Surface Ocean CO_2 Atlas (SOCAT) Community Event

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Surface Ocean CO_2 Atlas (SOCAT) Community Event

Convenors: Dorothee Bakker, Are Olsen, Kevin O'Brien, Maciej Telszewski, Bronte Tilbrook

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Abstract:
The Surface Ocean CO_2 Atlas (SOCAT) is an activity by the international marine carbon research community. This SOCAT Community Event is an event by and for the SOCAT Community. SOCAT aims to improve access to surface water CO_2 data by regular releases of quality controlled, synthesis and gridded fCO_2 (fugacity of carbon dioxide, similar to partial pressure) data products for the global oceans and coastal seas. SOCAT version 1 was publicly released in 2011, version 2 in 2013. Version 2 has 10.1 million surface water fCO_2 data from 2660 datasets between 1968 and 2011.

About 1940 datasets have been submitted to SOCAT version 3 with half of these new data. Version 3 extends the dataset to December 2013 and includes CO_2 measurements from alternative sensors and platforms. Quality control for version 3 will be carried out from September to November 2014. Regional groups may need quality control meetings. Any marine carbon scientist keen to become a quality controller should contact the respective regional group lead and Dorothee Bakker. **Quality control comments should be adequate and fully justify the dataset quality control flag.** New features in the version 3 quality control system will include: 1) Check-boxes will correspond to the criteria for dataset quality control flags; 2) A dataset quality control flag can only be submitted, if the corresponding check-boxes have been ticked and a text comment has been entered; 3) The Expocode of the cross-over dataset must be specified for submission of a dataset flag of A; 4) Adding a quality control comment without submitting a dataset quality control flag will be possible. Some changes have been made and are being made to the version 3 quality control system, as a direct consequence of the automation effort.

The automation system for data submission (for version 4) will be launched in late 2014/ early 2015. It will enable data providers to upload their data directly onto the SOCAT quality control system and to check their data using SOCAT quality control tools prior to submission to SOCAT.

Data providers should ONLY submit fully documented, good quality data to SOCAT. SOCAT version 4 will allow data providers to submit provisional dataset and WOCE flags for their CO_2 data. The participants agreed that from SOCAT version 4 onwards:

- **Additional surface water parameters will be accepted** by SOCAT.
- **Only directly measured, either discrete or continuous parameters** will be included.
- **Additional parameters will not be quality controlled.**
- **Additional parameters will be in separate output files.** Thus, there will be two types of output files, one with quality controlled surface water fCO_2 values, including sea surface temperature and salinity, and one with non-quality controlled ancillary data.

Further discussion is needed on how or when additional parameters will be made available, either during each SOCAT release or upon request only.

SOCAT carries out quality control for surface water fCO_2 only. Sea surface temperature (SST) and salinity are only checked in as far as this is relevant for (re-)calculation of surface water fCO_2. Salinity and SST in SOCAT data products have not been fully quality controlled! SOCAT urges data providers to provide fully calibrated, high quality salinity and SST data, as part of the surface water CO_2 data set.

The participants discussed opportunities and challenges for SOCAT. Topics included: 1) Acknowledgements and credits for data providers and funding agencies, 2) Collaboration with the Global Carbon Project, 3) Measuring the success of SOCAT and 4) Plans for SOCAT science. Acknowledgements and credits are essential for data gatherers, funding agencies and future SOCAT releases. The SOCAT data policy states that data providers should be consulted and considered for co-authorship, if SOCAT is used for a regional study. One measure of success is that SOCAT has been cited or named in more than 38 peer-reviewed scientific publications (2014 – 15; 2013 – 18; 2012 - 2; 2011 – 1; 2010 – 1; 2009 - 1) and 3 book chapters (2014). This list of peer-reviewed, scientific publications will be made available on the SOCAT website. SOCAT data products are used for a variety of scientific studies, notably process studies, quantification of the ocean carbon sink, its seasonal, year-to-year and decadal variation and the initialisation and validation of ocean carbon cycle models. An example is the Surface Ocean pCO_2 Mapping Intercomparison (SOCOM). The OceanGHG Flux project (http://www.oceanflux-ghg.org), a European Space Agency project, heavily relies on SOCAT. The Global Carbon Project used one data product based on SOCAT version 2 in its 2013 Global Carbon Budget and will use four such products for the 2014 Budget (Le Quéré et al., 2014). The Community Event updated SOCAT scientists on recent progress, welcomed new members, enabled discussion of SOCAT strategy and informed the SOCAT agenda for the next 24 months.

Chair: Bronte Tilbrook, Rapporteur: Steve Jones

1 Introduction and Aims of the SOCAT Community Event (Dorothee Bakker)

Dorothee Bakker, chair of the SOCAT global group, welcomes the participants, introduces SOCAT and lists the aims of the SOCAT Community Event. The Surface Ocean CO_2 Atlas (SOCAT) is an activity by the international marine carbon research community. The SOCAT Community Event is an event by and for the SOCAT Community.

The SOCAT Community Event has these aims:

- Update the SOCAT Community on SOCAT progress;
- Welcome new members;
- Get feedback from the SOCAT Community;
- Set the SOCAT strategy and agenda for the next 2 years.

These key questions will addressed:

- How do we promote efficient quality control (version 3)?
- How does data submission via the automation system work (version 4)?
- Should SOCAT products include additional parameters (version 4)?
- How do we promote SOCAT science?

These key questions will be addressed in three sessions:
Session 1 SOCAT version 3 quality control
Session 2 Automation for version 4
Session 3 Future SOCAT

After setting out the aims of the meeting Dorothee Bakker asks in a brief show of hands which participants have provided data to SOCAT, which participants have been quality controllers or would like to become one, who is a using SOCAT and who is new to SOCAT. All categories are present at the Community Event (Appendix 2).

Dorothee Bakker provides an overview and update on SOCAT. SOCAT aims to improve access to surface water CO_2 data by regular releases of quality controlled, synthesis and gridded fCO_2 (fugacity of carbon dioxide, similar to partial pressure) data products for the global oceans and coastal seas. SOCAT version 2, public since June 2013, contains 10.1 million surface water fCO_2 data from 2660 datasets between 1968 and 2011. The SOCAT website (http://www.socat.info/) provides access to all SOCAT data products and tools. Powerful online viewers at the NOAA-PMEL Live Access Server enable interactive interrogation of the SOCAT synthesis and gridded products. The products are available in various formats, e.g. text, NetCDF and Ocean Data View. Matlab code is available for reading some of these formats. SOCAT versions 1 and 2 were documented in three publications: Pfeil et al. (2013), Sabine et al. (2013) and Bakker et al. (2014).

SOCAT has a large number of contributors (Appendix 3). Quality control (Session 1) is carried out by regional groups. Quality control for version 3 will be carried out from September to November 2014. Dorothee Bakker asks whether the regional groups need meetings for

version 3 quality control. Anyone keen to become a quality controller should contact the respective regional group lead and Dorothee Bakker. Version 3 extends the dataset to December 2013 and includes CO_2 measurements from alternative sensors and platforms. The dataset quality control flags were revised for SOCAT version 3 to enable inclusion of data from alternative sensors and platforms, as described in Wanninkhof et al. (2013).

The automation system will streamline SOCAT data submission, quality control and releases. Automated data submission (for version 4) will be launched in late 2014 or early 2015 (Session 2).

The Global Carbon Project has asked access to data submitted to SOCAT for use in the Global Carbon Budget 2014, prior to SOCAT quality control of these data. A consultation by email and at a CarboChange project meeting has given these results:

24 – I am in favour, incl. 2 with a concern on 1-author policy;
05 – I have no opinion (yet)/ I have to know more;
05– I am against, incl. 2 with 'wait until SOCAT fits GCP timescale';
34 – Total

The collaboration between SOCAT and the GCP will be discussed in Session 3.

SOCAT data products are used for a variety of scientific studies, notably process studies, quantification of the ocean carbon sink, its seasonal, year-to-year and decadal variation and the initialisation and validation of ocean carbon cycle models. Dorothee Bakker identifies five scientific presentations at the IMBER Open Science Conference using SOCAT data products. An example is the Surface Ocean pCO_2 Mapping Intercomparison (SOCOM), led by Christian Rödenbeck. It is still open to contributions from data-based pCO_2 mapping products. The OceanGHG Flux project (http://www.oceanflux-ghg.org), a European Space Agency project, heavily relies on SOCAT. SOCAT has been cited or named in more than 38 peer-reviewed scientific publications (2014 – 15; 2013 – 18; 2012 - 2; 2011 – 1; 2010 – 1; 2009 - 1) and 3 book chapters (2014).

The SOCAT data policy asks users to recognise the contribution of SOCAT data contributors and quality controllers in the form of invitation to co-authorship or citation of relevant articles and to cite the relevant SOCAT ESSD publication, documenting the data product. Acknowledgements and credits for data providers will be discussed in Session 3.

Finally Dorothee Bakker asks participants to sign a card for Steve Hankin of NOAA-PMEL. Steve has been active in SOCAT since 2007 and has been responsible for designing the SOCAT online quality control system, the interactive viewers and the automation system. Kevin O'Brien has replaced Steven Hankin on the SOCAT global group.

Discussion: Introduction and Aims of the SOCAT Community Event

Dick Feely asks whether this presentation will be made public, e.g. for NOAA Programme managers. Dorothee Bakker replies that the presentation will be made public.

2 Session on SOCAT version 3 quality control (Rik Wanninkhof, Ute Schuster, Are Olsen)

In this session we present the secondary quality control (QC) process of the Surface Ocean CO_2 Atlas and seek input from the SOCAT community on what level of quality is required for different uses of SOCAT, such as quantification of sea-air CO_2 fluxes on various time and space scales, patterns of ocean acidification and extrapolation of laboratory and mesocosm findings on the effects of ocean acidification. The session aims to widen the uses of SOCAT and solicit feedback on current secondary quality control practices, in particular how to include new sensors, how the dataset quality control flags are used in creating data-based mapping products and other applications. We also encourage more groups to become involved in the community-based secondary quality control efforts.

2.1 Update on version 3 (Benjamin Pfeil, Karl Smith, Kevin O'Brien)

Benjamin Pfeil provides an update on SOCAT version 3. About 1850 datasets collected between 1957 and 2013 have been submitted for version 3 (Figure 2.1). Most data providers followed requests from SOCAT and the wider marine carbon community to submit data directly to the Carbon Dioxide Information Analysis Center (CDIAC). The data submissions include many updates of data submitted to earlier SOCAT versions, as data providers have implemented recommendations and feedback from SOCAT quality control. The data submissions include data from alternative sensors.

