SOCAT Update and Road Ahead

IOCCP side event
at the 10th International Carbon Dioxide Conference (ICDC10),
Interlaken, Switzerland
Wednesday 23 August 2017, 13:00-14:30

Convenors: Dorothee Bakker, Kim Currie, Are Olsen
Minutes: Steve Jones
Report: Dorothee Bakker with input from speakers and Penelope Pickers

Introduction (Dorothee Bakker)
Dorothee Bakker provided an update on ongoing activities in SOCAT:

- SOCAT has its 10th anniversary in 2017 and celebrates this today at ICDC10.
- The automation of data upload has enabled annual SOCAT releases from version 4 onwards.
- SOCAT releases in June are timed for the annual Global Carbon Budget.
- The SOCAT website (**www.socat.info**) has been updated.
- The ongoing automation of uploading metadata is a top priority. Target is completion by summer 2018, in time for version 7. Kevin O'Brien will provide an update.
- Update of the 'Cookbook' for quality control is a high priority. Aim is to complete this in time for the bulk of the version 6 quality control. Siv Lauvset will discuss this revision.
- **Data submission for SOCAT version 6 ends on 15 January 2018 and V6 quality control ends on 31 March 2018**.

Authorship policy for the Global Carbon Budget - Dorothee Bakker reflected on ongoing discussions between Corinne Le Quéré, Are Olsen and herself on the authorship policy for the Global Carbon Budget's ESSD articles. She summarized the discussion as follows: One authorship will be offered per research group for providing surface ocean fCO_2 ocean measurements that make **a significant contribution** to the Global Carbon Budget, notably data holdings:

- with SOCAT data set quality flags of A to D (only),
- with at least 30 days of surface ocean fCO_2 measurements at sea in the year preceding the budget,
- that are made available in full.

Additional requests will be considered, for example authorship for:

- a 2nd group member for very large data providers,
- a provider of a significant data holding that does not quite meet the threshold criteria.

This policy may be refined further. Please, keep these authorship discussions honest and polite.

Discussion topics during this SOCAT hour - Dorothee highlighted topics on the possible future inclusion of parameters in SOCAT and/or the creation of products parallel to SOCAT to be discussed later in the meeting. She provided an overview of the status of these discussion items (Table 1). She emphasized that SOCAT needs to prioritize, that actions take volunteers and time to implement and that the annual SOCAT releases should not be put at risk.

Discussion

Rik Wanninkhof asked for a description of the options for submitting data to a data centre during SOCAT data upload. Dorothee Bakker clarified that the automated data upload system for SOCAT offers the data provider three options with respect to submission of the original data and metadata:

1) Immediate data submission to NCEI/OCADS (formerly CDIAC) (by SOCAT),
2) Data submission to NCEI/OCADS upon release of the next SOCAT version (by SOCAT),
3) The data provider takes responsibility for submission of the original data to a data centre for archival and for public release.

The data provider needs to select option 1, 2 or 3 before submission of the data set to the SOCAT quality control system.

Table 1: Discussion items on the possible future inclusion of parameters in SOCAT and/or products parallel to SOCAT and the status of these discussions.

What	Status	Who
Other surface ocean parameters (nutrients, DIC, TA, etc.)	In 2014 the SOCAT community agreed to include additional parameters without quality control and release these parameters in a separate file (SOCAT, 2014). The SOCAT global group proposes to start with GLODAP parameters and units, as defined in (Olsen et al., 2016) for V7.	Kevin O'Brien, Karl Smith, global group
Surface ocean CH_4, N_2O	Ongoing discussion since 2015 (SOCAT and SOCOM, 2015). The intention is a data product using the LAS infrastructure, parallel to, but independent from SOCAT.	Tobias Steinhoff, MEMENTO scientists, global group
Atmospheric CO_2	Discussions on the inclusion of atmospheric CO_2 data in SOCAT have taken place since 2014 (Appendix 6 in SOCAT, 2014). The scope and quality control need discussion.	Jonathan Bent, Penelope Pickers, Ingrid Van der Laan-Luijkx, Tobias Steinhoff, Rik Wanninkhof, others to be named, all SOCAT scientists
Calculated surface ocean fCO_2 from new observing platforms	New item for discussion. The SOCCOM community has asked whether calculated surface ocean fCO_2 from floats might be included in SOCAT.	All SOCAT scientists

