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SOCAT QUALITY CONTROL
HAVE YOU EVER WONDERED …

› what the difference between complete metadata for «traditional» instruments and complete metadata for «alternative» instruments really is?

› what «clear description of the calibration» methods actually mean?

› exactly how to judge when a cross-overs is high quality (for flag A)?

› if there is such a thing as «good enough» quality for a cross-over?
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 \( x_{CO_2} \) analysis, not \( f_{CO_2} \) 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.

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.
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.
Flags A, B, C and E require complete metadata. 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 ($x$CO$_2$, $p$CO$_2$, $f$CO$_2$);
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 ($x$CO$_2$, $p$CO$_2$, $f$CO$_2$);
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.
2.3 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.
QUESTIONS?

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