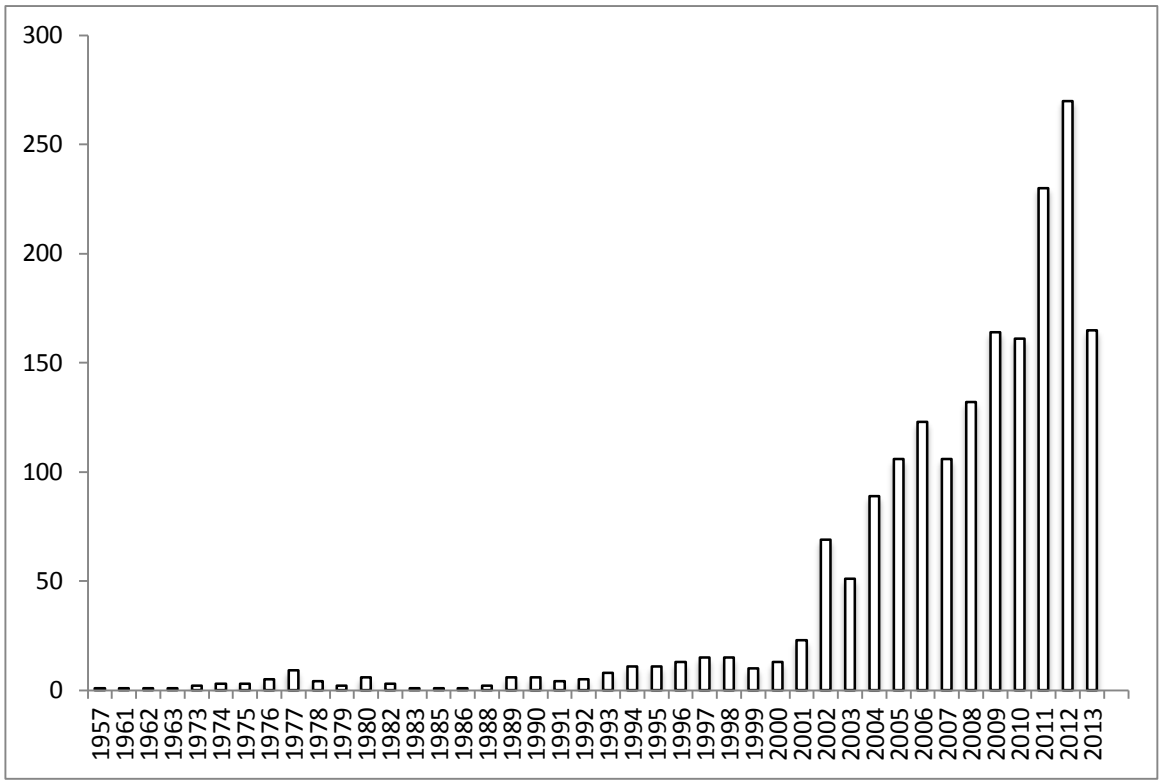


Figure 2.1. The number of new and updated files submitted to SOCAT version 3 by year.

Benjamin Pfeil highlights several changes in data entry for version 3 in comparison to version 2. He and his colleague Camilla Landa are using the dashboard at NOAA-PMEL for uploading the data into the SOCAT quality control system. This provides a test for the SOCAT automation system (Session 2). The Matlab routines for (re-)calculation of fCO_2 at sea surface temperature used for versions 1 and 2 have been converted to centralised routines at the automation dashboard for version 3. A range checker, being developed by Steve Jones, Karl Smith and Kevin O'Brien, is used for identification of out-of-range data. Thus basic quality control issues are being identified by the automation system, which will reduce the work for the quality controllers.

The quality control system on the Live Access Server (LAS) in version 3 will have the same capabilities as in version 2. However, it will look slightly differently and have a better performance. The quality control system will need to be tested by experienced quality controllers, before general quality control opens.

2.2 Version 3 and 4 time table (Dorothee Bakker)

Dorothee Bakker presents the time table for versions 3 and 4:
Time table for version 3:

- V3 1940 cruises, 1957-2013 on quality control system (July 2014)
- V3 Tests of quality control system (Aug 2014)
- V3 Quality control by regional groups (1 Sep- 30 Nov 2014)
- V3 QC meetings and web seminars by regional groups
- V3 Quality control complete (30 Nov 2014)
- V3 Early release (spring 2015)
- V3 Public release (summer 2015)

Timetable for version 4

- V4 Submit data to CDIAC (any time)
- V4 Tests of automated data upload (autumn'14)
- V4 Data submission system live (late '14/early '15)

Any marine carbon scientist keen to become a quality controller should contact the respective regional group lead and Dorothee Bakker. The SOLAS Open Science Conference from 7 to 11 September 2015 in Kiel, Germany, is a possible venue for the public release of SOCAT version 3.

Discussion: Version 3 and 4 time table
Maciej Telszewski and Benjamin Pfeil comment that the large amount of data submitted to version 3 imply a major quality control effort with the potential to miss the quality control deadline. Rik Wanninkhof queries whether any group will be overwhelmed by the quality control and how realistic the time table is. Maciej Telszewski asks what the proportion is of data submissions in the various quality control regions (Appendix 3). Dorothee Bakker replies that many datasets will cross the coastal region, similar to versions 1 and 2.

Dorothee Bakker wonders whether the regional groups need quality control meetings. Such meetings may promote quality control. Maciej Telszewski comments that the coastal group has had problems in completing its heavy quality control load in version 1. A quality control workshop by the coastal region was highly successful for version 2. Ute Schuster raises the possibility of web seminars (webinars) or video-conferences for quality control by regional groups.

2.3 Revised dataset quality control flags in version 3 (Rik Wanninkhof)

Rik Wanninkhof introduces secondary quality control in SOCAT. In secondary quality control the submitted dataset is reviewed in context of specific metrics relating to environment, instrument, completeness of metadata and neighbouring cruises. The secondary quality control is largely based on instrumental requirements and provides a letter code for each dataset, determined by a prescribed protocol. The letter code (A-F, S, X) is based on the type of instrument and calibration procedure, as described in the accompanying metadata using standardised metadata forms. For version 3 the letter codes have been revised to include a semi-quantitative estimate of uncertainty of the measurements in the dataset (Appendix 4) (Wanninkhof et al., 2013). A flag of E has been added to accommodate **alternative sensors** (Appendix 4), whose accuracy is difficult to estimate with current procedures. The accuracy estimates are based on side-by-side comparisons of instruments in both laboratory settings, such as multi-national comparison efforts, and in the field by deploying several instruments on the same platform. Only datasets deemed acceptable are included in the SOCAT data products.

Cross-overs, comparison of data in the same location and time span determined from a time-space correlation estimate (Appendix 4), are a significant component of secondary quality control. There only is a true intersect (in time and space), when a ship is right next to mooring or another ship. A **high-quality cross-over** is now required for a flag of A (Appendix 4) (Wanninkhof et al., 2013), a revision of the requirement of an acceptable cross-over in versions 1 and 2. Most coastal data will not receive a flag of A, because of small-scale variability.

Discussion: Revised dataset quality control flags in version 3
Bronte Tilbrook wonders how the submission of alternative sensor data to version 3 will impact on the quality control process. Dorothee Bakker notes that sensor data included in SOCAT versions 1 and 2 need to be quality controlled following the revised flagging scheme.

Are Olsen comments that dataset flags encourage marine carbon scientists to improve the quality of data collection and data reporting. Hopefully the proportion of higher quality flags (A, B) will increase over time. Rik Wanninkhof confirms that data quality has improved from SOCAT version 1 to version 2 (Bakker et al., 2014).

2.4 Planned quality control for version 3 in practice (Ute Schuster)

Ute Schuster emphasizes that **quality control comments should be adequate** and fully justify a dataset quality control flag (Appendix 5). An adequate record of why a dataset passed (or failed) certain quality control criteria is critical, so that another quality controller or the data provider can assess how the initial quality controller came to his/her conclusion and exactly what was checked.

Steve Jones wonders whether the quality control system should require a text comment when a dataset quality control flag is entered. Are Olsen asks whether check-boxes can be added to the quality control form. Such check-boxes would define the dataset quality control flag (A-F, S, X), i.e. what quality control criteria the dataset has passed or failed. Steven van Heuven argues that check-boxes alone are not sufficient and that the quality controllers also need a text box for comments on why a dataset did or did not meet certain criteria.

Karl Smith confirms that for version 3 quality control:

- There will be check-boxes corresponding to the criteria for dataset quality control flags;
- A dataset quality control flag can only be submitted, if the corresponding check-boxes have been ticked and a text comment has been entered.
- The Expocode of the cross-over dataset must be specified for a flag of A.
- Adding a quality control comment without submitting a dataset flag will be possible.

Reiner Schlitzer asks for clarification on the types of quality flags in SOCAT. Rik Wanninkhof clarifies that there are dataset quality control flags (A-F, S, X) (Appendix 5) and WOCE flags for individual fCO_2 values (2: good, 3: questionable, 4: bad). **The quality control flags only reflect the quality of recommended fCO_2** and do not apply to other parameters. Most SOCAT synthesis data products only report fCO_2 values with a WOCE flag of 2. Values with flags of 3 and 4 are available upon request via the Cruise Data Viewer. The gridded data products only have data points with a WOCE flag of 2 (Bakker et al., 2014). Quality control comments for datasets with flags of A-D (A-E in version 3) are made public via the Table of Cruises on the Cruise Data Viewer.

Rik Wanninkhof asks how many users of SOCAT data products actually look at the dataset quality control flags. Essentially none of the participants use these dataset flags. Christian Rödenbeck has so far only used WOCE flags and wonders whether he should also use the dataset flags. Rik Wanninkhof replies that dataset flags of A-C give an assessment of the instrument standards, rather than an assessment of the individual measurements. Are Olsen adds that many datasets with a flag of D are of good quality, but have incomplete metadata. Therefore users might not need to consider the dataset flags. Ute Schuster adds that if a user would want an uncertainty of less than 2 µatm, the user should use datasets with flags of A or B.

Are Olsen suggests that dataset quality control flags A-E should be added to the SOCAT synthesis data product available via Ocean Data View (ODV) (Bakker et al., 2014). Reiner Schlitzer will look into this.

Reiner Schlitzer queries whether it would be useful to add the quality control comments to all SOCAT synthesis files. A discussion follows with some in favour and others not seeing the need for this. Are Olsen comments that addition of quality control comments as text strings will complicate manipulation of the files in e.g. Matlab and therefore argues against the addition of quality control comments to synthesis files.

