

Individual data set files at PANGAEA in SOCAT version 5



The **SOCAT individual data set files** are available at Pangaea for all data sets with flags of A, B, C, D and E. The files are available in text format. A full description of the files is in Bakker et al. (2016). Below follows a short description, as well as two tables from Bakker et al. (2016).

The files contain all data points, including those data missing recommended $f\text{CO}_2$ values and those with a WOCE flag indicating questionable (3) or bad (4) recommended $f\text{CO}_2$ values. The files also contain other parameters, such as atmospheric pressure from reanalysis, climatological salinity and the atmospheric CO_2 mole fraction. Metadata reported by the data provider accompany the files and links to the original data sets are provided. The quality assessments given by the Data Set quality control (QC) flag and WOCE flag only apply to the recommended $f\text{CO}_2$ value ($f\text{CO}_2\text{rec}$).

Data Set QC flag: Criteria for assigning Data Set QC flags are based on the expected accuracy of the recommended $f\text{CO}_2$ data. All criteria need to be met for assigning a data set QC flag.

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. The parameters are listed in order of reference (with algorithm 1 as the favourite). The algorithm has been reported in the SOCAT global and regional output files.

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). If the World Ocean Atlas (WOA) Sea Surface Salinity is missing for an observation, but was needed for recomputing $f\text{CO}_2$, a value of 35.0 was used.

Table 2. Data set quality control (QC) flags in version 3 (Wanninkhof et al., 2013b; Olsen et al., 2015). All criteria need to be met for assigning a flag of A to E. Data sets with flags of A to E have been made public. Data sets with a flag of A to D are included in the global synthesis and gridded products (Table 8). Changes relative to versions 1 and 2 are in bold. Flag (ID) refers to the data set quality control flag with its numerical identifier (ID) provided between brackets. Calculation of “recommended $f\text{CO}_2$ ” ($f\text{CO}_2\text{rec}$) is explained in Sect. 4.2.

Flag (ID)	Criteria for version 3
A (11)	(1) Accuracy of calculated $f\text{CO}_2\text{rec}$ (at SST) is better than $2\ \mu\text{atm}$. (2) A high-quality cross-over^{1,2} with another data set is available. (3) Followed approved methods/SOP ³ criteria. (4) Metadata documentation complete. (5) Data set QC was deemed acceptable.
B (12)	(1) Accuracy of calculated $f\text{CO}_2\text{rec}$ (at SST) is better than $2\ \mu\text{atm}$. (2) Followed approved methods/SOP criteria. (3) Metadata documentation complete. (4) Data set QC was deemed acceptable.
C (13)	(1) Accuracy of calculated $f\text{CO}_2\text{rec}$ (at SST) is better than $5\ \mu\text{atm}$. (2) Did or did not follow approved methods/SOP criteria. (3) Metadata documentation complete. (4) Data set QC was deemed acceptable.
D (14)	(1) Accuracy of calculated $f\text{CO}_2\text{rec}$ (at SST) is better than $5\ \mu\text{atm}$. (2) Did or did not follow approved methods/SOP criteria. (3) Metadata documentation incomplete. (4) Data set QC was deemed acceptable.
E (17)	Primarily for alternative sensors (1) Accuracy of calculated $f\text{CO}_2\text{rec}$ (at SST) is better than $10\ \mu\text{atm}$. (2) Did not follow approved methods/SOP criteria. (3) Metadata documentation complete. (4) Data set QC was deemed acceptable.
S (15) (Suspend)	(1) More information is needed for data set before flag can be assigned. (2) Data set QC revealed non-acceptable data. (3) Data are being updated (part or the entire data set).
X (15) (Exclude)	The data set duplicates another data set in SOCAT.
N (No flag)	No data set flag has yet been given to this data set.
U (Update)	The data set has been updated. No data set flag has yet been given to the revised data.

