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Discussions

An update to the Surface Ocean CO_2 Atlas (SOCAT version 2)

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An update to the Surface Ocean CO_2 Atlas

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Abstract

The Surface Ocean CO_2 Atlas (SOCAT) is an effort by the international marine carbon research community. It aims to improve access to carbon dioxide measurements in the surface oceans by regular releases of quality controlled and fully documented synthesis and gridded fCO_2 (fugacity of carbon dioxide) products. SOCAT version 2 presented here extends the data set for the global oceans and coastal seas by four years and has 10.1 million surface water fCO_2 values from 2660 cruises between 1968 and 2011. The procedures for creating version 2 have been comparable to those for version 1. The SOCAT website (http://www.socat.info/) provides access to the individual cruise data files, as well as to the synthesis and gridded data products. Interactive online tools allow visitors to explore the richness of the data. Scientific users can also retrieve the data as downloadable files or via Ocean Data View. Version 2 enables carbon specialists to expand their studies until 2011. Applications of SOCAT include process studies, quantification of the ocean carbon sink and its spatial, seasonal, year-to-year and longer-term variation, as well as initialisation or validation of ocean carbon models and coupled-climate carbon models.

Data coverage and parameter measured

Repository-Reference: Individual cruise files and synthesis product:
doi:10.1594/PANGAEA.811776
Gridded products: doi:10.3334/CDIAC/OTG.SOCAT_V2_GRID
Available at: http://www.socat.info/
Coverage: 79° S to 90° N; 180° W to 180° E
Location Name: Global Oceans and Coastal Seas
Date/Time Start: 16 November 1968
Date/Time End: 26 December 2011

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1 Introduction

Human activity is releasing large quantities of the greenhouse gas carbon dioxide (CO_2) into the atmosphere. As a result, the atmospheric CO_2 mole fraction has increased from 280 $\mu mol\,mol^{-1}$ in pre-industrial times (Jansen et al., 2007) to 397 $\mu mol\,mol^{-1}$ in April 2013 (Tans and Keeling, 2013). The rapid, ongoing change in the atmospheric composition by greenhouse gas emissions is predicted to increase global mean temperature by 1.5 to 5.0 °C by the end of the century (Peters et al., 2013). Such warming would be accompanied by sea level rise, increased storm frequency, melting of ice caps and sea ice, changes in precipitation patterns and ocean acidification (Solomon et al., 2007) to name only the most prominent examples. Already many changes in the Earth's climate are apparent, such as the decline in Arctic sea ice extent (Stroeve et al., 2007), warming in Alaska, near the Antarctic Peninsula (Vaughan et al., 2003; Mulvaney et al., 2012) and of the upper ocean (Levitus et al., 2005).

The oceans absorb a substantial part of the CO_2 emissions by human activity, thereby mitigating climate change. From pre-industrial times to 1994 the oceans have taken up 118 ± 19 Pg C from the atmosphere (Sabine et al., 2004). This is equivalent to roughly 50 % of CO_2 emissions from fossil fuel burning and cement production or 30 % of the total anthropogenic emissions, if CO_2 emissions from land use change are included. Recent estimates indicate that the oceans are a contemporary sink for roughly 27 % of the annual CO_2 emissions by fossil fuel combustion, cement production and land use change (Le Quéré et al., 2013). Uncertainty in the land use change emissions leads to a large error estimate for the proportion of the anthropogenic emissions taken up by the oceans.

There is uncertainty on how much CO_2 the oceans will absorb in a warming climate of the future (e.g. Jones et al., 2013). Considerable year-to-year, decadal and long-term variation has been demonstrated by CO_2 uptake in the North Atlantic Ocean (Corbière et al., 2007; Schuster and Watson, 2007; Thomas et al., 2008; Schuster et al., 2009;

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McKinley et al., 2011), the North Sea (Thomas et al., 2007), the North Pacific Ocean (Takamura et al., 2010), the Equatorial Pacific Ocean (Ishii et al., 2004, 2009; Feely et al., 2002, 2006; Park et al., 2006, 2012) and the Southern Ocean (Le Quéré et al., 2007; Metzl, 2009) with large differences between ocean regions (Le Quéré et al., 2010; Lenton et al., 2012).