Dick Feely notes that a ship-based dataset may be good quality for the duration of the cruise, but that a mooring dataset can be good for a while and bad later. Dick wonders how SOCAT quality control deals with this. Dorothee Bakker comments that the individual fCO_2 values in the first part of the dataset might be flagged as good (WOCE flag of 2) and the second part as bad (flag of 4). Bronte Tilbrook adds that once bad data points have been flagged as bad, the dataset may still receive a flag of A-E.

Bronte Tilbrook asks whether it is possible to automatically add figures of cross-over properties as supplementary information for a dataset. Karl Smith replies that this capability will be considered for version 4.

Chair: Kim Currie, Rapporteur: Ingunn Skjelvan

2.5 Other issues for SOCAT version 3 quality control (Rik Wanninkhof)

Rik Wanninkhof continues the discussion on WOCE flags for individual (re-)calculated fCO_2 values (2, 3, 4) and dataset quality control flags (A-F, S, X) (Appendix 5). Only (re-)calculated fCO_2 values have a WOCE flag. Other parameters (e.g. sea surface temperature, equilibrator temperature, salinity) do not have WOCE flags. SOCAT should ask data providers to provide provisional dataset quality control flags and WOCE flags during data submission and to justify the flags with clear comments. The participants agree that SOCAT version 4 will allow the data provider to submit provisional dataset flags and WOCE flags with their data.

SOCAT carries out quality control for surface water fCO_2 only. Salinity and sea surface temperature are checked only in as far as this is relevant for (re-)calculation of surface water fCO_2. Therefore sea surface temperature and salinity in SOCAT data products have not been quality controlled. SOCAT urges data providers to provide fully calibrated, high quality and high accuracy salinity and sea surface temperature.

Rik Wanninkhof discusses sea surface temperature (SST) and the temperature correction for (re-)calculated fCO_2. The NOAA-AOML team flags surface water CO_2 data as 3 (questionable) or 4 (bad), if warming between the water intake and the equilibrator exceeds 1°C or cooling exceeds 0.5°C. This is a good diagnostic for rapid flushing of the equilibrator. Sea surface temperature in SOCAT is defined as the temperature at the sea water intake and depends on the position of the SST sensor which differs from ship to ship. The degree of warming (or

cooling) depends on SST and warming is likely to be higher in high latitude regions. The temperature correction introduces uncertainty in (re-)calculated fCO_2. There are different relationships to correct for warming (e.g. Mehrbach et al., 1973; Goyet and Poisson, 1989; Takahashi et al., 1993). Also it takes time for seawater to travel from the intake to the equilibrator, typically 1 to 5 minutes. Not all data providers correct for this delay. Rik Wanninkhof notes that mapping techniques for fCO_2, e.g. for the creation of basin-wide fCO_2 maps, often use remotely sensed sea surface temperature.

Rik Wanninkhof asks whether SOCAT should therefore focus on fCO_2 at the equilibrator temperature and pressure (fCO_2_Tequ_ Pequ), rather than on fCO_2 at SST and atmospheric pressure. Several participants comment that this is **not** advisable. It is questionable whether the users can handle the conversion from fCO_2 at Tequ to fCO_2 at SST.

Dorothee Bakker comments that the SOCAT uses different temperature criteria for quality control from those mentioned by Rik Wanninkhof. For example, the Southern Ocean group applies a criterion that warming should be less than 3°C and deems cooling unlikely (Bakker et al., 2014). A comment is made that a stepwise temperature correction (steps of 0.5°C) might be made for temperature differences between 1.5°C and 3.0°C.

Rik Wanninkhof describes the (re-)calculation of fCO_2 at sea surface temperature from the reported surface water xCO_2, pCO_2 or fCO_2 value in SOCAT. There is a strict order of preference for the input parameter with the mole fraction of CO_2 in dry air at equilibrator temperature (xCO_2water_equi_dry) as the preferred input parameter (Pfeil et al., 2013; Bakker et al., 2014). However, quality control and adjustments by the data provider are often not properly incorporated, as the following example illustrates:

'As part of the quality control process, each dataset is compared with the Marine Boundary Layer (MBL) data from GlobalView-CO_2. The CO_2 air data from this mooring deployment were on average -3.7 ± 0.8 µmol/mol below the MBL data and therefore a correction of +4 µmol/mol was applied to the air and seawater xCO_2(wet) data from the mooring.'

Discussion: Other issues for SOCAT version 3 quality control

A comment is made that the xCO_2 submitted should be truly dry and not partly dried. Steven van Heuven notes that Pierrot et al. (2009) state that Li-COR versions LI-6262, LI-7000, and LI-840 all perform a correction for dilution by water vapour:

"The system can accommodate three models, according to the user's need: the LI-6262, LI-7000, and LI-840. The LI-840, having a lower accuracy and higher signal-to-noise ratio, will likely not meet the specified accuracy of 0.2 ppm for atmospheric air samples, but some users find it adequate for their needs. The CO_2 measurements are corrected for the dilution by water vapor and band-broadening pressure effect by the firmware internal to the analyser such that they report a dry mole fraction. The sample gas is dried to a water mole fraction of about 2 ppt, making this correction small and minimizing the errors associated with it."

However, this is only correct for version LI-6262. Rik Wanninkhof confirms this. The LI-6262 and LI-840 have an option for a band broadening correction. The data reduction program by Denis Pierrot has been changed and can now do calculations for both types of Li-CORs (those with and without the vapour correction).

Chair Siv Lauvet, Rapporteur: Ingunn Skjelvan

2.6 Discussion of version 3 quality control (Ute Schuster)

Ute Schuster emphasizes the importance of consistent quality control and the need to enter comments for all quality control steps, for example on each property check, on each crossover check (while noting the Expocode) and on the adequacy of the metadata. Dorothee Bakker promises to update the quality control cookbook for version 3, bringing together the revision of the quality control flags (Appendix 5) (Wanninkhof et al., 2013) with relevant sections in SOCAT publications (e.g. Bakker et al., 2014) and recommendations from this meeting (Appendix 6).

A suggestion is made that data submitters need clear instructions (a cook book) on how to calculate, adjust, perform initial quality control and submit data. Ute Schuster comments that the European ICOS (Integrated Carbon Observation System) program has funding for bringing groups together in order to unify datasets and carry out primary quality control. Rik Wanninkhof and Kim Currie stress that data providers need to carry out their own quality control prior to submission to SOCAT. **Data providers should ONLY submit fully documented, good quality data to SOCAT**

3 Session on Automation for version 4 (Kevin O'Brien, Steve Jones)

In this session, we present and discuss the advances in automating the various SOCAT processes. The completion of SOCAT versions 1 and 2 demonstrated that the process for data entry, quality control and releasing new versions of the SOCAT collection is too labour intensive to sustain. An 'automation' plan was therefore agreed upon for streamlining the process as much as possible (SOCAT, 2012a, 2012b). The automation will reduce work for data managers and quality controllers and will streamline SOCAT releases.

3.1 Automation for version 4 and implications for version 3 quality control (Kevin O'Brien, Steve Jones, Karl Smith)

Kevin O'Brien presents the automation system for SOCAT version 4. The presentation and a series of videos provide an overview of the automation system, from submission of data through quality control, to data archival and release. From version 4 onwards, scientists will be able to upload and submit their data directly into the SOCAT quality control system (Figures 3.1 and 3.2). As part of the upload, an automated 'parameter range check' will be run to find obvious errors in the data. Data providers will have access to visualisations of their data for identification and correction of quality issues in the data. Tools in the automation system will enable the scientists to inform the system about the parameters and units in their uploaded files. Plots of cross-overs with other datasets can be seen in the Preview Dataset part of the dashboard. Standardised metadata will be required. Tools for entering, editing and checking metadata will be provided. The automation system for data upload is scheduled to be available in late 2014 or early 2015 for SOCAT version 4.

Demonstration videos of automated data upload will be made available online and possibly in web seminars (or webinars).

As a result of the automation system, changes have been made to the quality control system (for version 3) (Figure 3.3). For the quality controllers these changes will not be very visible. However, the system needs to be tested. Therefore, a small number of experienced quality controllers will need to verify smooth operation of the quality control system in **August 2014** before general **quality control starts on 1 September 2014**.

The SOCAT Community reacts very positively to the slick automation system and makes a few excellent suggestions for minor changes to the system.

