Surface Ocean CO_2 Atlas (SOCAT) side event: Release of Version 2 and Science Highlights

9th International Carbon Dioxide Conference,
Beijing International Convention Center, Beijing, China
Tuesday 4 June 2013, 12:15-13:15

Organising committee:
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Event sponsors:
IOCCP, Korean Institute of Ocean Science and Technology (KIOST)

Chairs:
Dorothee Bakker, Maciej Telszewski

Report:
Steve Jones (UEA, UK), Dorothee Bakker

Program

1) On behalf of SOCAT sponsors (Maciej Telszewski)*
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Apologies
*Presentation available on SOCAT website (http://www.socat.info/)

1) On behalf of SOCAT sponsors by Maciej Telszewski*

Welcome at this lunch-time side-event on the Surface Ocean CO_2 Atlas (SOCAT) at the 9th International Carbon Dioxide Conference (ICDC9). The session consists of the release of SOCAT version 2, an outlook towards future SOCAT versions, two short science talks on SOCAT highlights and a discussion. The Surface Ocean CO_2 Atlas is an effort by the international marine carbon research community since 2007. 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 has more than 100 contributors and data providers. It has multiple funding sources, but no long-term funding. SOCAT scientists have participated in 10 meetings over 6 years and numerous teleconferences. For inclusion of your surface water fCO_2 data in SOCAT, submit your data and metadata to CDIAC in IOCCP recommended formats (http://cdiac.ornl.gov/oceans/submit.html). Join the SOCAT quality control (QC) effort and other SOCAT activities! Please, cite and acknowledge SOCAT, data providers and contributors. Version 1 has been documented in two articles (Pfeil et al., 2013; Sabine et al., 2013). The International Carbon Coordination Project, the Surface Ocean Lower Atmosphere Study (SOLAS) and the Integrated Marine Biogeochemistry and Ecosystem Research program (IMBER) support SOCAT.

Discussion

No questions or comments.

2) Release of SOCAT version 2 by Benjamin Pfeil*

The Surface Ocean CO_2 Atlas has been initiated in 2007 at Unesco with two aims:

- To provide a global surface ocean data set of recalculated fCO_2 in a uniform format with 2nd level quality control;
- A global gridded product of monthly surface water fCO_2 means, with minimal temporal or spatial interpolation (i.e. bin averages).

These data products are to be made public with regular updates. Fully documented and transparent methods are to be used (Bakker et al., 2012). Regional groups and a global group have been established.

SOCAT version 1 has been made public in September 2011 and contains 6.3 million surface water fCO_2 data from the global oceans and coastal seas originating from 1851 cruises between 1968 and 2007 (Pfeil et al., 2013; Sabine et al., 2013). The data are available as recalculated fCO_2 in individual cruise files and concatenated synthesis files, and as gridded fCO_2 means. In addition to the recalculated fCO_2 data, the original CO_2 data, as reported by the data provider, are available in the individual cruise files. All data products are citable using DOIs (digital object identifiers). Interactive, online data viewers (via a Live Access Server) enable easy interrogation and visualisation of the SOCAT products. The SOCAT products can be downloaded in a variety of formats, including in Ocean Data View format. The SOCAT website (http://www.socat.info/) provides access to the SOCAT products, downloadable files and interactive data viewers.

Version 2 contains 10.1 million fCO_2 data from 2660 cruises and extends the data set to December 2011. New data in version 2 are mainly from the years 2006 to 2011. The methods followed for creating version 2 close follow those for version 1. Improvements include more consistent quality control and better documentation. The SOCAT website provides access to all version 2 products and tools, which are similar to those for version 1. The capabilities of the gridded data viewer have

been expanded and include the SOCAT coastal mask. A manuscript describing version 2 will shortly be submitted to Earth System Science Data (Bakker et al., 2013).

The global group has these participants for version 2: Dorothee Bakker (lead), Benjamin Pfeil, Steve Hankin, Are Olsen, Alex Kozyr, Denis Pierrot, Nicolas Metzl and Maciej Telszewski. Regional group leads for version 2 are: Ute Schuster (North Atlantic), Nathalie Lefèvre (Tropical Atlantic), Jeremy Mathis (Arctic Ocean), Yukihiro Nojiri (North Pacific), Cathy Cosca (Tropical Pacific), Vedula Sarma (Indian Ocean), Bronte Tilbrook and Nicolas Metzl (Southern Ocean), Simone Alin, Burke Hales and Wei-Jun Cai (coastal seas). The stellar contributions of Karl Smith, Ansley Manke, Kevin O'Brien and numerous quality controllers should also be mentioned.