Measurements of CO_2 in the surface oceans (generally as the mole fraction of CO_2 (xCO_2), partial pressure (pCO_2), or fugacity (fCO_2)) enable estimation of CO_2 air-sea fluxes and their variability. Underway measurements of fCO_2 can be made on the surface water supply of ships, including ships of opportunity on commercial routes. The number of CO_2 measurements increased over the past four decades (Fig. 1) (Sabine et al., 2010). Data collection started in the late 1960s and 1970s, increased in the 1980s and intensified from the 1990s onwards. Roughly four times more data were collected during the 2000s than in the 1990s. The growth in data collection partly resulted from large international research programmes, for example JGOFS (Joint Global Ocean Flux Study) and WOCE (World Ocean Circulation Experiment) and regional funding initiatives. The development of autonomous instrumentation for the continuous measurement of surface water fCO_2 (e.g. Körtzinger et al., 1996; Cooper et al., 1998; Pierrot et al., 2009), the intercomparison of such instrumentation at sea (Körtzinger et al., 1996, 2000) and its installation on voluntary observing ships (e.g. Cooper et al., 1998; Lüger et al., 2004; Schuster and Watson, 2007; Watson et al., 2009; Monteiro et al., 2010; Takamura et al., 2010; Lefèvre et al., 2013) and on moorings and drifters (Bakker et al., 2001; Emerson et al., 2011; Wada et al., 2011) have played an important role in the increase in data collection.

Quantification of regional and global annual mean ocean CO_2 uptake requires observations of surface water fCO_2 with adequate spatial and temporal coverage (Sweeney et al., 2000; Lenton et al., 2006). Studies of year-to-year, decadal and longer-term trends in air-sea CO_2 uptake require consistent, multi-decade data records of surface ocean fCO_2 (e.g. Schuster and Watson, 2007; Takamura et al., 2010; Park et al., 2012). Statistical techniques and modelling have been deployed for basin-wide estimation of

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air-sea CO_2 fluxes from surface water fCO_2 observations, for example a diffusion-advection based interpolation scheme (Takahashi et al., 1997, 2009), (multiple) linear regression (Boutin et al., 1999; Cosca et al., 2003; Sarma et al., 2006; Olsen et al., 2008; Chen et al., 2011; Chierici et al., 2012), neural network approaches (Lefèvre et al., 2005; Telszewski et al., 2009; Hales et al., 2012; Landschützer et al., 2013; Nakaoka et al., 2013) and a diagnostic model (Rödenbeck et al., 2013a).

Uniform procedures for the collection, reporting, processing and archiving of CO_2 data, as well as public release of data are required for creating global and regional, long-term, consistent surface ocean fCO_2 synthesis products. Takahashi and co-workers have constructed an impressive series of surface ocean CO_2 climatologies, the most recent one for the climatological year 2000 (Takahashi et al., 2009), and now provide annual updates to their global surface ocean pCO_2 data set (Takahashi et al., 2013). The Surface Ocean CO_2 Atlas (SOCAT) (Bakker et al., 2012; Pfeil et al., 2013; Sabine et al., 2013) complements this work. The SOCAT and Takahashi data sets benefit from standardisation and intercomparison of measurement and reporting protocols, as well as discussions between data providers and quality controllers on reporting standards and data quality (Dickson et al., 2007; IOCCP, 2008, 2012; SOCAT, 2011, 2012a, b; Wanninkhof et al., 2013a). Both data sets have contributed towards more rapid availability of ocean carbon data for synthesis products and policy-related assessments.

SOCAT aims to create, make publicly available and archive (IOCCP, 2007):

- A 2nd level quality-controlled, global surface ocean fCO_2 data set following internationally agreed-upon procedures and regional review;

- A gridded data product of mean monthly surface water fCO_2 on a 1° latitude by 1° longitude grid with minimal temporal or spatial interpolation using the 2nd level quality-controlled, global surface ocean fCO_2 data set.