Automated data upload (Camilla Landa)
Camilla Landa provided the following overview of automated data upload for SOCAT:

All data for SOCAT must be uploaded and submitted through the Upload Dashboard. Use of the Upload Dashboard has been demonstrated at previous meetings. This talk will highlight the advantages for Data Providers (DPs) of uploading and submitting their data themselves using the Upload Dashboard. Since SOCAT version 4 there have been two ways for the DPs to get their data into SOCAT: They can upload and submit their data through the Upload Dashboard, or they can ask a SOCAT Data Manager (DM) to do this for them. The percentage of data sets uploaded and submitted by Data Providers themselves has increased from 25% to 53% from SOCAT version 4 to 5, respectively.

Direct data upload and submission on the Upload Dashboard by the DPs has these advantages for Data Providers:

- The Upload Dashboard runs a sanity checker on the uploaded data; this includes checking for outliers, date time issues, and other things, and it also provides various property-property plots. This means that a Data Provider gets immediate feedback on the quality of their data. The Data Provider, who knows the data best, is the best person to interpret this feedback. A Data Manager uploading data will only inform the DP about serious issues, not about smaller issues, and will not have the time or expertise to evaluate the property-property plots. Also, since the Data Provider knows their data best, they are more likely to correctly identify the data column types or missing values during data upload.
- The Data Provider can upload and submit their data when convenient. SOCAT allows data submission all year round, thereby a Data Provider receives the quality feedback immediately. By contrast, a Data Manager will upload data in December-January, briefly before the submission deadline, which means that the Data Provider has to wait for quality feedback. They might receive this feedback when they are busy and do not have time to deal with it.
- The Data Providers who submit data themselves are likely to save time. They do not need to exchange e-mails with a Data Manager.
- The Upload Dashboard provides an overview of previously submitted datasets for each Data Provider. This makes it easy for the Data Providers to keep track of what they have already submitted.

The help page on the new SOCAT website (https://www.socat.info/index.php/socat-help/) has a video showing how to upload and submit data on the Upload Dashboard, and a document describing the process. Information on how new users can get a login also is on the site. Questions can also be sent to submit@socat.info.

Discussion
Liqing Jiang queried whether SOCAT has mechanisms for automating metadata processing in the upload system. Camilla Landa responded that such automation of metadata processing is being developed and that this is the subject of the video talk by Kevin O'Brien.

Rik Wanninkhof expressed the thanks of the SOCAT data providers to Benjamin Pfeil and Camilla Landa for their work on data upload. The automated system helps a lot, but the people behind it providing support are extremely important. Dorothee Bakker extended this thanks to Kevin O'Brien and Karl Smith at NOAA-PMEL who developed the software for the automated data upload. [Retrospective comment by Dorothee Bakker: And last but not least: Steve Jones also contributed to the automation of the data upload.]

Truls Johannessen pointed out that Bergen's work on data upload is funded through the ICOS OTC.

Automation of metadata upload (Kevin O'Brien)

Kevin O'Brien (NOAA-PMEL, USA) discussed progress on SOCAT metadata automation in a pre-recorded video. The aim of the automation is to automate quality control of the metadata, in order to improve the metadata quality and to reduce the quality control effort. The closure of CDIAC meant loss of support for the Online Metadata Editor (OME), which SOCAT had been planning to use. Instead, work funded in part by the NOAA Ocean Acidification Program (OAP) will now provide an OME-like editor for OAP data, which will be modified for SOCAT after its release to the OAP community in autumn 2017. SOCAT will use this as the new editor, while still supporting any OME-based XML files coming out of existing automated processes. Kevin showed an example of the SOCAT automated metadata form. The objective is to have the automated metadata upload in place for SOCAT version 7. Kevin welcomes volunteers for beta-testing the automated metadata upload.

There were no questions following the video presentation by Kevin O'Brien.

