

SOCAT QC Cookbook for SOCAT participants

Are Olsen & Nicolas Metzl

2009

PLAN

We are now at version 1.3 of the SOCAT dataset. This is frozen, is the version that will be QC'ed and resides at the LAS.

By frozen we mean that NO NEW data will be added. If you have new data (cruises), these can be submitted to Benjamin but will not be included in v1.3. They will be included in future versions of SOCAT.

It is still possible to revise the data in v1.3, but this must follow procedures so that we maintain some control, see last section of this document.

For explanation of the various parameters in the SOCAT data files see documentation available at the www.socat.info page.

SOCAT QC PROCESS

The SOCAT QC process will lead to the following:

1. A “Wanninkhof flag” will be assigned to each cruise, i.e. data file.
2. Each fCO₂_rec datum will be flagged using WOCE flags 2 (good), 3 (questionable) or 4 (bad). This will be done line by line in each data file.

Wanninkhof flags

The Wanninkhof flags provide information on the expected quality of each cruise and must be assigned to each cruise in the QC process. To assign the “Wanninkhof” flag you must evaluate both the data and metadata. The flags and criteria are (the criteria have been revised somewhat from the original given in IOCCP, 2008, mainly to make the flags unique and consistent):

Category A (11):

- 1) followed approved methods / SoP criteria
- 2) metadata documentation complete
- 3) 2nd level QC performed and deemed acceptable + comparison with other data performed and deemed acceptable

Category B (12):

- 1) followed approved methods / SoP criteria
- 2) metadata documentation complete
- 3) 2nd level QC performed and deemed acceptable

Category C (13):

- 1) did not follow approved methods / SoP criteria
- 2) metadata documentation complete
- 3) 2nd level QC performed and deemed acceptable (including if possible comparison with other data)

Category D (14):

- 1) did or did not follow approved methods/SOP criteria (for sure, or could not be evaluated)
- 2) metadata documentation incomplete
- 3) 2nd level QC performed and deemed acceptable (including if possible comparison with other data)

Category F (15): (F for “failure”)

- 1) did or did not follow approved methods / SoP criteria (for sure, or could not be evaluated)
- 2) metadata documentation complete or incomplete
- 3) 2nd level QC revealed non-acceptable data

Category S: (S for “suspend”)

- 1) did or did not follow methods / SoP criteria
- 2) metadata documentation complete or incomplete
- 3) 2nd level QC revealed non-acceptable data, but data are being updated (all cruise or part of the cruise)

Category X (15): (X for “exclude”)

- 1) the cruise (all data) are duplicates of another set of data in SOCAT.

On Approved methods/SoP criteria

These are required of category A and B cruises (2 μ atm or better), have been specified to (IOCCP, 2009):

- Continuous measurements, not discrete;
- Based on $x\text{CO}_2$ analysis, not $f\text{CO}_2$ calculated from other carbon parameters; Detection based on an equilibrator and IR (infrared)/ GC (gas chromatograph);
- The calibration included at least 2 non-zero gas standards, traceable to WMO standards;
- The equilibrator temperature was measured to within 0.05°C;
- The seawater temperature was measured to within 0.05°C;
- The equilibrator pressure was measured to within 0.5 hPa;

These criteria follow the recommendations from the 2002 Miami workshop

<http://www.aoml.noaa.gov/ocd/gcc/uwpc02/workshops/>

All of these needs to be fulfilled for flag A and B:

Note that equilibrator pressure accuracy of 0.5 hPa is sufficient for seawater $f\text{CO}_2$. For high accuracy atmospheric data, the atmospheric pressure (outside the ship) needs to be determined to 0.1 hPa.

Also, on installations where only the outside air pressure is recorded and used for the seawater $f\text{CO}_2$ calculation, the required accuracy of 0.5 hPa is never met because of the overpressure that is normally maintained within ships. In the calculation of $f\text{CO}_2$ this has been taken into account by adding 3hPa (a very approximate correction proposed by Takahashi and Sutherland (2007)) whenever atmospheric pressure and not equilibrator pressure was reported in the data files.

On metadata.

There exist several metadata formats and forms in the community.

By complete metadata we mean that they should provide the following information:

- Time
- Region
- Method & reported data (xCO₂, pCO₂, fCO₂)
- Standards: number used, their approximate concentration and traceability
- List of sensors and their accuracy. At least equilibrators and intake temperature, equilibrators pressure,

And the accuracy of any other data in the file (for instance salinity, but note that the sensitivity of the xCO₂ to fCO₂ calculation, to salinity is very small, so high accuracy salinity data is not needed to meet the 2 µatm criterion (example, xCO₂ of 360 ppm and 20°C and 1 atm yields fCO₂ of 347.22 and 347.24 at salinity 30 and 35, respectively))

This information must appear either in the metadata themselves (preferable) or in a publication cited in metadata.

