

The quality assessments given by the Cruise QC flag and WOCE flag only apply to the recomputed $f\text{CO}_2$ value ($f\text{CO}_2\text{rec}$).

A short description can be found in this document for detailed information about the recomputed $f\text{CO}_2$ value and the meaning of the Cruise QC flag, the source of the CO_2 parameter ($f\text{CO}_2\text{rec_src}$), and the WOCE flags ($f\text{CO}_2\text{rec_flag}$ values) see:

Pfeil, B.; Olsen, A.; Bakker, D. C. E.; et al. (2013) A uniform, quality controlled Surface Ocean CO_2 Atlas (SOCAT). Earth System Science Data, 5(1), 125-143, doi:10.5194/essd-5-125-2013

Short description extracted from the above paper:

The SOCAT individual cruise data files contain all data points, including those data missing recomputed $f\text{CO}_2$ values and those with a WOCE flag indicating questionable (3) or bad (4) recomputed $f\text{CO}_2$ values

Cruise QC flag

Criteria for assigning cruise flags based on the expected quality of the recommended $f\text{CO}_2$ data (revised after Olsen and Metzl, 2009). All criteria need to be met for assigning a cruise flag. SOP is Standard Operating Procedures (Dickson et al., 2007).

Cruise flag (ID)	Criteria
A (11)	1. Followed approved methods or SOP criteria and 2. Metadata documentation complete and 3. Extended QC was deemed acceptable and 4. A comparison with other data was deemed acceptable.
B (12)	1. Followed approved methods or SOP criteria and 2. Metadata documentation complete and 3. Extended QC was deemed acceptable.
C (13)	1. Did not follow approved methods or SOP criteria and 2. Metadata documentation complete and 3. Extended QC was deemed acceptable (including comparison with other data if possible).
D (14)	1. Did or did not follow approved methods or SOP criteria and 2. Metadata documentation incomplete and 3. Extended QC was deemed acceptable (including comparison with other data if possible).
S (Suspend)	1. Did or did not follow methods or SOP criteria and 2. Metadata documentation complete or incomplete and 3. Extended QC revealed non-acceptable data 4. Data are being updated.
X (15) (Exclude)	The cruise (data set) duplicates another cruise (data set) in SOCAT.
N (No flag)	No cruise flag has yet been given to this cruise.
U (Update)	The cruise data have been updated. No cruise flag has yet been given to the revised data.

Source: Pfeil et al., 2013

Source for recomputing $f\text{CO}_2$:

Surface water CO_2 parameters reported in the original data files, which have been used for the calculation of recommended $f\text{CO}_2$ ($f\text{CO}_2\text{rec}$) at sea surface (or intake) temperature (Pfeil and Olsen, 2009). The parameters are listed in order of preference (with index 1 as the favourite). The index has been reported in the SOCAT global and

regional output files as “fCO2rec_src”. Ancillary parameters have been used for NCEP (National Centers for Environmental Prediction) atmospheric pressure (Kalnay et al., 1996) and WOA (World Ocean Atlas) salinity (Antonov et al., 2006).

Index	Reported CO ₂ parameter	Unit	Extra variable
1	xCO2water_equi_dry	μmol mol ⁻¹	
2	xCO2water_SST_dry	μmol mol ⁻¹	
3	pCO2water_equi_wet	μatm	
4	pCO2water_SST_wet	μatm	
5	fCO2water_equi	μatm	
6	fCO2water_SST_wet	μatm	
7	pCO2water_equi_wet ¹	μatm	NCEP Pressure
8	pCO2water_SST_wet ¹	μatm	NCEP Pressure
9	xCO2water_equi_dry ²	μmol mol ⁻¹	WOA Salinity
10	xCO2water_SST_dry ²	μmol mol ⁻¹	WOA Salinity
11	xCO2water_equi_dry ¹	μmol mol ⁻¹	NCEP Pressure
12	xCO2water_SST_dry ¹	μmol mol ⁻¹	NCEP Pressure
13	xCO2water_equi_dry ^{1,2}	μmol mol ⁻¹	NCEP Pressure, WOA Salinity
14	xCO2water_SST_dry ^{1,2}	μmol mol ⁻¹	NCEP Pressure, WOA Salinity

¹ Atmospheric pressure was not reported in the original data file.

² Salinity was not reported in the original data file.

* Not used for data reporting as an approach with a lower index was available.

Source: Pfeil et al., 2013

If the World Ocean Atlas (WOA) Sea Surface Salinity is missing for an observation, but was needed for recomputing fCO₂, an approximated value of 35.0 was used.

We kindly ask colleagues:

- 1) To send references for their publications using SOCAT to submit@socat.info to be listed on the website
- 2) To generously acknowledge the contribution of SOCAT PIs, regional group leaders, SOCAT QC-ers and data PIs in the form of invitation to co-authorship, acknowledgement or reference to relevant papers as appropriate.

- 3) To cite all version SOCAT version 2 products as:

Bakker, D.C.E et al. (2013) An update to the Surface Ocean CO₂ Atlas, Earth Syst. Sci. Data, to be submitted

- 2) To report problems to submit@socat.info

For further advice, please, contact any of the SOCAT PIs.

References:

- Antonov, J. I., Locarnini, R. A., Boyer, T. P., Mishonov, A. V., and Garcia, H. E.: World Ocean Atlas 2005, in: Volume 2: Salinity, edited by: Levitus, S., NOAA Atlas NESDIS 62, US Government Printing Office, Washington, DC, 182 pp., 2006.
- Dickson, A. G., Sabine, C. L. and Christian, J. R. (eds.): Guide to best practices for ocean CO₂ measurements. PICES special publication 3, 191 pp, 2007.
- Kalnay, E., Kanamitsu, M., Kistler, R., Collins, W., Deaven, D., Gandin, L., Iredell, M., Saha, S., White, G., Woollen, J., Zhu, Y., Chelliah, M., Ebisuzaki, W., Higgins, W., Janowiak, J., Mo, K. C., Ropelewski, C., Wang, J., Leetmaa, A., Reynolds, R., Jenne, R., and Joseph, D.: The NCEP/NCAR 40-year reanalysis project, *B. Am. Meteorol. Soc.*, 77, 437–470, 1996.
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