Surface water CH_4 and N_2O using SOCAT infrastructure (Tobias Steinhoff)

Tobias Steinhoff summarized the discussions with Hermann Bange, Annette Kock (for MEMENTO, MarinE MethanE and NiTrous Oxide) and Benjamin Pfeil, on the possible setup of a system for surface ocean methane (CH_4) and nitrous oxide (N_2O) using SOCAT infrastructure. There is a growing need for observing other greenhouse gases besides CO_2, e.g. CH_4 and N_2O. During the last years instruments have become available that can measure N_2O and CH_4 with the same frequency as is common for CO_2 measurements by infrared instruments. They can be used in existing setups for surface ocean CO_2 measurements without much effort. This results in data sets that have CO_2 and N_2O and/or CH_4 measurements combined. There is interest from the observationalist and modelling community to combine these data streams.
These questions need addressing, before using the SOCAT infrastructure for MEMENTO data sets:

- Can MEMENTO use the SOCAT LAS system for CH_4 and N_2O?
- What changes would be needed?
- How would the quality control be done for the CH_4 and N_2O data?

We do not want to risk the very high reputation that SOCAT has for its high quality data.

Discussion
Rik Wanninkhof queried the expected data volume and whether the data would include data from Ships of Opportunity in near real time. Tobias Steinhoff did not want to hazard a guess on data volume. [Retrospective comment by Tobias Steinhoff: To date there are approximately 400 data submissions with 120,000 data points for N_2O in MEMENTO. Roughly 90% of these data are surface data.]

Tobias Steinhoff stressed that that several data providers are measuring CO_2 and CH_4/N_2O in parallel, and that these currently have to split their data streams and submit to multiple locations. Andrew Watson wondered whether we are trying to integrate these projects simply for the convenience of data providers? Data users will use N_2O data for different purposes than SOCAT CO_2 data, with different criteria, so it may not fit the data users to integrate them. Tobias Steinhoff responded that this requires discussion. We are looking at how we might collaborate. Where there is overlap and synergy we should work on combining systems, but we should not force integration where it is not appropriate.

[Retrospective comment by Dorothee Bakker: Such a system would be parallel to, but independent from SOCAT. The MEMENTO scientists would take responsibility for the N_2O and CH_4 set up and quality control.]

SOCAT quality control (Siv Lauvset)
Siv Lauvset provided a summary of known issues where the SOCAT quality control cookbook (Olsen et al., 2015) needs clarification. These are:

- The difference between complete metadata for 'traditional' (infrared, gas chromatograph, cavity ringdown spectrometer) instruments and for 'alternative' (sensor) instruments,
- A 'clear description of the calibration' methods,
- How to judge when a cross-over is high-quality (for flag A),
- Is there such a thing as 'good enough' quality for a cross-over?
- Consistency in when bracketing by calibration gases is needed and how many non-zero calibration gases are needed:
  - 'For a flag of A or B the calibration has to include at least two non-zero gas standards, traceable to World Meteorological Organisation (WMO) standards'*,
  - 'For flags of C and D for infrared-based systems this means at least two calibration gases, such that the samples is bracket 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.'
- Use of references to publications as single source of metadata. References can be used in addition to metadata, but should not be used instead of 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 the metadata.'
- Clarification how warming of up to 3°C affects the data accuracy (and thus the data set flag).
  - 'Warming should be less than 3°C.'

*[Retrospective note by Rik Wanninkhof: Based on 2017 GGMT meeting (Switzerland, 28/08-01/09/2017), we need to be more specific on what WMO scale the standards are traceable to, e.g. WMO-X2006.]

Discussion
Rik Wanninkhof agreed with Siv Lauvset that there is a clear need to update the cookbook. However, Rik would prefer a complete review of the quality control procedures, rather than simply ironing out the inconsistencies.

Adrienne Sutton expressed a concern that quality control might suffer if cruise flags were to be upgraded as a result of a crossover.

Masao Ishii wondered if the quality control criteria cover cavity ringdown systems. Siv Lauvset responded that these are included in the existing quality control procedures.