One may compare SOCAT with its successive releases to the Great Wall snaking up and down and disappearing in the haze. SOCAT has reached another high point with the release of version 2. The path to future SOCAT versions is circuitous and eventually disappears in the distance. The lack of central funding is a key difference between the building of the Great Wall and the SOCAT community effort.

Version 2 is hereby made public!

Benjamin Pfeil thanks data contributors, the SOCAT team, especially regional and global group leaders, members and data centers involved! Special thanks to SOCAT Global Group leader Dorothee Bakker.

Discussion

Rik Wanninkhof (Atlantic Oceanographic and Meteorological Laboratory, National Atmospheric and Oceanographic Administration (NOAA-AOML), USA): We need to be sure that SOCAT is not seen as the data owner exclusively. The data is still owned by the many data providers. There is a risk that simply citing SOCAT in publications will imply that SOCAT is the data owner.

Benjamin Pfeil: The SOCAT database includes full traceability. For the individual cruise DOIs the originating Principal Investigators (PIs) are the lead authors.

Rik Wanninkhof: This issue is something that should be stressed by SOCAT, so that end users of the product(s) are aware of this issue.

Dorothee Bakker: If a particular study is examining a localised region, users should consider citing the individual PIs as well as the entire SOCAT database. Such projects should also consider inviting those PIs to be part of the study to help give them recognition for their data and gain their specific expertise.

Andrew Lenton (CSIRO Marine and Atmospheric Research, Australia): Is it appropriate to provide an acknowledgement, to make the contributions of the data providers more explicit?

Maciej Telszewski: Using a citation is probably more powerful, as citations feed into authors' impact factors and other metrics.

Andrew Watson (UEA, UK): The citation is certainly more important, as that is what funding bodies examine when considering where to spend their money.

2) SOCAT sensors, automation and vision by Dorothee Bakker* with input from Steve Hankin and Rik Wanninkhof

Alternative sensor data in SOCAT:
The sensor team consists of Rik Wanninkhof (lead), Nick Bates, Are Olsen, Tobias Steinhoff, Adrienne Sutton and Dorothee Bakker. Observations from alternative platforms and alternative sensors do not fit well in the current quality assessment scheme (Wanninkhof et al., 2013). In the future there will be more data from alternative approaches. How can we incorporate alternative sensor data in SOCAT, while maintaining adequate quality control and documentation? Examples of alternative sensors include CARIOCA, SAMICO2, PSI CO2-pro, Contros HydroC, Seaology / MApCO_2 and SubCtech Ocean Pack. A draft white paper (Wanninkhof et al., 2013) has been available for community feedback on the SOCAT website. Recommendations include:

Technology:
- Encourage manufacturers to provide on board calibration/standardisation routines;
- Obtain more information on long term deployments over ranges of environmental conditions (through side-by-side studies);
- Improve understanding of membrane (bio-fouling);

SOCAT documentation:
- Update metadata forms to reflect specific sensor criteria;
- Include platform type in the documentation;
- Revise dataset quality control flags based on accuracy of analyses at sea;
- Enable entry of provisional dataset flags during data submission (NA-NF).

Proposed changes to dataset quality control flags

Flag A	: Strict cross-over definition;
Flags C and D	: (At sea) accuracy < 5 µatm;
Flag E (NEW)	: Mainly for alternative sensors, (at sea) accuracy < 10 µatm;
Flag NA-NF (NEW)	: Flags by the data contributor prior to independent quality control.

Feedback is being incorporated into the paper, which will then be presented for approval by the SOCAT community.

SOCAT automation
The automation team consists of Steve Hankin (lead), Steve Jones, Karl Smith, Alex Kozyr, Ansley Manke, Kevin O'Brien, Benjamin Pfeil, Roland Schweitzer, Dorothee Bakker and Are Olsen. The automation of SOCAT aims to reduce the effort required for SOCAT in order to make SOCAT sustainable. At present much manual effort is needed to organise and reformat the data. PIs have commitments to various data centers. The automation system (Poster 140, Hankin et al.) will provide:
- Automated data submission;
- Tools for initial quality control by data provider;
- An option to make original data public via CDIAC prior to SOCAT release.

Tools and functions in the automation system will include: Metadata entry and edit; Metadata checker (e.g. spelling); File upload with version tracking; Identification of columns; A ranger

checker for data values; Computation of recommended fCO_2; Preliminary WOCE flagging; Visualisation and analysis; and Cross-over detection.