The first SOCAT release was made public as versions 1.4 and 1.5, here jointly referred to as version 1, in September 2011 (Bakker et al., 2012). SOCAT version 1 contains 6.3 million surface fCO_2 data points from 1851 cruises in the global oceans and coastal seas between 1968 and 2007 (Fig. 1; Table 1). This version was documented in two complementary publications (Pfeil et al., 2013; Sabine et al., 2013). Surface water fCO_2 values at sea surface temperature (fCO_2_rec, with "rec" indicating recommended fCO_2) have been (re-)calculated from the original CO_2 values reported by the data provider, following a strict calculation protocol. Pfeil et al. (2013) describe the procedures for putting the data into a uniform format, (re-)calculation of surface water fCO_2 and 2nd level quality control (QC). Sabine et al. (2013) detail the gridding of the fCO_2 values on a 1° latitude by 1° longitude grid with a higher 0.25° latitude by 0.25° longitude resolution product for the coastal seas.

2 SOCAT version 2

2.1 An update of version 1

Version 2 of SOCAT has been made public on 4 June 2013 at the 9th International Carbon Dioxide Conference in Beijing, China (SOCAT, 2013b). SOCAT version 2 contains 10.1 million surface fCO_2 values from 2660 cruises for the global oceans and coastal seas between November 1968 and December 2011 (Figs. 1 and 2; Table 1). Version 2 has an additional 809 cruises relative to version 1, mostly from 2006 to 2011. About 70 cruises contained in version 1 were removed from version 2 upon identification of data quality concerns. The data in version 2 originate from 109 different ships and 4 time series, moorings, and drifters. Figure 3 shows the number of fCO_2 values from the 30 ships and time series with the most intense data collection effort.

The procedures for the retrieval and formatting of these data, for the (re-)calculation of surface water fCO_2, for quality control, and for the creation of data products were analogous to those used in version 1 (see Pfeil et al., 2013; Sabine et al., 2013). During primary quality control basic problems in the data were identified, for example unrealistic positions, times and orders of magnitude. Second level quality control consisted of

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assigning a quality control flag to each data set and a WOCE flag to individual surface water fCO_2 values (see Sect. 2.3.2).

Version 2 has three different data products (Table 2):

1. Individual cruise files of surface water fCO_2 in a uniform format which have been subject of 2nd level quality control;

2. A synthesis data set of surface water fCO_2 for the global oceans and coastal seas;

3. Global gridded products of surface water fCO_2 means.

These data products are much the same as products reported with version 1 (Pfeil et al., 2013; Sabine et al., 2013).

SOCAT is a community effort of seagoing ocean carbon scientists and data managers without central funding. SOCAT is 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). The numerous SOCAT contributors have donated their time and data to this effort (Figs. 3 and 4; Tables 3, 4 and 5).

Users of the SOCAT data products are requested to (SOCAT, 2013a, b):

1. Recognise the contribution of SOCAT scientists, data contributors and quality controllers in the form of invitation to co-authorship, or citation of relevant scientific articles by data contributors;

2. Cite all SOCAT data products by reference to publications documenting SOCAT;

3. Send references of publications using SOCAT products to submit@socat.info.

Regular updates of the SOCAT products are planned (IOCCP, 2007; Bakker et al., 2012; Pfeil et al., 2013). The SOCAT website (http://www.socat.info/) provides access

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to the data products together with online visualisation tools, data documentation, meeting reports, publications and a list of contributors. This publication documents SOCAT version 2, in particular differences relative to version 1. Section 2.2 highlights where version 2 differs from version 1 (Table 1) and Sect. 2.3 provides a summary of the procedures followed for creating version 2. Section 2.4 describes the data products and tools available for version 2 (Table 2).

2.2 Key differences between versions 1 and 2

2.2.1 Time stamp and version numbering

The time stamp for SOCAT version 1 products did not contain seconds (Table 1) (Pfeil et al., 2013). In some cases this resulted in multiple entries for a given time stamp. Such multiple entries were averaged in the global and regional synthesis data files (version 1.5), but not in the individual cruise files (version 1.4). Two version numbers (version 1.4 and 1.5) highlight the different treatment of multiple entries for the same time stamp in these version 1 data products.