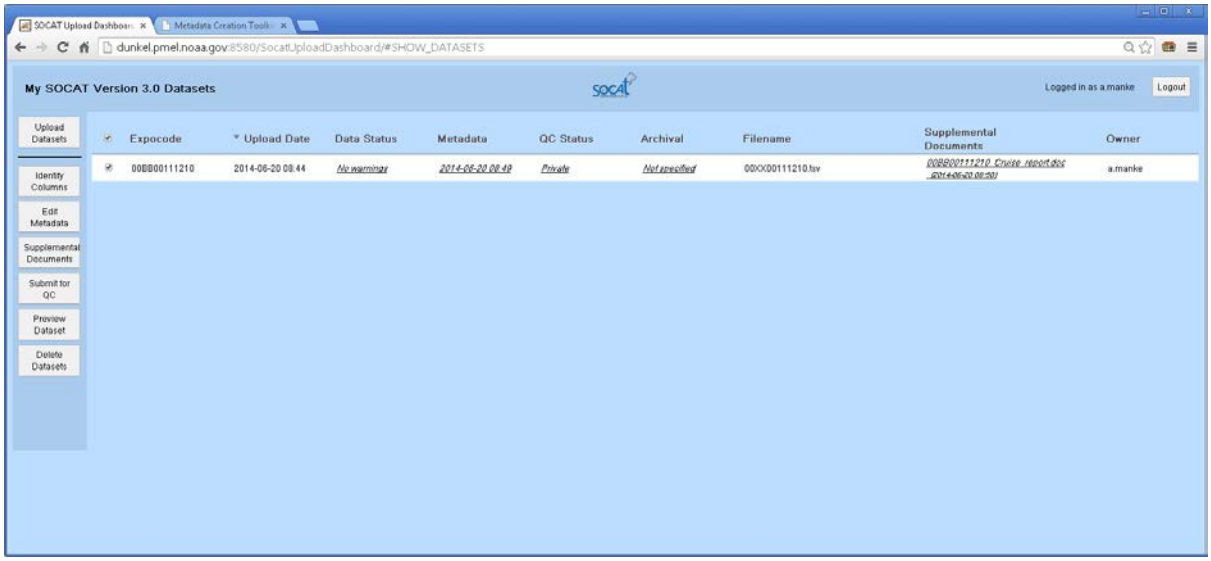
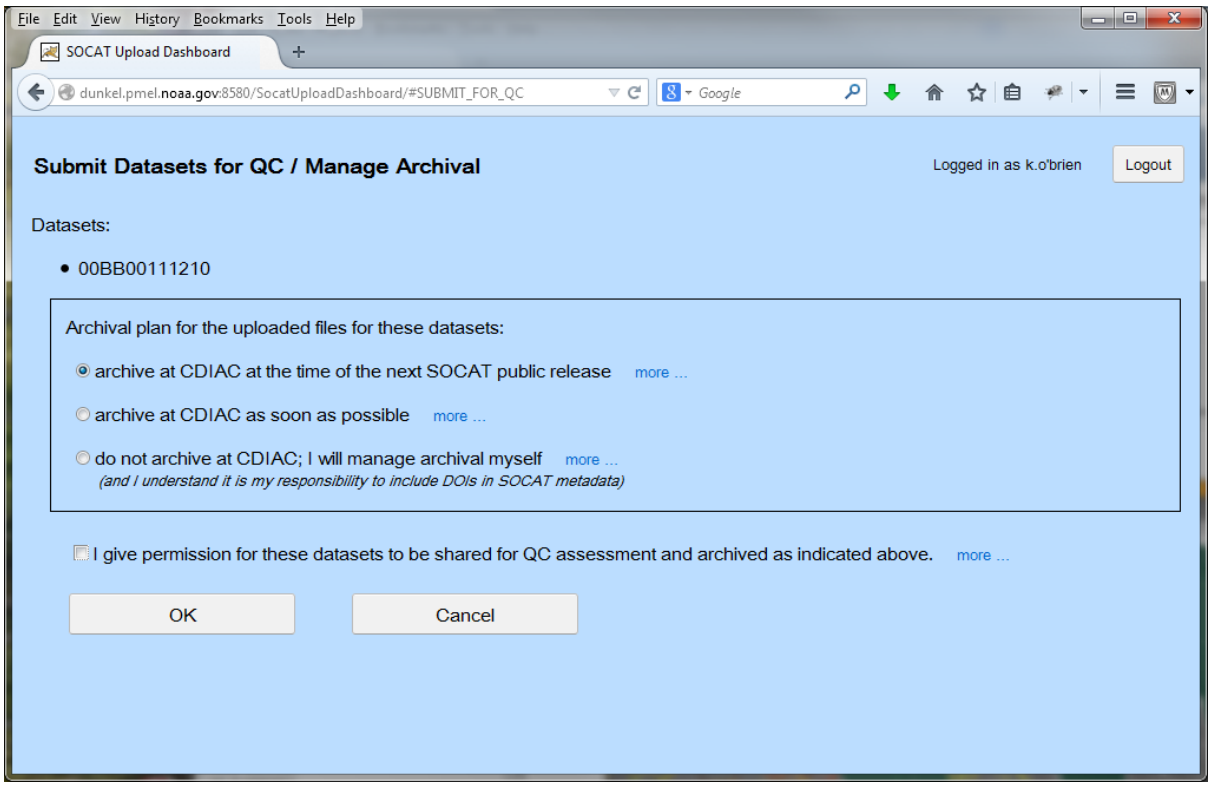


Figure 3.1. The dashboard for automated data submission for SOCAT version 4.



Figur 3.2. Submission of a dataset for quality control via the SOCAT dashboard. This window makes the data provider choose one of three options for archival of the original (uploaded) data files prior to submission of the dataset(s).

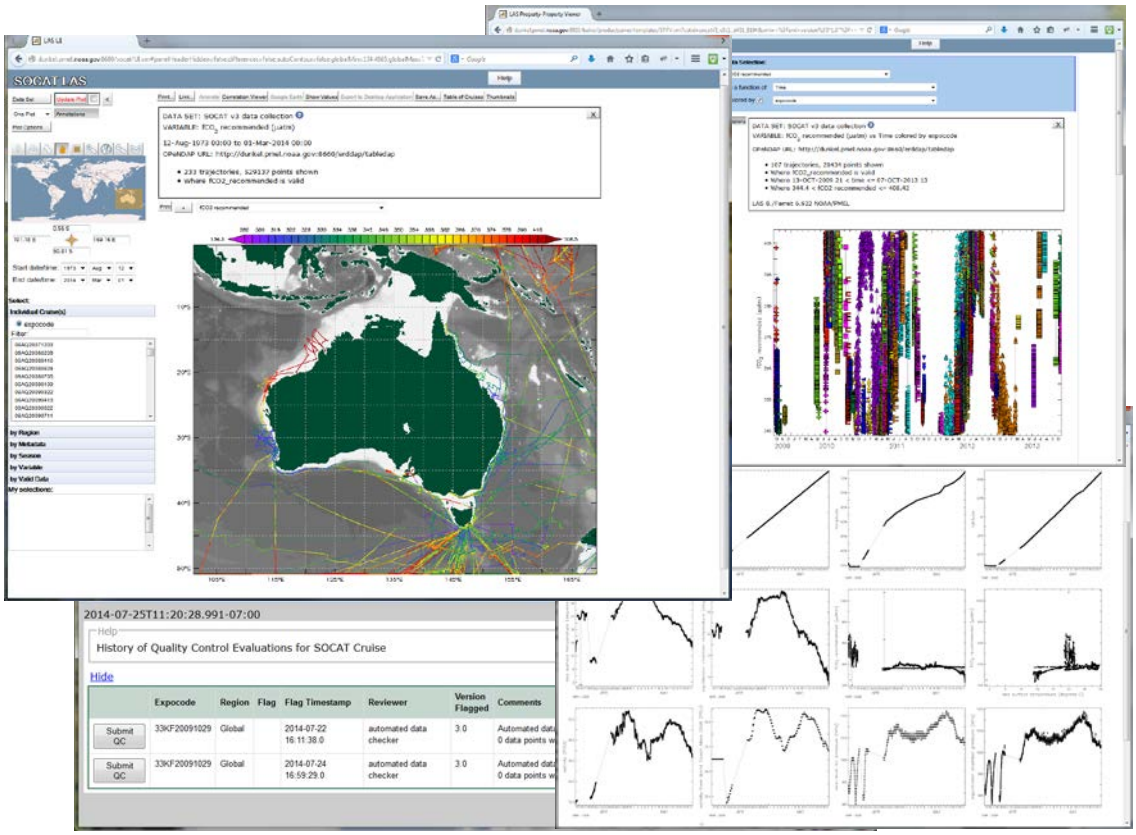


Figure 3.3. SOCAT version 3 QC will be done using version 8.1 of the Live Access Server (LAS). Above is a collection of LAS version 3 quality control tools, including the main LAS user interface, the correlation viewer, the thumbnail viewer and Table of Cruises.

Discussion: Automation for version 4 and implications for version 3 quality control

Kevin O'Brien recommends this sequence through the data submission scheme: Dataset entry, range checking, metadata entry, add supplemental documents, preview dataset, submit and archive (at CDIAC as default). It is possible to upload the data via the automation system without actually submitting the data. If erroneous values are found when running the data through the range checker, the dataset needs to be corrected prior to submission. The system currently accepts data as comma or tab separated value (csv, tsv) files. In the future, this may be extended to include other formats (such as NetCDF, for example). It is possible to upload several datasets in one go.

Steve Jones is creating the range checker (or sanity checker) for the data upload system. The range checker will provide a list of important error messages. Steve Jones and Ute Schuster are testing this system on version 3. It will be fully operational for version 4. Kevin O'Brien suggests that these tests may be further expanded by adding Denis Pierrot's and Are Olsen's Matlab code for quality control to the automation system, thus providing data providers

with additional quality control checks prior to data submission. Ute Schuster wonders, if geographical range checks can be added, e.g. certain sea surface temperatures do not occur in the Southern Ocean. Making these tools available will hopefully encourage data providers to carry out all possible quality control checks before data submission.

Dorothee Bakker asks for a tick box to be added for the data provider to consent that the data can be used for data-policy relevant products, such as the Global Carbon Budget, before the formal SOCAT release, as discussed in 2012 (SOCAT, 2012b).

The data provider needs to provide the correct Expocode (4-character ship or mooring identifier plus start date of cruise or deployment) during data upload. This is a challenging task. Benjamin Pfeil comments that Expocodes might change. Even more complicated is that all US buoys have the same 4-character code, making it extremely difficult to distinguish between the mooring sites. Benjamin Pfeil and Dorothee Bakker will create a short guideline on how to create an Expocode for data providers to SOCAT version 4.

Chair: Ute Schuster, Rapporteur: Steven van Heuven

4 Session on Future SOCAT (Dorothee Bakker, Are Olsen, Maciej Telszewski)

The Surface Ocean CO_2 Atlas requires input from the SOCAT community on its future direction. This session contains discussions of opportunities and challenges for SOCAT.

4.1 Science highlights from regional leads and key participants (Dorothee Bakker)

Five contributors present science highlights using SOCAT:

Jaard Hauschildt (GEOMAR), a Master Student with Tobias Steinhoff, applied the SOCAT data base for investigating mesoscale variability of fCO_2 and sea surface temperature in the tropical Northeastern Atlantic Ocean for his thesis. (Slide presented by Dorothee Bakker)

Claire Lo Monaco (LOCEAN) uses SOCAT fCO_2 data around Kerguelen Island (Southern Ocean) for quantification of air-sea CO_2 fluxes in HNLC (high-nutrient low-chlorophyll) waters and iron-fertilised waters (LoMonaco et al., in preparation). SOCAT Southern Ocean data are also used in a SCAR (Scientific Committee on Antarctic Research) report on Southern Ocean Acidification (in preparation).

Jeremy Mathis (NOAA-PMEL), Jessica Cross (UAF), and Wiley Evans (NOAA-PMEL, UAF) present syntheses of CO_2 fluxes in the Gulf of Alaska (Evans and Mathis, 2013), the Bering Sea (Cross et al., in review, JGR Oceans) and the Western Arctic Ocean (Evans et al., in preparation). The relative importance of regions is rather different from earlier thinking.

Shin-ichiro Nakaoka and Yukihiro Nojiri (NIES) present SOCAT-relevant science for the North Pacific Ocean. NIES submitted 113 datasets from 2011 to 2013 to SOCAT version 3, including 80 cruises on the *Pyxis* and 38 on the *Trans Future 5*. Highlights include monthly maps of surface water pCO_2 and dissolved inorganic carbon for the North Pacific Ocean (Nakaoka et al., 2013; Yasunaka et al., 2013, 2014). Mapping of nutrient concentrations is in progress (Yasunaka et al., in preparation).

Steven van Heuven (RUG) and Mario Hoppema (AWI) (re-)submitted 14 and 28 cruise legs with pCO_2 on the RV *Polarstern* to SOCAT versions 2 and 3, respectively. The data originate from the Atlantic and the adjacent Southern and Arctic Oceans. Atmospheric CO_2 mixing ratios from 2007 to 2014 on *Polarstern* compare well to data from Scripps CO_2 network stations. Annual trends in surface water pCO_2 by latitude exhibit large variation with high uncertainty in the Weddell Sea and North Sea.

