreviations are: Pequ – equilibrator pressure, SOP – standard operating procedures, SST – sea surface temperature, Tequ – equilibrator temperature.

Examples of (barely) 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 C) 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 datasets.
3) Flag C. Metadata complete. A flag C was given because 1) the accuracy of pCO2/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. Hence flag D.
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. Hence flag E.
6) Flag F (or S). No information is provided on the calibration of these sensor data. The data provider has been asked to update information on the pre-deployment calibration.
7) Flag S. File lacks surface water CO_2 measurements. The data provider has been consulted.
8) Flag S. SST has not been reported, such that Tequ was used in calculation of fCO_2rec. Dataset suspended in consultation with data provider.
9) Flag X. This dataset overlaps with dataset 11FF20200808. This is an older version of the same dataset. The data provider has been consulted.

Examples of poor, inadequate quality control comments:

1) Flag A. No comment.
   (*Lacks comments on 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 comment on data quality deemed acceptable and metadata complete*).
4) Flag D. Metadata incomplete.
   (*Lacks comment on data quality deemed acceptable, what is missing in metadata.*)
5) Flag E. A spectrophotometric sensor has been used.
   (*Lacks comment on accuracy of pre-deployment calibration, metadata complete, data quality.*)
6) Flag F (or S). An infrared sensor has been used.
   (*Lacks comment on grounds for suspension, e.g. no information on pre-deployment calibration. Has the data provider been consulted?*)
7) Flag S. Data quality not good.
   (*Lacks explanation on the nature of the problem. Has the data provider been consulted?*)
8) Flag X. This dataset overlaps with another dataset.
   (Which other dataset? Has the data provider been consulted?)