SOCAT version 2 products include seconds, as reported by the data contributor, in the time stamp for all newly added and updated cruises (Table 1). However, a time stamp including seconds is still not available most of the version 1 cruises. For these cruises seconds were added artificially to the time stamp to avoid the problem of multiple entries. The next version of SOCAT will include seconds, as reported by the data contributor, for all cruises.

The CO_2 measurements for a dozen historical cruises are listed as taken at midnight or their time stamp in fractional days contains insufficient decimals for retrieving minutes and seconds. Artificial seconds, in some cases including tenths or hundreds of a second, were generated for these valuable data, such that they can remain in SOCAT version 2. Every effort will be made to retrieve a more adequate time stamp for these cruises for future versions. Unlike version 1, which has version 1.4 and 1.5 data products, version 2 data products have a single version number.

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2.2.2 Expocodes

SOCAT uses twelve character expocodes (Swift, 2008) as stable and unique data set identifiers. For example, 49P120101218 indicates a cruise on the Japanese (49) ship of opportunity Pyxis (P1) with the first day of the cruise on 18 December 2010. In contrast to version 1, expocodes have also been assigned for moorings and drifters in version 2, by registering a "vessel code" at International Council for the Exploration of the Sea (ICES) in collaboration with the National Oceanographic Data Center (NODC) and the British Oceanographic Data Centre (BODC) (Table 1).

2.2.3 Creation of an Arctic regional designation

Quality control in SOCAT is carried out by groups organised according to region. Figure 5 shows the regions for SOCAT version 2 (Table 4). These regions have been operationally defined and do not necessarily follow common oceanographic definitions. Version 1 had regions for the coastal seas, the North Atlantic, Tropical Atlantic, North Pacific, Tropical Pacific, Indian Ocean and Southern Ocean (Pfeil et al., 2013). Arctic data were part of the North Pacific and North Atlantic Oceans and the coastal region. Given the importance of Arctic research and the rapid increase in the quantity of Arctic fCO_2 values, an Arctic region has been defined for version 2 (Figs. 1b, 5 and 6; Table 1) (SOCAT, 2012b). The Arctic region includes both shelf seas and the deep ocean. It encompasses all waters north of 70° N for 100° W to 43° E (Atlantic sector) and north of 66° N elsewhere.

2.2.4 WOCE flags for individual fCO_2 values

During quality control individual fCO_2 values are assigned WOCE flags: 2 (good), 3 (questionable) or 4 (bad) with 2 (good) being the default setting (Pfeil et al., 2013). Flags 3 and 4 might indicate an erroneous time or position stamp, an unrealistic seawater temperature, strong warming of the water between intake and equilibrator or a

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large pressure difference between the equilibrator and the atmosphere. Outliers in parameters required for the timing, location and calculation of fCO_2 values are given flags of 3 and 4.

About 0.2 % of the fCO_2 values were assigned a flag of 3 or 4 during version 1 quality control. Unintentionally these fCO_2 values were reported with a flag of 2 in version 1 products. The earlier version 1 flags of 3 and 4 have been re-instated in version 2. Flags of 2, 3 and 4 have been assigned to individual fCO_2 values in version 2 (Table 1). Individual cruise files contain surface water fCO_2 values with flags of 2, 3 and 4, while synthesis files only include fCO_2 values with a flag of 2 (Tables 2, 6).

2.2.5 SOCAT output files

The data set quality control flags A to D have been added as numerical values 11 to 14 to the synthesis files in version 2 (Tables 1 and 6). The distance to a major land mass is a new parameter in the files. Atmospheric CO_2 mole fractions from the 2012 GLOBALVIEW-CO2 are reported in version 2 output files; this represents an update from the 2008 GLOBALVIEW-CO2 values which were reported for version 1.