4.2 Addition of extra parameters in SOCAT version 4 or later? (Are Olsen)

Are Olsen proposes to make extra parameters available via the SOCAT system. Frequent requests are made to add extra parameters to SOCAT, e.g. surface water nutrients, oxygen,

dissolved inorganic carbon (DIC), alkalinity, methane and nitrous oxide and isotope data. At present additional parameters submitted to SOCAT, alongside surface water xCO_2, pCO_2 or fCO_2, are archived, but they are not quality controlled and not included in the SOCAT data products. Extra parameters are needed for understanding mechanisms of fCO_2 changes. An increase in fCO_2 may be related to enhanced remineralisation or variable upwelling, as shown by work of Nicolas Metzl. Such research requires nutrient data. Jerry Tjiputra et al. analysed fCO_2 growth rates and causes thereof in 14 regions by looking at SST, salinity, DIC and alkalinity. This analysis shows that in several regions the loss of alkalinity increases fCO_2, suggesting that the uptake of anthropogenic carbon is smaller than expected based on analysis of fCO_2 alone. There is an increasing necessity for understanding climate-carbon feedbacks and for more information on regional uptake rates of anthropogenic carbon. All this has relevance for ocean acidification, which partly explains why the Global Ocean Observing System (GOOS) wants measurements of the full carbonate system, rather than just fCO_2 (Framework for Ocean Observing (FOO), 2012), describing carbonate parameters as 'essential variables'.

Discussion: Addition of extra parameters in SOCAT version 4 or later?
Dorothee Bakker reminds all that in 2012 regional and global leads agreed to only include quality controlled parameters in SOCAT version 3 (SOCAT, 2012b). SOCAT regional leads had major concerns on the extra quality control effort required for the inclusion of additional parameters. Are Olsen comments that SOCAT already includes non-quality controlled salinity data. Rik Wanninkhof suggests including additional parameters, while stating clearly which data have not been quality controlled.

Ute Schuster comments that SOCAT only carries out quality control for surface water fCO_2. Ute suggests collecting all the parameters and recruiting experts from other communities for quality control of additional parameters. The SOCAT community should not on its own undertake quality control of additional parameters. Kim Currie recommends carrying out a quick quality assessment of the additional parameters during data submission and only allowing good quality data in.

Steven van Heuven argues that SOCAT needs to get the point across that these additional parameters have not been quality controlled and should not be used until they have been quality controlled. Colm Sweeney proposes to put error estimates on all measurements, such that users can filter data by their uncertainty. Rik Wanninkhof replies that SOCAT already does this for fCO_2 with the dataset quality control flags.

Dick Feely reminds the participants that the Global Ocean Acidification Observing Network (GOA-ON) requires a second carbonate system parameter (Newton et al., 2014). The second parameter could be, for example, continuous DIC, discrete DIC or continuous pH and is essential for analysis of trends in ocean acidification. SOCAT should therefore include ancillary parameters.

Benjamin Pfeil suggests involving the GOA-ON community in quality control, using the GOA-ON infrastructure and getting funding from GOA-ON. For the time being SOCAT might accept and archive ancillary data, but maybe not yet distribute them. There is a case for storing all data centrally, even if these data have not been quality controlled. The technical

capability for storing those small datasets is valuable in itself. SOCAT can provide the infrastructure for archiving these data. Scientists may figure out how to process them later. Steven van Heuven expresses concern that SOCAT might become a black hole for ancillary parameters. Benjamin Pfeil comments that this will not be the case as original data files uploaded via the automation system (version 4) will be made available through CDIAC either instantly (upon data submission) or during the release of the next SOCAT version, depending on the preference of the data provider.

Steven van Heuven comments that dissemination of additional parameters may stimulate collection efforts in the wider community. Rik Wanninkhof adds that acceptance of additional parameters might act as an incentive for contributors to shape up their efforts, for e.g. oxygen and chlorophyll data.

Rik Wanninkhof comments that the number of discrete nutrient measurements is small in comparison to continuous surface water fCO_2 measurements. The time lag and flushing time of the equilibrator complicate co-location of nutrient data with fCO_2 data. Rik Wanninkhof recommends a distinction between continuous and discrete data. Are Olsen recommends a label for different types of data, e.g. 1 for discrete data and 2 for sensor data.

Are Olsen wonders whether SOCAT should also collect surface water datasets of discrete DIC and alkalinity from small process studies and ships of opportunity where no parallel underway fCO_2 measurements are made? Rik Wanninkhof cautions against including CTD samples as co-locating surface water fCO_2 values with CTD data is often problematic.

During the discussion a consensus builds that SOCAT can accept incoming ancillary data. Are Olsen asks whether there indeed is consensus to include ancillary data, but make it very clear that these data are not quality controlled and might range from very poor quality to highly valuable data. Nobody objects.

In conclusion, the participants agree that from SOCAT version 4 onwards:

- **Additional surface water parameters measured alongside surface water fCO_2 or other carbonate chemistry parameters will be accepted** by SOCAT, for example, but not limited to, nutrients and additional carbonate chemistry parameters.
- **Only directly measured, discrete or continuous parameters** will be included.
- **Additional parameters will not be quality controlled.**
- The absence of quality control for additional parameters will be clearly stated.
- **Additional parameters will be in separate files.** Thus, there will be two types of output files, one with quality controlled surface water fCO_2 values, including sea surface temperature and salinity, and one with non-quality controlled ancillary data.
- Ancillary data will not be provided in gridded form.

Further discussion is needed on how or when additional parameters will be made available, either during each SOCAT release or upon request only.

The above decision by the SOCAT Community to accept many more parameters has implications for the SOCAT automation system. On behalf of the LAS group, Kevin O'Brien agrees that the above is a good idea, and that this will be implemented in version 4 or

version 5 depending on time schedules. This will also allow the dashboard to be integrated with Ocean Acidification data.

N.B. The inclusion of atmospheric CO_2 data in SOCAT version 3 was discussed on 17 June 2014 (Appendix 6).

4.3 Acknowledgments and credits for data providers (Rik Wanninkhof)

Rik Wanninkhof reminds the SOCAT Community that acknowledgements and credits are essential for data gatherers and funding agencies. Without acknowledgements there will be no funding for future data collection. As a community we need to provide clear guidelines for citing the data and crediting the data originators. For large datasets (e.g. SOCAT, Takahashi's LDEO dataset, GLODAPv2) sometimes the synthesis product is of worse quality than the original datasets, as quality control by data providers has not been taken into account. Rik Wanninkhof recommends that:

- Data providers should be consulted, if SOCAT or another synthesis product is used for regional studies;
- Original data rather than synthesis products should be used for regional studies;
- Synthesis products are appropriate for global studies.

Rik Wanninkhof also comments that data providers need to publish their own data in order to obtain sufficient citations (credit) for their data.

Andrew Watson comments that other communities have solved this differently, e.g. the ATLAS Collaboration working on the Large Hadron Collider has 2,884 authors on hundreds of scientific publications.

Andrew Watson: 'If you go to Web of Science and search for publications authored by both someone called "Aad" and someone called "Abbott," you get about 300 hits, Most of these papers are by members of the ATLAS Collaboration, in the field of particle physics. If you click on any one of these publications, and hit the "more" link beside the first few authors shown, you get the full author list, which has several thousand names each with their affiliations. If you use Web of Science to search on publications by any one of these names, it finds these papers. Iin other words, all the names are properly recognised as authors by the search, and presumably they all put them on their CVs.'

Andrew advocates that the SOCAT community adopts this model, such that everyone who uses SOCAT has **all** of SOCAT contributors as co-authors. Not many in the audience are in favour of Andrew's recommendation. Steve Jones queries **what is sufficient**, if citing the relevant SOCAT ESSD publication is not sufficient. Why go to such lengths?

Colm Sweeney adds that maintaining the lists of publications using SOCAT (as presented in the Introduction by Dorothee Bakker) is very important. Program managers love such lists. Rik Wanninkhof would like this list to be made available on the SOCAT website. Dorothee Bakker and Benjamin Pfeil are happy to do so.

Several participants, including Maciej Telszewski, Ute Schuster, Are Olsen and Rik Wanninkhof, would like to ask users for their name, email address, research objective and timeline prior to any downloads of SOCAT data products. Benjamin Pfeil comments that SOCAT has both offline and online products, so how could one assemble such information by data users? Furthermore doi-listed data products do not allow to ask for such information prior to data download.

Are Olsen suggests to prominently mention the funding source as a column in the SOCAT data files. The meeting participants comment that this might be easy for individual dataset files, but difficult to realize in synthesis files.

Colm Sweeney comments that the atmospheric CO_2 community has learned how to deal with the acknowledgement issue. SOCAT would do well to discuss details with that community, represented at the meeting by Colm Sweeney. The atmospheric community asks users to put specific sentences in the acknowledgements. Maybe the SOCAT community can do the same? SOCAT should prepare a list of recommendations for acknowledgements and credits. N.B. The SOCAT data policy asks users to use certain sentences in the acknowledgements (Appendix 7).

Following this discussion Rik Wanninkhof has drawn up a list of practical suggestions on how SOCAT may improve acknowledgements and credits for data providers and funding agencies (Appendix 8). Several suggestions can be adopted fairly easily. Others are may be more difficult from a technological point and may take more time to implement. Finally some may be too difficult or may require further discussion.

Chair Colm Sweeney, Rapporteur: Peter Landschützer

4.4 SOCAT and the Global Carbon Project (Corinne Le Quéré via WebEx, Steve Jones)

Corinne Le Quéré presents the Global Carbon Project (GCP) and the annual Global Carbon Budgets (GCB) via a WebEx presentation. The GCP used one data product based on SOCAT version 2 in its 2013 Global Carbon Budget (Le Quéré et al., 2014). The 2014 budget will be released by 22 September 2014, on time for the New York Climate Summit. The 2015 budget is particularly important, because of COP 21 (Conference of the Parties) in Paris. The carbon budget for the IPCC AR6 is very important, as it will be used by the cumulative carbon quota to meet climate targets.

The GCP would like early access to the most recent one or two years of data submitted to SOCAT for its annual Global Carbon Budget. For these recent data the GCP team will use recalculated fCO_2 data in a uniform format, but without the full SOCAT quality control. Steve Jones will carry out automated quality control. The data will only be used for estimates of the annual, global ocean carbon sink and not for any other purpose. For the 2014 budget SOCAT version 2 will be cited and new data will be cited separately. The data will be provided to creators of data-based flux products for estimates of the annual ocean carbon sink. Authorship will be granted to one data provider per group for data from 2012 and 2013

(20 people so far). All contributors of data that is not yet public will be consulted by the GCP prior to the use of these data.