¹ A cross-over between two data sets is defined as an equivalent distance of less than 80 (Pfeil et al., 2013). This criterion combines distance and time as $([\Delta x^2 + (\Delta t \times 30)^2]^{0.5}) \leq 80$ with distance x in kilometres and time t in hours. One day of separation in time is equivalent (heuristically) to 30 km of separation in space. ² 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 $0.3\ ^\circ\text{C}$ and a maximum $f\text{CO}_2\text{rec}$ difference of $5\ \mu\text{atm}$. Inconclusive cross-overs with the temperature or $f\text{CO}_2\text{rec}$ difference between the data sets exceeding $0.3\ ^\circ\text{C}$ or $5\ \mu\text{atm}$, respectively, do not receive a flag of A. High-quality cross-overs are rare in coastal waters, near sea ice and in regions of freshwater influence, as a result of high spatial variation, not for lack of measurement quality (Sect. 4.4). ³ Seven approved methods or SOP (standard operating procedure) criteria need to be fulfilled for a data set quality control flag of A and B (Sect. 4.4) (after Pfeil et al., 2013). In version 3, the accuracy requirement for equilibrator pressure has been relaxed to 2.0 hPa from 0.5 hPa in earlier SOCAT versions. The six other criteria are the same in SOCAT versions 1, 2 and 3.

Table 6. Algorithms and surface water CO₂ parameters used in the calculation of recommended *f*CO₂ (*f*CO₂rec) at sea surface temperature in version 3 (after Pfeil et al., 2013). Algorithm 1 was the preferred method, followed by algorithm 2 and so forth. The algorithm used for each data set is stated in the output files (Table 9). In the case of incomplete reporting, NCEP (National Centers for Environmental Prediction) atmospheric pressure (Kalnay et al., 1996; NCEP, 2014) and WOA (World Ocean Atlas) 2005 salinity (Antonov et al., 2006) were applied.

Algorithm	CO ₂ parameter	Unit	Data set percentage (%)	Extra variable
1	<i>x</i> CO ₂ water_equi_dry	μmol mol ⁻¹	59.1	–
2	<i>x</i> CO ₂ water_SST_dry	μmol mol ⁻¹	12.5	–
3	<i>p</i> CO ₂ water_equi_wet	μatm	7.2	–
4	<i>p</i> CO ₂ water_SST_wet	μatm	3.0	–
5	<i>f</i> CO ₂ water_equi	μatm	0.4	–
6	<i>f</i> CO ₂ water_SST_wet	μatm	12.2	–
7	<i>p</i> CO ₂ water_equi_wet ¹	μatm	0.4	NCEP pressure
8	<i>p</i> CO ₂ water_SST_wet ¹	μatm	6.1	NCEP pressure
9	<i>x</i> CO ₂ water_equi_dry ²	μmol mol ⁻¹	2.9	WOA salinity
10	<i>x</i> CO ₂ water_SST_dry ²	μmol mol ⁻¹	3.1	WOA salinity
11	<i>x</i> CO ₂ water_equi_dry ¹	μmol mol ⁻¹	0.3	NCEP pressure
12	<i>x</i> CO ₂ water_SST_dry ¹	μmol mol ⁻¹	0.5	NCEP pressure
13	<i>x</i> CO ₂ water_equi_dry ^{1,2}	μmol mol ⁻¹	0.05	NCEP pressure, WOA salinity
14	<i>x</i> CO ₂ water_SST_dry ^{1,2}	μmol mol ⁻¹	0.2	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.

We expect that users of SOCAT data products:

- 1) Generously acknowledge the contribution of SOCAT data providers and investigators in the form of invitation to co-authorship**, reference to relevant scientific articles by data providers or by naming data providers in the acknowledgements.

Specifically, in regional studies invite large data providers, who frequently possess valuable expert knowledge on data and region, to collaborate at an early stage, which may lead to an invitation of co-authorship.

We recognize that co-authorship is only justified in case of a significant scientific contribution to a publication and that provision of data on its own does not warrant co-authorship.

- 2) Cite SOCAT and its data products as:**

Version 5: Bakker et al. (2016);
 Version 4: Bakker et al. (2016);
 Version 3: Bakker et al. (2016);
 Version 2: Bakker et al. (2014);
 Version 1 (synthesis data products): Pfeil et al. (2013);
 Version 1 (gridded data product): Sabine et al. (2013) and Pfeil et al. (2013).

- 3) Include in the acknowledgements:**

‘The Surface Ocean CO₂ Atlas (SOCAT) is an international effort, endorsed by the International Ocean Carbon Coordination Project (IOCCP), the Surface Ocean Lower Atmosphere Study (SOLAS) and the Integrated Marine Biosphere Research (IMBeR) program, to deliver a uniformly quality-controlled surface ocean CO₂ database. The many researchers and funding agencies responsible for the collection of data and quality control are thanked for their contributions to SOCAT.’

- 4) Report problems to submit@socat.info.
- 5) Inform submit@socat.info of publications in which SOCAT is used.
Please, contact the SOCAT investigators for further advice.

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