2.3 Procedures for creating version 2

2.3.1 Data entry and (re-)calculation of recommended fCO_2

Version 2 contains 809 more cruises than version 1. The new cruises were either submitted directly to SOCAT or were retrieved from public websites hosted by the Carbon Dioxide Information Analysis Center (CDIAC), PANGAEA®, institutes and projects. As in version 1, most surface water CO_2 values have been measured by equilibration of a headspace with seawater and subsequent analysis of the CO_2 content of the headspace (Pfeil et al., 2013). Historical measurements generally used gas chromatographic analysis, while more recent measurements are based on infrared detection. SOCAT versions 1 and 2 include a small number of historical, discrete surface water

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fCO_2 measurements. SOCAT products do not include fCO_2 calculated from other carbon parameters, such as pH, alkalinity or dissolved inorganic carbon. A small number of fCO_2 observations (0.08 % in version 2) are from measurements by a spectrophotometric method using a pH-sensitive dye.

As in version 1, all data were assembled in a uniform file format (Pfeil et al., 2013). Primary quality control was carried out at this stage. Surface water fCO_2 values at sea surface temperature, also known as recommended fCO_2 (fCO_2_rec), were recalculated following a single set of equations and an order of preference for the CO_2 input parameter (Pfeil et al., 2013). Climatological values of salinity and atmospheric pressure from re-analysis were used in the calculation of recommended fCO_2, if the data contributor did not report in situ salinity and pressure (Pfeil et al., 2013).

2.3.2 Secondary quality control

Secondary quality control of the version 2 data was carried out by 24 marine carbon scientists from eight countries (Fig. 4). Procedures for 2nd level quality control were defined in a series of workshops (IOCCP, 2008, 2009, 2010; Pfeil et al., 2013). The regional group members assigned data set quality control flags and WOCE flags. All new and updated data sets were subject to this quality control. The criteria and procedures for quality control were identical between versions 1 and 2 (Pfeil et al., 2013). Each data set was assigned a separate data set flag A, B, C, D, S (Suspend) or X (Exclude) for each region it crossed. As a final step in the quality control process the quality controllers needed to resolve any "conflicting" data set flags between regions and decide on the "agreed" flag for a data set. Only data sets with a flag A, B, C or D are included in SOCAT version 2 products, as was also the case for version 1.

The data set quality control flags in SOCAT versions 1 and 2 were developed for automated shipboard measurement of surface water fCO_2, mainly by infrared detection and at sea standardisation using compressed calibration gases with a range of CO_2 concentrations (IOCCP, 2008; Pfeil et al., 2013). Much weight is put on whether approved methods or standard operating procedures (AOML, 2002; Dickson et al., 2007;

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Pierrot et al., 2009) were followed by making this a pre-requisite for flags A and B (Pfeil et al., 2013). Frequent calibration of shipboard fCO_2 measurements is undertaken with three or more non-zero calibration gases, e.g. every 2.5–3 h (Pierrot et al., 2009), to characterise the non-linearity in detector response. The fCO_2 values from cruises with flags of A and B are judged to have an accuracy of ±2 µatm or better.

Complete metadata documentation is required for data set quality control flags of A, B and C. Comparison to other data is carried out, if possible. The overall quality of the data needs to be deemed acceptable for flags of A, B, C and D (Pfeil et al., 2013). Surface water fCO_2 measurements from moorings and drifters were quality controlled for versions 1 and 2 using the existing data quality control criteria.

Overall data quality and reporting of metadata has improved from version 1 to version 2 which we attribute to the SOCAT effort. In the first version, 41 % of cruises were assigned a flag of A or B, 22 % obtained a flag of C and 37 % received a flag of D. Version 2 has a larger proportion of cruises with flags of A or B (48 %) and smaller proportions of cruises with a flag of C (18 %) and D (33 %).