The aim is to have the automation system ready by January 2014 and to have the automation system fully operational for version 4. Initially large data providers will be invited to submit data via the automation system.

A provisional time table for SOCAT version 3 has been set as:
31 December 2013 : Cut-off date for data submission to CDIAC for version 3;
January-March 2014 : Data submission via automation system (invitation only);
October 2014 : Quality control complete;
June 2015 : Release (provisional).
Data can be submitted to CDIAC at all times. Data providers are strongly encouraged to continuously submit their data to CDIAC, as these data become available. This reduces peaks in the workload for Benjamin Pfeil for ingesting data into SOCAT. The 31 December deadline is a cut-off date for data to be considered for inclusion in version 3.

Regional and global group leads discussed in July 2012 whether additional parameters, e.g. nutrients, pH, DIC (dissolved inorganic carbon), TA (total alkalinity) should be included in SOCAT (SOCAT, 2012). The group leads decided:

- No extra parameters until version 4 or later.
- Only include extra parameters, if they can be quality controlled and if sufficient manpower and/or automation is in place to do this QC.

The SOCAT global group has decided to archive all additional parameters submitted to SOCAT, even if they are not included in the SOCAT products.

Discussion
Rik Wanninkhof: Is it possible to include a ΔfCO_2 (fCO_2water – fCO_2air) column in the SOCAT data products?

Dorothee Bakker: It shouldn't be difficult to do: the GLOBALVIEW atmospheric CO_2 value is already stored, so it's a simple calculation.

Colm Sweeney (Earth System Research Laboratory, National Atmospheric and Oceanographic Administration, USA): Is there an intention to add in situ atmospheric CO_2 measurements to the SOCAT data products?

Dorothee Bakker: If the data are included in the original data files, they are kept in the SOCAT archive. At present atmospheric CO_2 measurements are not quality controlled and are not included in the SOCAT data products.

Colm Sweeney: The revised data set quality control flags for alternative sensors are specified in terms of 'accuracy', which is a term with many different definitions. Is 'repeatability' a better goal for this?

Rik Wanninkhof: Virtually all terms are loaded and/or frequently misunderstood.

4) Variability of the global ocean carbon sink from 1998-2007 (2011) using SOCAT by Peter Landschützer, Nicolas Gruber, Dorothee Bakker and Ute Schuster

Abstract
The global ocean provides a major sink for atmospheric carbon dioxide (CO_2), but this sink is known to show strong variability on different time scales. Here we use the existing underway network of observations in the global ocean to estimate this sink and its temporal variations, benefitting from a continuous improvement of the quantity and quality of the observation of sea surface CO_2 data, as available via the Surface Ocean CO_2 Atlas (SOCAT) v1.5 database. In particular, we combine two neural network methods to reconstruct basin-wide monthly maps of the sea surface partial pressure of CO_2 (pCO_2) from 1998 through 2007 at a resolution of 1° latitude x 1° longitude. These estimates are used to compute air-sea CO_2 flux maps using a bulk gas exchange parameterization and high-resolution wind speeds. The evaluation with independent time series data in the different ocean basins shows that our estimates reconstruct the pCO_2 reasonably well. We estimate a mean CO_2 uptake by the ocean of 1.32 ± 0.52 PgC/yr, excluding the Arctic Ocean and coastal regions. Initial results show strong seasonal and inter-annual variability with a minimum ocean uptake in 2001 of 0.75 ± 0.35 PgC/yr up to a maximum uptake in 2006 of 1.9 ± 0.72 PgC/yr. Taking into account recently derived estimates of 0.45 ± 0.18 PgC/yr for the outgassing of riverine derived carbon and a mean Arctic Ocean sink of 0.12 ± 0.06 PgC/yr, we estimate a mean anthropogenic CO_2 uptake of 1.89 ± 0.55 PgC/yr from 1998-2007.

Discussion
No questions.

5) Global sea-air CO_2 flux variability estimated from SOCAT pCO_2 observations by Christian Rödenbeck, Dorothee Bakker, Nicolas Metzl, Are Olsen, Chris Sabine, Nicolas Cassar, F. Reum, Ralph Keeling and Martin Heimann

Abstract
A temporally and spatially resolved estimate of the global surface-ocean CO_2 partial pressure field and the sea-air CO_2 flux is presented, obtained by fitting a simple data-driven diagnostic model of ocean mixed-layer biogeochemistry to surface-ocean CO_2 partial pressure data from the SOCAT data base.