Discussion: SOCAT and the Global Carbon Project

Dick Feely asks how the observations and models are evaluated in the Global Carbon Budget. Corinne Le Quéré answers that all model results are normalised to the mean annual ocean carbon sink of 2.2 PgC/yr (Denman et al., 2007, IPCC AR4). Models provide the trend and interannual variability in the global ocean carbon sink.

Rik Wanninkhof queries how the GCP distinguishes between anthropogenic and natural CO_2 fluxes. Corinne Le Quéré replies that some, but not all estimates include riverine carbon inputs. The GCP corrects estimates, where necessary, for the riverine flux, estimated as 0.45 PgC/yr (Jacobsen et al., 2007). The correction creates additional uncertainty. The uncertainty in the mean is larger than the uncertainty in the interannual variability of the ocean carbon sink.

Colm Sweeney enquires how the GCP uses SOCAT. Corinne Le Quéré responds that in the 2013 budget included one data-based method using SOCAT for estimating the ocean carbon sink (the diagnostic ocean mixed layer scheme by Rödenbeck et al., 2013; Le Quéré et al., 2014). For the 2014 budget four data-based methods (Rödenbeck, Landschützer, Nakaoka, Zeng) will use SOCAT. All methods used in the Global Carbon Budget need to be published prior to their use by the GCP.

Rik Wanninkhof comments that the data-based approaches are very different and asks how the GCP determines uncertainties. Corinne Le Quéré responds that the GCP is developing a method to check consistency between methods and components of the budget. A preliminary analysis has been carried out. Uncertainty is based on the consistency between the data-based methods. Christian Rödenbeck clarifies that his diagnostic ocean mixed layer scheme, used in the 2013 Global Carbon Budget, is not an atmospheric inversion and is based on SOCAT (Rödenbeck et al., 2013).

Andrew Watson comments that insight from the models can help data providers, for example on the riverine carbon input. Modellers and observers should collaborate more. Corinne Le Quéré replies that something similar has been done on the land. The GCP effort using both data-based methods and models is a springboard for the future. The exchange of information can go both ways.

N.B. Early data access for the 2015 Global Carbon Budget was not discussed. Global and regional leads will discuss this and, if necessary, hold a Community-wide consultation in late 2014.

4.5 Measuring the success of SOCAT (Maciej Telszewski)

Maciej Telszewski gives a brief introduction. SOCAT is a great success, but how can we measure the success of SOCAT? How can we quantify the impact of the SOCAT community effort? Is data more available thanks to SOCAT? Has the use of SOCAT improved the latest Global Carbon Budget? Are models improved? Are decisions more informed? Is society better informed? Do we reach out to various communities and can we measure the value of this outreach? Should SOCAT develop some sort of success indices? This kind of information is important when discussing the surface ocean observing system as a whole. If we can quantify the usefulness of SOCAT, we can use it to justify the need for a (sustained and improved) observation network, and the need for instrument development.

Discussion: Measuring the success of SOCAT
Christian Rödenbeck provides an example where SOCAT has an impact: A novel data-based product using SOCAT is now available and provides a constraint on interannual variability of the ocean carbon sink.

Colm Sweeney comments that we should ask: Where can SOCAT play a role? What is needed that is not there and that SOCAT can provide? Clearly there is a role for observation-based estimates in, for example, the Global Carbon Budget.

Rik Wanninkhof asks for clarification of the slide on the Framework for Ocean Observing (FOO, 2012). Maciej Telszewski responds that he will discuss this with Rik Wanninkhof later.

4.6 Plans for SOCAT science (Dorothee Bakker)

Dorothee Bakker lists possible SOCAT science applications. These include:

- Quantification of the ocean carbon sink and its variation;
- Studies of ocean carbon cycling and ocean acidification;
- Initialisation and validation of ocean carbon cycle models;
- Constraints for atmospheric inverse models used in global carbon budgets.

Christian Rödenbeck will present the Surface Ocean pCO_2 Mapping intercomparison (SOCOM) at the IMBER meeting. SOCOM is an intercomparison of data-based mapping products, mainly SOCAT. SOCOM is open to additional data-based products, thus if you have one, talk to Christian.

Dorothee Bakker queries how we can promote SOCAT science. Is SOCAT used enough? Would the community favour, e.g. a series of publications, regional publications or a special issue? Dorothee asks the participants for feedback to the SOCAT global and regional leads during the remainder of the IMBER meeting.

5 Conclude (Dorothee Bakker)

Dorothee Bakker thanks all the participants for the constructive, informative and enjoyable SOCAT Community Event. In particular she thanks the chairs, the rapporteurs, session leads and presenters. The participants thank her.

6 Outcomes and action items

Outcomes
Outcome: Data providers should ONLY submit good quality data to SOCAT.

Outcome: SOCAT quality control comments should be adequate and fully justify the dataset quality control flag.

Outcome: SOCAT version 4 will allow data providers to submit provisional dataset flags and WOCE flags for surface water fCO_2 values.

Outcome: SOCAT urges data providers to provide fully calibrated, high quality salinity and sea surface temperature.

Outcome: From SOCAT version 4 onwards:

- **Additional surface water parameters will be accepted** by SOCAT.
- **Only directly measured, either discrete or continuous parameters** will be included.
- **Additional parameters will not be quality controlled.**
- **Additional parameters will be in separate files.** Thus, there will be two types of output files, one with quality controlled surface water fCO_2 values and one with non-quality controlled ancillary data.

Further discussion is needed on how or when additional parameters will be made available, either during each SOCAT release or upon request only.

Action Items
Action Item: The presentation with an overview and update on SOCAT will be made public. Responsible: Dorothee Bakker and Benjamin Pfeil. Timeframe: Immediate.

Action Item: Update the quality control cookbook for version 3. Responsible: Dorothee Bakker. Time frame: August-September 2014.

Action Item: Verification of the smooth operation of the quality control system before general quality control for version 3 starts. Responsible: Experienced quality controllers. Time frame: August 2014.

Action Item: A short guideline for data providers on how to create an Expocode for SOCAT version 4. Responsible: Benjamin Pfeil, Dorothee Bakker. Time frame: late 2014.

Action Item: Demonstration videos of automated data upload available online and/or in webinars. Responsible: Kevin O'Brien, Karl Smith. Time frame: late 2014 / early 2015.

Action Item: A list of scientific, peer-reviewed publications citing SOCAT will be regularly maintained and made available on the SOCAT website. Responsible: Dorothee Bakker and Benjamin Pfeil. Timeframe: Continuous.

Action Item: Discussion of and implementation, where possible, of recommendations for credits and acknowledgements for data providers and funding agencies. Responsible: Dorothee Bakker, SOCAT global group. Time frame: late 2014.

Action Item: Discussion of and, if necessary, a Community-wide consultation on early data access for the 2015 Global Carbon Budget. Responsible: Dorothee Bakker, global and regional group leads. Time frame: late 2014.

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Appendix 1: Agenda

SOCAT Community Event on Monday 23 June 2014
Convenors: Dorothee Bakker (UEA), Are Olsen (UiB), Kevin O'Brien (NOAA-PMEL), Maciej Telszewski (IOCCP), Bronte Tilbrook (CSIRO)

09:00-10:30 *Chair: Bronte Tilbrook, Rapporteur: Steve Jones*

Introduction and Aims of the SOCAT Community Event

09:00 Introduction and Aims of the SOCAT Community Event (Dorothee Bakker)

SOCAT version 3 quality control (Session leads: Rik Wanninkhof, Ute Schuster, Are Olsen)

09:15 Update on version 3 (Benjamin Pfeil, Karl Smith, Kevin O'Brien)
09:30 Version 3 and 4 time table (Dorothee Bakker)
09:45 Revised quality control flags in version 3 (Rik Wanninkhof)
10:00 Planned quality control for version 3 in practice (Ute Schuster)

10:30-11:00 Coffee

11:00-12:00 *Chair: Kim Currie, Rapporteur: Ingunn Skjelvan*
11:00 Other issues for SOCAT version 3 quality control (Rik Wanninkhof)

12:00-13:00 Lunch

13:00-14:30 *Chair Siv Lauvet, Rapporteur: Ingunn Skjelvan*

Automation for version 4 (Session leads: Kevin O'Brien, Steve Jones)

13:00 Automation for version 4 and implications for version 3 quality control (Kevin O'Brien, Steve Jones, Karl Smith)

SOCAT version 3 quality control (continued)

14:00 Discussion of version 3 quality control (Ute Schuster)

14:30-16:00 *Chair: Ute Schuster, Rapporteur: Steven van Heuven*

Future SOCAT (Session leads: Dorothee Bakker, Are Olsen, Maciej Telszewski)

14:30 Science highlights from regional leads and key participants
15:00 Addition of extra parameters in version 4 or later? (Are Olsen)
15:30 Acknowledgments and credits for data providers (Rik Wanninkhof)

16:00-16:30 Tea

16:30-17:50 *Chair Colm Sweeney, Rapporteur: Peter Landschützer*
16:30 SOCAT and the Global Carbon Project (Corinne Le Quéré via WebEx, Steve Jones)
17:15 Measuring the success of SOCAT (Maciej Telszewski)
17:30 Plans for SOCAT science (Dorothee Bakker)
17:45 Conclude (Dorothee Bakker)