Andrew Watson commented that one should correct to a 'consistent, representative' sea surface temperature as proposed by Goddijn-Murphy and co-authors, rather than correct to the inlet temperature as currently done in SOCAT. Jamie Shutler expressed a concern that users of SOCAT do not understand this temperature issue. Jamie proposed to warn users of SOCAT data products or alternatively to recalculate SOCAT fCO_2 values with the correction by Goddijn-Murphy et al. (2015). [Retrospective note by Dorothee Bakker: Goddijn-Murphy et al. correct fCO_2rec values (at the intake temperature) reported by SOCAT to the equilibrator temperature and then correct to the true, 'consistent and averaged' sea surface temperature (Goddijn-Murphy et al., 2015; Woolf et al., 2016).]

Siv Lauvset added that the lack of thorough quality control of salinity data in SOCAT is a substantial problem.

Atmospheric CO_2 (Jonathan Bent)
Jonathan Bent introduced initial thoughts on the inclusion of atmospheric CO_2 in SOCAT. Jonathan in collaboration with Penelope Pickers (University of East Anglia) and Ingrid Van der Laan- Luijkx (Wageningen University& Research) has produced a set of possible quality control flags for air measurements that he showed. Jonathan and Penelope are keen to work with the SOCAT community to incorporate quality controlled atmospheric XCO_2 (CO_2 mole fraction) measurements as part of the SOCAT holdings. Here are two, very preliminary, draft, pilot examples of what a flagging system might look like:

A3(viii)	**Low/undefined accuracy, moderate precision** · No target tank measurements, intercomparison activities or companion flask measurements made so accuracy is undetermined. · Hourly ±1σ standard deviation on 'low variability sample air' is ≤ **XXXX** but ≥ **XXXX**. Dataset does not contain evidence of step changes/leaks. · No specific calibration protocols followed for atmospheric CO_2 data (i.e. no limited range on calibration scale, no requirement for dry cylinders in natural air, or less than three PSSes).

A1(i)	**High accuracy, high precision** · Compatibility of dataset meets WMO NH/SH goal as quantified by Target tank and/or intercomparison activities (NH = ± 0.1 ppm; SH = ± 0.05 ppm). · Hourly ±1σ standard deviation on 'low variability sample air' is ≤ **XXXX** and on target tank or other cylinder air is ≤ **XXXX**. Dataset does not contain evidence of step changes/leaks. · Regular calibration of measurement system using a suite comprising a minimum of three NOAA scale Primary Secondary Standards (PSSes) of dry, natural air. PSSes span the ambient range of atmospheric CO_2 values by not more than ± 50 ppm (i.e. for atmospheric CO_2 of 400 ppm in 2017, maximum scale range does not exceed 350-450 ppm). · Air that is not fully dried is being corrected for H_2O dilution effects, and water correction is robust.

Many pCO_2 systems would currently qualify for this type of flag A3(viii).

The flag A1(i) is probably quite daunting right now, but is the highest possible flag, and is designed to be future proofed (and is determined by what the ultimate atmospheric scientific goals are).

There are a number of considerations for moving forwards:

- A set of atmospheric flags should only be implemented after full consultation with both the oceanic and atmospheric measurement communities.
- This is a great opportunity for our two communities to work closer together (we could both learn a lot from each other).
- There are lots of fine details to be discussed another time (e.g. drying issues, inlet lines, number of calibration gases, participation in intercomparison programs, etc.).
- [Retrospective comment by Penelope Pickers after the GGMT side session: The ocean community would like an SOP (Standard Operating Procedures) document for making the atmospheric measurements. Rik Wanninkhof would like the SOP to be a priority.]

In particular, Jonathan and colleagues would like input on:

- Is this worth your consideration?
- How much data is there already?
- How many people are needed for quality control?

- Include all atmospheric CO_2 data or just some?
- Timeline: flagging, software automation…
- Same flags as for surface ocean CO_2 or not?
- Would the audience like to look at our flagging recommendations?

Discussion

Are Olsen queried the requirements stating that measurements should be taken every hour. Recommendations for underway measurements and incorporated in GO (General Oceanics) systems operations procedures, for example, typically measure atmospheric CO_2 every 3rd hour. Will this kind of frequency be sufficient? Jonathan Bent responded that every 3 hours would probably be sufficient, but that this will need more discussion. Another issue is the need for a flag that states whether measurements are open ocean ('background') or coastal. We would want more frequency at the coast.