2.4 Version 2 data products and tools

2.4.1 Surface water fCO_2 in the SOCAT data products

The SOCAT data products provide access to recommended surface ocean fCO_2 values in a uniform format for the global oceans and coastal seas. Three different SOCAT data products are available: individual cruise files, synthesis files and gridded files. All data products can be accessed via the SOCAT website (http://www.SOCAT.info/) or via the web-links provided below and in Table 2. The version 2 data products ressemble those for version 1 (Pfeil et al., 2013; Sabine et al., 2013). The key differences between the version 1 and 2 products have been discussed in Sect. 2.2 and are listed in Table 1. Two interactive online tools, the Cruise Data Viewer and the Gridded Data Viewer, facilitate interrogation of the global synthesis product and the gridded data products, respectively. These data products and tools are discussed below.

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2.4.2 Individual cruise files

Individual cruise files provide surface water $f\mathrm{CO_2}$, the parameters used to (re-)calculate $f\mathrm{CO_2}$ and the original $\mathrm{CO_2}$ parameter(s) reported by the data contributor (Table 6). The files for data sets with flags A, B, C and D include all surface water $f\mathrm{CO_2}$ values with WOCE flags of 2, 3 and 4. Individual cruise data files are archived at PANGAEA® (http://doi.pangaea.de/10.1594/PANGAEA.811776) (Table 2). Each cruise has a digital object identifier (doi). Metadata provided by the data contributor accompany the cruise files.

As in version 1, the individual cruise and synthesis files include the climatological values of salinity and atmospheric pressure from re-analysis (Table 6). The files also contain values for the water depth, the distance to a major land mass and the atmospheric $\mathrm{CO_2}$ mole fraction interpolated from GLOBALVIEW-CO2 (2012). Version 2 is made available via PANGAEA® to the World Data System (WDS) of the International Council for Science (ICSU), to the Group of Earth Observations (GEO) Portal and to the Global Earth Observation System of Systems (GEOSS).

2.4.3 Global synthesis product

A global synthesis product of surface ocean $f\mathrm{CO_2}$ values has been created by merging the individual cruise files. The product is available as a global file or as regional files for the various SOCAT regions (Tables 2 and 4). The synthesis files only contain cruise files with flags A, B, C and D and surface water $f\mathrm{CO_2}$ values with WOCE flag 2 (Table 6). The synthesis files do not contain the original $\mathrm{CO_2}$ values. Each line in the files lists the doi-number of the corresponding individual cruise file at PANGAEA® , thus giving access to the metadata and the original $\mathrm{CO_2}$ values (Sect. 2.4.1). The global and regional files are publicly available as compressed zip text files via CDIAC (http://cdiac.ornl.gov/ftp/oceans/SOCATv2/). The regional files contain only data from within that region, so that data from most cruises are split between several regional files. The global synthesis

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product is also available in Ocean Data View format (http://odv.awi.de/en/data/ocean/socat_fCO2_data).

The Cruise Data Viewer (http://ferret.pmel.noaa.gov/SOCAT2_Cruise_Viewer/), an interactive tool on a Live Access Server, enables interrogation of the global synthesis product. The user can search and subset the global SOCAT data set by year, month, day, region, parameter, expocode, cruise name, vessel, and data set quality control flag. One may define search limits, for example salinity below 30 or sea surface temperature above 10 °C. The user can include data with a WOCE flag of 3 (questionable) and 4 (bad), find metadata, read quality control comments, create property-property plots and download data. Figures 2 and 7 have been made with the Cruise Data Viewer.

2.4.4 Gridded products

Several gridded products of surface ocean fCO_2 means with minimal interpolation are available (doi:10.3334/CDIAC/OTG.SOCAT_V2_GRID). Surface water fCO_2 values with a flag of 2 have been put on a 1° latitude by 1° longitude grid in four ways: per year, monthly per year, monthly per decade, and per climatological month from 1970 to 2011 (Table 2). A higher resolution of 0.25° latitude by 0.25° longitude is available as monthly means per year for the coastal region (Fig. 5; Table 4). The procedures for gridding the data are similar between versions 1 and 2 (Sabine et al., 2013).