Appendix 2: Participants

1. Dorothee Bakker, University of East Anglia, UK, d.bakker@uea.ac.uk (Convenor)
2. Alejandro Bianchi, Servicio de Hidrografia Naval, Argentina, abianchi@hidro.gov.ar
3. Jessica Cross, University of Alaska Fairbanks, USA, jncross@alaska.edu
4. Kim Currie, National Institute of Water and Atmospheric Research, New Zealand, kim.currie@niwa.co.nz
5. Andrea Fassbender, University of Washington, USA; afassben@uw.edu
6. Richard Feely, Pacific Marine Environmental Laboratory, National Oceanic and Atmospheric Administration, USA; richard.a.feely@noaa.gov
7. Véronique Garçon, Laboratoire d'Etudes en Géophysique et Océanographie Spatiales, France, veronique.garcon@legos.obs-mip.fr
8. Dennis Hansell, University of Miami, USA, dhansell@rsmas.miami.edu
9. Mario Hoppema, Alfred Wegener Institute for Polar and Marine Research, Germany, mario.hoppema@awi.de
10. Truls Johanessen, University of Bergen, Norway, truls@gfi.uib.no
11. Steve Jones, University of East Anglia, UK, s.jones3@uea.ac.uk
12. Atsushi Kojima, Japan Meteorological Agency, Japan, kojima-ats@met.kishou.go.jp
13. Naohiro Kosugi, Meteorological Research Institute, Japan, nkosugi@mri-jma.go.jp
14. Alex Kozyr, Carbon Dioxide Information Analyis Center, USA, kozyra@ornl.gov
15. Camilla Landa, University of Bergen, Norway, Camilla.Landa@gfi.uib.no
16. Peter Landschützer, ETH Zürich, Switzerland, peter.landschuetzer@usys.ethz.ch
17. Siv Lauvset, University of Bergen, Norway, siv.lauvset@gfi.uib.no
18. Timothy Liu, NASA California Institute of Technology, USA, w.t.liu@jpl.nasa.gov
19. Claire LoMonaco, Laboratoire d'Océanographie et du Climat, France, claire.lomonaco@locean-ipsl.upmc.fr
20. Jeremy Mathis, Pacific Marine Environmental Laboratory, National Oceanic and Atmospheric Administration, USA, jeremy.mathis@noaa.gov
21. Shin-ichiro Nakaoka, National Institute for Environmental Studies, Japan, nakaoka.shinichiro@nies.go.jp
22. Kevin O'Brien, Pacific Marine Environmental Laboratory, National Oceanic and Atmospheric Administration, USA (Convenor), kevin.m.obrien@noaa.gov
23. Are Olsen, University of Bergen, Norway (Convenor), are.olsen@gfi.uib.no
24. Abdirahman Omar, Uni Research, Norway, abdir.omar@uni.no
25. Benjamin Pfeil, University of Bergen, Norway, benjamin.pfeil@gfi.uib.no
26. Christian Rödenbeck, Max Planck Institute for Biogeochemistry, Germany, christian.roedenbeck@bgc-jena.mpg.de
27. Reiner Schlitzer, Alfred Wegener Institute for Polar and Marine Research, Germany, reiner.schlitzer@awi.de
28. Ute Schuster, University of Exeter, UK, u.schuster@exeter.ac.uk
29. Ingunn Skjelvan, Uni Research, Norway, ingunn.skjelvan@uni.no
30. Karl Smith, Pacific Marine Environmental Laboratory, National Oceanic and Atmospheric Administration, USA, karl.smith@noaa.gov
31. Colm Sweeney, Earth System Research Laboratory, National Oceanic and Atmospheric Administration, USA, colm.sweeney@noaa.gov

32. Maciej Telszewski, International Ocean Carbon Coordination Project, Poland m.telszewski@ioccp.org (Convenor)
33. Bronte Tilbrook, CSIRO Oceans and Atmosphere, Australia, bronte.tilbrook@csiro.au (Convenor)
34. Steven van Heuven, University of Groningen, The Netherlands, svheuven@gmail.com
35. Rik Wanninkhof, Atlantic Oceanographic and Meteorological Laboratory, National Atmospheric and Oceanographic Administration, USA, rik.wanninkhof@noaa.gov
36. Andrew Watson, University of Exeter, andrew.watson@exeter.ac.uk
37. Fang Zuo, IMBER Regional Project Office, China, fzuo@sklec.ecnu.edu.cn (IT and photo)

Remote:

1 Corinne Le Quéré, University of East Anglia, UK, c.lequere@uea.ac.uk

Appendix 3: Key participants and regional group leads

Table A3.1 Key activities and their participants in SOCAT versions 3 and 4 to date. Names underlined indicate those attending the SOCAT Community Event. Bold identifies new group members.

Activity	Key Participants
Global group	Bakker (chair), **Currie**, Kozyr, Metzl, **O'Brien**, Olsen, Pfeil, Pierrot, Telszewski
Website www.socat.info	Pfeil
Data entry and calculations	Pfeil, Olsen
Data management	Kozyr, Pfeil
Live Access Server	O'Brien, Smith, Hankin
Community Event	Bakker, O'Brien, Olsen, Telszewski, Tilbrook
Alternative sensors (version 3)	Wanninkhof, Steinhoff, Bakker, Bates, Boutin, Olsen, Sutton
Automation (version 4)	O'Brien, Smith, Hankin, S. Jones, Kozyr, Pfeil, Bakker, Olsen, Pierrot, Schuster, Shresta, Devarakondra

Table A3.2. Regional group leads for version 3. The regions are the same as in version 2 (Bakker et al., 2014). Names underlined indicate those attending the SOCAT Community Event.

Region	Definition	Lead(s)
Coastal Seas	Less than 400 km from land; between 30°S and 70°N for 100°W to 43°E; between 30°S and 66°N elsewhere	Alin, Cai, Hales
Arctic Ocean	North of 70°N for 100°W to 43°E; north of 66°N elsewhere, incl. coastal waters	Mathis
North Atlantic	30°N to 70°N	Schuster
Tropical Atlantic	30°N to 30°S	Lefèvre
North Pacific	30°N to 66°N	Nojiri
Tropical Pacific	30°N to 30°S	Cosca
Indian Ocean	North of 30°S	Sarma
Southern Ocean	South of 30°S, incl. coastal waters	Tilbrook, Metzl

Appendix 4: Dataset quality control flags for SOCAT version 3

Table A4.1. Dataset quality control flags for SOCAT version 3 (from Wanninkhof et al., 2013). Changes relative to SOCAT versions 1 and 2 are in bold. fCO_2rec is (re-)calculated fCO_2 at sea surface temperature.

Flag	Criteria[a]
A (11)	(1) Accuracy of calculated fCO_2rec (at SST) is better than 2 µatm. (2) **A high-quality cross-over[b,c]** with another dataset is available. (3) Followed approved methods/SOP[d] criteria. (4) Metadata documentation complete. (5) Dataset QC was deemed acceptable.
B (12)	(1) Accuracy of calculated fCO_2rec (at SST) is better than 2 µatm. (2) Followed approved methods/SOP criteria. (3) Metadata documentation complete. (4) Dataset QC was deemed acceptable.
C (13)	(1) **Accuracy of calculated fCO_2rec (at SST) is better than 5 µatm** (2) Followed approved methods/SOP criteria. (3) Metadata documentation complete. (4) Dataset QC was deemed acceptable.
D (14)	**(1) Accuracy of calculated fCO_2rec (at SST) is better than 5 µatm.** (2) Did or did not follow approved methods/SOP criteria. (3) Metadata documentation incomplete (4) Dataset QC was deemed acceptable.
E (17)	**(Primarily for alternative sensors)** **(1) Accuracy of calculated fCO_2rec (at SST) is better than 10 µatm.** (2) Did not follow approved methods/SOP criteria. **(3) Metadata documentation complete.** (4) Dataset QC was deemed acceptable.
F (15)	(1) Does not meet A through E criteria listed above.
S (Suspend) (15)	(1) More information is needed for dataset before flag can be assigned (2) Dataset QC revealed non-acceptable data and (3) Data are being updated (part or the entire cruise).
X (Exclude) (15)	The dataset duplicates another dataset in SOCAT.
NA-NF	Submitted data to SOCAT that has not undergone independent dataset quality control as indicated by the "N". The NA though NF are the flags provided by the submitting group.

[a]The accuracy takes precedent over the criteria that follow.
[b]**A high-quality cross-over is defined** in version 3, as a cross-over between two datasets with a maximum cross-over equivalent distance of 80 km, a maximum difference in sea surface temperature of 0.3°C and a maximum fCO_2rec difference of 5 µatm. Inconclusive cross-overs, defined as having a temperature difference greater than 0.3°C or a fCO_2rec difference exceeding 5 µatm, will not have a flag A.
[c]**A cross-over is defined** as a distance of less than 80 km. This criterion combines distance and time as $([dx^2 + (dt*30)^2]^{0.5}) \leq 80$ km. One day of separation in time is equivalent (heuristically) to 30 km of separation in space.
[d]SOP or Standard Operating Procedure following Dickson et al. (2007).

Appendix 5: Examples of quality control comments

The examples below of adequate and poor quality control comments in SOCAT version 3 have been inspired by quality control comments in the Table of Cruises on the Cruise Data Viewer and adjusted to the revision of dataset quality control flags in version 3. All relevant quality control comments should be entered on the quality control system. Abbreviations are: Pequ – equilibrator pressure, SOP – standard operating procedures, SST – sea surface temperature, Tequ – equilibrator temperature.

Examples of (barely) adequate quality control comments in version 3.

1) Flag A. The system follows SOP criteria. Metadata is complete, includes information on calibration and accuracy of SST, Tequ and Pequ. The data quality looks good. The 55 km crossover with 49UU20201010 (Flag C) is high-quality with a SST difference of 0.2°C and a fCO_2rec difference of 4 µatm between both cruises.
2) Flag B. The system follows SOP criteria. The metadata is complete. The data quality looks good. The 55 km cross-over with 58XX2021212 (Flag B) is inconclusive with different SST (2°C) and fCO_2rec (50 µatm) on both cruises.
3) Flag C. Metadata complete. A flag C was given because 1) the accuracy of pCO2/fCO_2 (3 µatm) did not meet the SOP criteria (2 µatm) and the 2) Equilibrator temperature was not within 0.05°C. The data quality was deemed acceptable.
4) Flag D. The metadata do not state the accuracy of Pequ and Tequ. Data quality looks good. Inconclusive 55 km cross-over with 06AA20200202 (Flag A) in Channel: Very different SST (6°C) and fCO_2rec (50 µatm) on 2 cruises. Hence flag D.
5) Flag E. The measurements have been made with a spectrophotometric sensor with no in situ calibration gases, but having pre-deployment calibration with documented accuracy better than 10 µatm. The system does not follow SOP criteria. The metadata is complete and includes adequate information on pre-deployment calibration. The data quality was deemed acceptable. Hence flag E.
6) Flag F (or S). No information is provided on the calibration of these sensor data. The data provider has been asked to update information on the pre-deployment calibration.
7) Flag S. File lacks surface water CO_2 measurements. The data provider has been consulted.
8) Flag S. SST has not been reported, such that Tequ was used in calculation of fCO_2rec. Dataset suspended in consultation with data provider.
9) Flag X. This dataset overlaps with dataset 11FF20200808. This is an older version of the same dataset. The data provider has been consulted.

Examples of poor, inadequate quality control comments:

1) Flag A. No comment.
   (*Lacks comments on cross-over, SOP criteria and metadata.*)
2) Flag B. Data looks good.
   (*Lacks comments on SOP criteria and metadata*.)
3) Flag C. Discrepancy in intake temperature and salinity of actual intake and ship sensors may lead to offsets.
   (*Lacks comment on data quality deemed acceptable and metadata complete*).
4) Flag D. Metadata incomplete.
   (*Lacks comment on data quality deemed acceptable, what is missing in metadata.*)
5) Flag E. A spectrophotometric sensor has been used.
   (*Lacks comment on accuracy of pre-deployment calibration, metadata complete, data quality.*)
6) Flag F (or S). An infrared sensor has been used.
   (*Lacks comment on grounds for suspension, e.g. no information on pre-deployment calibration. Has the data provider been consulted?*)
7) Flag S. Data quality not good.
   (*Lacks explanation on the nature of the problem. Has the data provider been consulted?*)
8) Flag X. This dataset overlaps with another dataset.
   (Which other dataset? Has the data provider been consulted?)