The estimated seasonality is well-constrained from the data in most regions, and compares well to the widely used monthly climatology by Takahashi et al. (2009). Comparison to independent data tentatively supports the slightly higher seasonal variations in our estimates in some areas. From a comparison with an independent seasonal climatology of surface-ocean PO_4 concentration, the diagnostic model is shown to capture relevant surface-ocean biogeochemical processes reasonably well.

The estimated interannual variations are largest in the Tropical Pacific and tight to ENSO. The interannual signals from SOCAT data are compatible with signals from atmospheric oxygen data in the Tropics and the Southern hemisphere.

The global ocean CO_2 flux is estimated to be (-1.2 ± 0.25) PgC/yr (1990-2009 average, negative for uptake), in line with earlier pCO_2-based estimates. Individual years range between -1.88 PgC/yr (1992) and -0.45 PgC/yr (2001).

The SOCAT-based sea-air CO_2 flux estimates (which include seasonal, interannual, and daily variations) are available to other groups as a gridded product in digital form.

Discussion
Niki Gruber (ETH Zürich, Switzerland): In terms of connecting the fCO_2 data to ocean interior data, how important will other parameters being considered for future SOCAT versions (e.g. nutrients) be for the model?

Christian Rödenbeck: If all fCO_2 measurements have co-located additional parameter data, this will be extremely useful. How many fCO_2 measurements have such co-located additional parameters?

Rik Wanninkhof: 90% of the fCO_2 data only has sea surface temperature and salinity co-located data.

Niki Gruber: It is good that all extra data is being kept in the SOCAT archive, and are therefore accessible, even if they are not 'published' as part of the 'official' SOCAT data products.

6) Open Discussion: How to move SOCAT forward?
Zhaohui 'Aleck' Wang (Woods Hole Oceanographic Institution, USA): What is the overlap between the SOCAT and the Takahashi LDEO databases?

Dorothee Bakker: There is a large overlap. The main differences are:

- The LDEO database (v2012) contains 7 million fCO_2 measurements. SOCAT version 2 has 10.1 million;
- The LDEO database (v2012) extends to 2012; SOCAT version 2 is only to 2011.
- The LDEO database (v2012) contains a large amount of data off the US west coast, which are not in SOCAT. SOCAT is working on getting those included.

Benjamin Pfeil:

- SOCAT contains a much larger proportion of coastal data than the LDEO database.

Benjamin Pfeil: SOCAT is actively trying to include any fCO_2 measurements that are in the LDEO database but not in SOCAT. To meet the quality control (QC) requirements of SOCAT, the SOCAT data manager communicates directly with PIs rather than obtaining the data from Taro Takahashi.

Zhaohui Wang: Having a comparison between the two databases would help comparative analyses for some studies.

Vinu Valsala (Indian Institute of Tropical Meteorology (IITM), India): There should be an option to view the differences between the two databases.

Andrew Watson: Should Taro Takahashi address this issue, since SOCAT is much more transparent with respect to its data sources?

Dorothee Bakker: This is an issue that both databases should be addressing.

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Galen McKinley (University of Wisconsin, USA): Is there a SOCAT climatology product à la Takahashi et al. (2009)?

Dorothee Bakker: We are not aware of one. This is not a primary focus of the project.

Rik Wanninkhof: For information, a revised Takahashi climatology incorporating the 2012 data is being released shortly.

Maciej Telszewski: Early discussions in SOCAT decided that this sort of activity would most likely be undertaken by efforts external to SOCAT.

Dorothee Bakker: If any such external data products are produced from the SOCAT data products, the project will be very keen to know about them and link to them from the main SOCAT website (http://www.socat.info/). This will benefit both SOCAT and the derived products.

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Arne Körtzinger (GEOMAR, Germany): Have you discussed the inclusion of surface water concentrations of other greenhouse gases in SOCAT, notably methane and nitrous oxide?

Dorothee Bakker: This hasn't been discussed, but would have the same issues as the potential inclusion of other parameters such as nutrients.

Arne Körtzinger: PIs currently have to submit different subsets of their data to different places. It would be easier if all data could be submitted once to a single location.

Benjamin Pfeil: PIs are welcome to submit all their data to SOCAT, where it will be kept in the archive. If SOCAT decides to add such data to its output products in the future, we will extract them from the archive.

Arne Körtzinger: Many other projects dealing with these extra parameters already have their own QC processes in place. If SOCAT takes this path, the project should consult with those other projects.

7) End of the side event

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