Andrew Watson suggested that as a general approach to specifying requirements, it may be best to say what accuracy you want. We cannot assess accuracy [numerically] very easily, so you could follow SOCAT's example of assigning flags based on instrumentation quality, standards, traceability etc. The whole activity needs to be simplified as much as possible to minimise the additional workload on those doing the quality control. Jonathan Bent responded that it is important to get quality control resources in place from the atmospheric community to avoid putting extra work on existing SOCAT quality controllers.

Werner Kutsch noted that the ICOS RINGO project will be deploying a Picarro sensor on a ship to try to achieve the same accuracy and precision as land-based stations. This effort will need strong inputs from the atmospheric community.

Christian Rödenbeck queried what uses the ocean community would have for this atmospheric CO_2 data. Input to flux inversions is an obvious example, although high accuracy would be required. Are there any other uses, e.g. calculation of local CO_2 fluxes, and what accuracy would then be required? Jonathan Bent: Good point.

Ute Schuster commented that very high precision is not possible. Ocean scientists can get around 0.3 ppm, but 0.1 ppm is not possible now. Jonathan Bent agreed that getting to 0.1 ppm would be a longer term goal.

Ute Schuster suggested that we should aim to install separate atmospheric and ocean system on ships, but the ocean community cannot implement that with current resources.

[Retrospective comments by Penelope Pickers after the GGMT meeting:

- Ships would need to start assessing their accuracy. There are various options for doing this: Target Tanks, intercomparisons, co-located flask measurements, etc.
- Provision of the quality control resources should not solely be the responsibility of the atmospheric community. It would be better in the long term if this responsibility is either shared or mostly done by the ocean community.

- It might not be necessary to build separate systems for atmospheric CO_2 measurements.
- There are ships that are currently achieving a precision better than 0.3 ppm. But in any case, it is more important that the data are as accurate as possible, and we can worry about the precision later.]

Calculated surface water fCO_2 from new observing platforms (Rik Wanninkhof)
In his presentation Rik Wanninkhof made the case that surface calculated fCO_2 values from new observing platforms should not be included in SOCAT. While SOCAT could in theory provide such calculated fCO_2, we do not want to mix two data 'streams' of measured and calculated surface ocean fCO_2 in SOCAT. Having separate data streams from separate sources, with tools to allow merging of those streams, will be a better approach

Discussion
Dick Feely commented that the inaccuracies in calculated fCO_2 show that we have a fundamental misunderstanding of the CO_2 system. We need to work on this with the SOCCOM community. Rik Wanninkhof agreed and indicated a need for intercalibration studies to progress on this.

Ute Schuster queried what is wrong with having the pH measurements (from the new observing platforms) in SOCAT and let people use them as they wish, like SOCAT plans to do for dissolved inorganic carbon (DIC) and Alkalinity? SOCAT would not provide recalculated fCO_2. Rik Wanninkhof responded that there are many different ways to calculate the fCO_2, and that the users want an fCO_2 product with minimal effort.

Niki Gruber stated that maintaining the accuracy of SOCAT [which is a strong basis of its reputation] is crucial. He strongly recommend to take this on, even if through a separate database, and through this we could provide impetus to improve the accuracy of the calculation methods. For users, having data in one place is much easier and will increase data usage. Also, a lot of applications do not need the highest quality, e.g. anomaly analysis, so combining the two data sets would make sense. Rik Wanninkhof agreed that the SOCAT community should be actively engaged in this effort. SOCAT can be most useful in a verification and validation role. But SOCAT should remain an annual updated product of known quality, and we should not add calculated fCO_2 to that. Rik encouraged integration of separate data streams.

Benjamin Pfeil raised the need the infrastructure and funding for these products. Benjamin considered that excluding these projects from SOCAT might reduce our ability to get funding for SOCAT.

Are Olsen recommended forcing users to specify what precision of data they require when selecting data from different data streams. The tools will then filter all the available data accordingly.

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