Appendix 6: Inclusion of atmospheric CO_2 data

The inclusion of atmospheric CO_2 data in SOCAT was discussed in a Skype call on 17 June 2014. The call had these participants: Kevin O'Brien (chair), Dorothee Bakker, Steven Hankin, Are Olsen, Benjamin Pfeil, Ute Schuster, Karl Smith, Rik Wanninkhof

The group decided that:

1) Version 3 will contain atmospheric CO_2 data measured by the same instrument as the surface water CO_2 data. If two files (by the same instrument) have been reported, then Benjamin Pfeil will combine the files. Atmospheric CO_2 measured values (actual data) will be given a separate WOCE flag from surface water fCO_2 values. A separate comment box for atmospheric measured values may not be necessary. The atmospheric CO_2 data will be visible to the quality controllers. The WOCE flag accompanying the atmospheric CO_2 data will be empty (no flag given). Quality controllers will **not** be asked to quality control atmospheric CO_2 in version 3.

2) Atmospheric CO_2 data measured by a different instrument from the water data will not be included in version 3. The inclusion of such data needs further discussion, with regards to the (separate) metadata and Expocode.

Rik Wanninkhof wonders if automated quality control can be done by comparing the atmospheric CO_2 data to Global View CO_2. This would enable identification of offsets in atmospheric CO_2 (and hence in surface water fCO_2). The automated quality control needs further discussion for version 3.

Appendix 7: SOCAT data policy for SOCAT version 2 *(revised on 7 March 2014)*

Available on: http://www.socat.info/SOCAT_data_policy_public_release_v2.htm, http://cdiac.ornl.gov/ftp/oceans/SOCATv2/

The aim of this public release of version 2 of the Surface Ocean CO_2 Atlas (SOCAT) is to provide:
1. A synthesis product of the surface water fugacity of CO_2 (fCO_2) for the global oceans and coastal seas,
2. A gridded product of fCO_2 with no interpolation.

We kindly ask colleagues:
1) To report problems to submit@socat.info .

2) To generously acknowledge the contribution of SOCAT investigators, regional group leaders, quality controllers and data providers in the form of invitation to co-authorship, and/or reference to relevant scientific articles by data contributors.

Users of SOCAT data are requested to include in the acknowledgements:
'The Surface Ocean CO Atlas (SOCAT) is an international effort, supported by the International Ocean Carbon Coordination Project (IOCCP), the Surface Ocean Lower Atmosphere Study (SOLAS), and the Integrated Marine Biogeochemistry and Ecosystem Research program (IMBER), to deliver a uniformly quality-controlled surface ocean CO database. The many researchers and funding agencies responsible for the collection of data and quality control are thanked for their contributions to SOCAT.'

3) To inform submit@socat.info of publications in which SOCAT is used.

4) To cite SOCAT as:
Version 2 (synthesis and gridded data products):
Bakker, D. C. E., Pfeil, B., Smith, K., Hankin, S., Olsen, A., Alin, S. R., Cosca, C., Harasawa, S., Kozyr, A., Nojiri, Y., O'Brien, K. M., Schuster, U., Telszewski, M., Tilbrook, B., Wada, C., Akl, J., Barbero, L., Bates, N. R., Boutin, J., Bozec, Y., Cai, W.-J., Castle, R. D., Chavez, F. P., Chen, L., Chierici, M., Currie, K., De Baar, H. J. W., Evans, W., Feely, R. A., Fransson, A., Gao, Z., Hales, B., Hardman-Mountford, N. J., Hoppema, M., Huang, W.-J., Hunt, C. W., Huss, B., Ichikawa, T., Johannessen, T., Jones, E. M., Jones, S., Jutterstrøm, S., Kitidis, V., Körtzinger, A., Landschützer, P., Lauvset, S. K., Lefèvre, N., Manke, A. B., Mathis, J. T., Merlivat, L., Metzl, N., Murata, A., Newberger, T., Omar, A. M., Ono, T., Park, G.-H., Paterson, K., Pierrot, D., Ríos, A. F., Sabine, C. L., Saito, S., Salisbury, J., Sarma, V. V. S. S., Schlitzer, R., Sieger, R., Skjelvan, I., Steinhoff, T., Sullivan, K. F., Sun, H., Sutton, A. J., Suzuki, T., Sweeney, C., Takahashi, T., Tjiputra, J., Tsurushima, N., Van Heuven, S. M. A. C., Vandemark, D., Vlahos, P., Wallace, D. W. R., Wanninkhof, R. and Watson, A. J. (2014) An update to the Surface Ocean CO_2 Atlas (SOCAT version 2). Earth System Science Data 6: 69-90. doi:10.5194/essd-6-69-2014.

Version 1 (synthesis and gridded data products):

Pfeil, B., Olsen, A., Bakker, D. C. E., Hankin, S., Koyuk, H., Kozyr, A., Malczyk, J., Manke, A., Metzl, N., Sabine, C. L., Akl, J., Alin, S. R., Bates, N., Bellerby, R. G. J., Borges, A., Boutin, J., Brown, P. J., Cai, W.-J., Chavez, F. P., Chen, A., Cosca, C., Fassbender, A. J., Feely, R. A., González-Dávila, M., Goyet, C., Hales, B., Hardman-Mountford, N., Heinze, C., Hood, M., Hoppema, M., Hunt, C. W., Hydes, D., Ishii, M., Johannessen, T., Jones, S. D., Key, R. M., Körtzinger, A., Landschützer, P., Lauvset, S. K., Lefèvre, N., Lenton, A., Lourantou, A., Merlivat, L., Midorikawa, T., Mintrop, L., Miyazaki, C., Murata, A., Nakadate, A., Nakano, Y., Nakaoka, S., Nojiri, Y., Omar, A. M., Padin, X. A., Park, G.-H., Paterson, K., Perez, F. F., Pierrot, D., Poisson, A., Ríos, A. F., Santana-Casiano, J. M., Salisbury, J., Sarma, V. V. S. S., Schlitzer, R., Schneider, B., Schuster, U., Sieger, R., Skjelvan, I., Steinhoff, T., Suzuki, T., Takahashi, T., Tedesco, K., Telszewski, M., Thomas, H., Tilbrook, B., Tjiputra, J., Vandemark, D., Veness, T., Wanninkhof, R., Watson, A. J., Weiss, R., Wong, C. S., and Yoshikawa-Inoue, H.: A uniform, quality controlled Surface Ocean CO2 Atlas (SOCAT). Earth Syst. Sci. Data 5: 125-143, doi:10.5194/essd-5-125-2013, 2013.

Plus cite for the SOCAT version 1 gridded products:

Sabine, C. L., Hankin, S., Koyuk, H., Bakker, D. C. E., Pfeil, B., Olsen, A., Metzl, N., Kozyr, A., Fassbender, A., Manke, A., Malczyk, J., Akl, J., Alin, S. R., Bellerby, R. G. J., Borges, A., Boutin, J., Brown, P. J., Cai, W.-J., Chavez, F. P., Chen, A., Cosca, C., Feely, R. A., González-Dávila, M., Goyet, C., Hardman-Mountford, N., Heinze, C., Hoppema, M., Hunt, C. W., Hydes, D., Ishii, M., Johannessen, T., Key, R. M., Körtzinger, A., Landschützer, P., Lauvset, S. K., Lefèvre, N., Lenton, A., Lourantou, A., Merlivat, L., Midorikawa, T., Mintrop, L., Miyazaki, C., Murata, A., Nakadate, A., Nakano, Y., Nakaoka, S., Nojiri, Y., Omar, A. M., Padin, X. A., Park, G.-H., Paterson, K., Perez, F. F., Pierrot, D., Poisson, A., Ríos, A. F., Salisbury, J., Santana-Casiano, J. M., Sarma, V. V. S. S., Schlitzer, R., Schneider, B., Schuster, U., Sieger, R., Skjelvan, I., Steinhoff, T., Suzuki, T., Takahashi, T., Tedesco, K., Telszewski, M., Thomas, H., Tilbrook, B., Vandemark, D., Veness, T., Watson, A. J., Weiss, R., Wong, C. S., and Yoshikawa-Inoue, H. (2013)Surface Ocean CO2 Atlas (SOCAT) gridded data products, Earth Syst. Sci. Data, 5, 145-153, doi:10.5194/essd-5-145-2013.

For further advice, please, contact the SOCAT investigators.

Appendix 8: Recommendations for improving acknowledgments and credits

Rik Wanninkhof has provided these practical suggestions on how SOCAT may improve acknowledgments and credits for data providers and funding agencies on 22 July 2014.

The discussion on acknowledgments centred on clearly providing instructions as to how the work should be cited and the guidelines how SOCAT should be referenced assuring proper recognition of the data contributors and those involved in contextual quality control (secondary QC) of the datasets. All recognized that this issue is critical for investigators who put most their efforts on surface water CO_2 monitoring and for sustained funding of these efforts. A main criterion for continued funding often is utilisation of the data by others and submission to a centralised data holding such as SOCAT is important, but not sufficient. Consensus was not reached on all points, but a majority view did evolve.

1) Information on how to cite SOCAT should be made easily available.
   a) A separate box labelled How to cite SOCAT should be listed on the home page of www.socat.info. (This is currently buried under data use policy.)
   b) The references should be provided as Endnote/Procite reference files with a link to the ESSD publications.

2) A table should be linked to the home page of www.socat.info with a list of all contributing investigators and their source of funding.

3) Any person accessing the data should be required to provide e-mail address and to agree to a fair use policy by checking a box. SOCAT should create such a policy. An example of what AOML uses (copied from ESRL/CMD atmospheric data) is as follows:

   "These data are made freely available to the public and the scientific community in the belief that their wide dissemination will lead to greater understanding and new scientific insights. The availability of these data does not constitute publication of the data. We rely on the ethics and integrity of the user to assure that AOML receives fair credit for our work. Please send manuscripts using this data to AOML for review before they are submitted for publication so we can insure that the quality and limitations of the data are accurately represented."

4) Any investigator using a subset of data is encouraged to determine the major data submitters and acknowledge them.

5) It would be worthwhile to be able to extract data by submitting group/PI and funding agency.

6) There should be an easy way for data users to contact the data contributors to consult on data.