WOCE Flags

Flagging each individual fCO₂_rec datum using WOCE flags 2, 3 or 4 was something we decided to do after the Atlantic and Southern Ocean Regional meeting in June 2009. The primary motivation for this, is that it allows us to include cruises with some bad data lines in SOCAT. Without this flag, cruise data would have to be revised if there are some bad data lines. This is not always possible, which would force us to exclude the cruise. Using WOCE flags enables us (in a traceable way) to retain all of the data in the file, with any questionable/bad data flagged 3/4, so that they can be easily identified.

Please note that we only flag the fCO₂_rec data. These can be bad for several reasons (e.g intake or equilibrators temperatures, xCO₂ etc), but we do not distinguish between these.

HOW TO PRACTICALLY CARRY OUT QC

You should all know what cruises you are expected to QC. When in doubt, please contact your regional group leader.

The data and QC system resides at PMEL's LAS, enter at <http://access.pmel.noaa.gov/SOCAT> using your username and password (have you forgotten these? contact Jeremy.Malczyk@noaa.gov).

Use the LAS tools to find the cruise you will QC.

QC the cruise either online using the LAS tools or download the whole cruise and QC offline using your favorite software. The full data files for each cruise can be accessed by pressing the "table of cruises" button at the LAS.

During the QC several analyses should be made. I will not list them here but refer to the Atlantic and Southern Oceans Regional Meeting report (IOCCP, 2009).

When the QC is done and you are ready to assign the Wanninkhof flag,

1. find your cruise in the "Table of Cruises".
2. Press the enter QC button and you will arrive at "Table of Quality Control Records currently being applied to SOCAT Cruise xxxxx"

2. Press the submit QC button (some cruises may have several, one for each region the cruise covers, remember to use your region)
3. In the pop-up window specify:
 - Reviewer
 - QC flag (drop down menu)
 - If you want to override conflicting flags (check box)
 - Enter your comment for this cruise. The comment should briefly summarise the line of reasoning behind the flag choice.

4. After you have pressed “Submit this QC evaluation” button in the pop-up window, this window will close. At this stage it is time to upload any figures that support your decision. The “Table of Quality Control Records currently being applied to SOCAT Cruise xxxxx” has a column named “Upload/Download Documents”. Press the “Docs” button for your region. This takes you to the SUBVERSION (Polarion SVN) repository for the cruise. Using the buttons to the upper right you can upload files, create new directories with files, delete files (in case you regret) and download all uploaded files.

Please upload any files you have (figures supporting your decision for instance) here. Filename should start with Cruisename _YYYYMMDD_(brief description of contents) (for instance if the figure is pCO₂ vs SST for cruise Colibri_2006_1 uploaded Nov 6 2009, name the file “Colibri_2006_1_20061106_pco2_vs_SST”.) Also use the opportunity of the comment field to enter a more detailed description. (Right now it is not possible to provide author identification, LAS group working on this. Until this works, write your author name in comment field).

Assigning WOCE FLAGS

In addition to the Wanninkhof flags we will also use WOCE QC flags for each fCO₂_rec datum in each data file. Initially we will assume that all fCO₂_rec data are good (WOCE flag =2). Hence, if you find questionable or bad data in the file that you will like to flag 3 or 4 you prepare comma separated text file containing:

```
"sta      WOCE_flag (other than 2)"
```

The “sta” variable is the first parameter in each data file, a synthetic counter for each file.

e.g. if you suggest that sta 41086 and 41091 of 0404SFC_PRT should be flagged 3 , the file should look like

```
41086      3
41091      3
```

Save as comma separated file with name Cruisename _YYYYMMDD_ WOCEflags (i.e for the example: 0404SFC_PRT_20091116_ WOCEflags.csv - if file was prepared Nov 11 2009 (filename very important, since the loading of these files will be automated). This file should be uploaded to the SUBVERSION repository for each cruise. Please note that to do this correctly you need to evaluate every datum of the cruise, i.e. using daily/hourly etc subsampling is no good.

REVISING DATA ALREADY IN THE DATABASE.

If the cruise should be revised (i.e. a new and revised version should be uploaded to SOCAT), set the quality flag to suspend and add a comment that the cruise is suspended awaiting revision. Then make sure that Benjamin gets a copy of the revised

datafile which can replace the suspended one. When this has been done, Benjamin will remove the “Suspend” flag and the revised version should be QC’ed.

References:

- IOCCP (2009), *Surface Ocean CO₂ Atlas Project, Atlantic and Southern Oceans Regional Meeting, Norwich, UK, 25-26 June 2009*, IOCCP Report Number 13, available at http://ioc3.unesco.org/ioccp/FinalRpts/WR222_eo.pdf
- IOCCP (2008), *Surface Ocean CO₂ Atlas (SOCAT) project – SOCAT-2 meeting, UNESCO, Paris June 16-17 2008*, available at http://ioc3.unesco.org/ioccp/Docs/SOCAT2_Final2.pdf
- Takahashi , T. and S. C. Sutherland (2007), *Global Ocean Surface Water Partial Pressure of CO₂ Database, Measurements Performed during 1968-2006*, CDIAC, Oak, Ridge, TN.