Gridded fCO_2 values are reported as unweighted means and as cruise-weighted means (Sabine et al., 2013). In an unweighted mean all the fCO_2_rec values in a grid cell have been given equal weight in calculating the mean. In a cruise-weighted mean, first averages of the fCO_2_rec data per cruise have been calculated within a grid cell, before averages of the cruise means have been determined. Grid cells without fCO_2 values are empty. No correction has been made for the expected long-term increase in surface water fCO_2, thus care should be taken in use of the decadal and climatological gridded products. Furthermore, the gridded products may have a temporal bias in grid cells with uneven temporal data coverage. For example, an annual gridded product will have a strong seasonal bias, if only summertime fCO_2 values are available.

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Gridded fCO_2 products can be accessed as NetCDF files from CDIAC (http://cdiac.ornl.gov/ftp/oceans/SOCATv2/SOCATv2_Gridded_Dat/), in Ocean Data View format (http://odv.awi.de/en/data/ocean/socat_fCO2_data) and via the Gridded Data Viewer (http://ferret.pmel.noaa.gov/SOCAT_gridded_viewer/) (Table 2).

Several new gridded products and variables are available via the Gridded Data Viewer for version 2. The number of different years has been added as a variable in the monthly climatological gridded dataset. Data sets now show the 400 km continental margin mask at 1 min resolution, as used in SOCAT, and the distance to the nearest major land mass from 0 to 1000 km at 20 min resolution. The Gridded Data Viewer has an option for animation of gridded products. The visualisation tools of the Gridded Data Viewer have been expanded. The interface now includes a comparison capability for up to four gridded data sets. This enables the user to visualise, for example, gridded data products in SOCAT versions 1 and 2 in a multiple-plot view.

3 Spatial and temporal data coverage

SOCAT version 2 includes surface ocean fCO_2 values collected between 1968 and 2011 for the global oceans and coastal seas (Figs. 1 and 2). Data availability has increased over time for most ocean regions (Figs. 1b and 6). A notable exception is the Indian Ocean north of 20° S, for which data are available from the 1990s, but where few subsequent observations have been made. Marked increases in data collection are apparent in the Arctic Ocean and the Gulf of Mexico (Fig. 1b). For example, version 2 has a total of 40 cruises in the Arctic Ocean, of which 10 cruises were conducted in 2011 alone. Data coverage remains sparse south of 30° S (Fig. 2). The seasonal data distribution of fCO_2 for the period 2000 to 2009 is shown in Fig. 7. The maps demonstrate the near-absence of wintertime data from the high-latitude regions. The southwest Ross Sea (Southern Ocean) has about 20 months of observations spanning five months from austral spring to autumn (Fig. 8).

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The installation of automated fCO_2 systems on voluntary observing ships and Antarctic supply ships has greatly improved the data availability for coastal regions along shipping routes (Fig. 9). For example, between 2000 and 2009 more than 40 individual cruises have crossed the 1° latitude by 1° longitude grid boxes in the Florida Straits, the English Channel, off the coast of Japan and close to the Antarctic Peninsula.

The number of months of the year and total months with fCO_2 values per 1° by 1° grid cell shed light on data collection activities for 1970 to 2011 (Fig. 8). High data density along shipping routes highlights the repeat fCO_2 observations. For example, numerous grid boxes east of Japan have observations in all months of the year for more than 50 months in total, reflecting an intense CO_2 observational effort over a large number of years. This on-going data collection effort is critical for the quantification of the variability and trends in CO_2 air-sea exchange.

4 Future plans

4.1 Progress towards version 3

Surface water CO_2 values and accompanying metadata can be submitted to CDIAC in the IOCCP-recommended formats (http://cdiac.ornl.gov/oceans/submit.html) at all times. Ideally data are submitted as they become available. The SOCAT global group sets deadlines for consideration of data in specific SOCAT versions, for example the deadline for submission to SOCAT version 3 is 31 December 2013. Version 3 quality control is scheduled to take place during the summer and autumn of 2014 with the release of version 3 planned for mid-2015.

4.2 Quality control flags for new instrumentation and alternative sensors

The SOCAT data quality control flags have been primarily designed for shipboard, continuous surface water CO_2 measurements by gas chromatography or infrared detection (Pfeil et al., 2013). Since the definition of these flags, high-precision and stable cavity ring-down spectroscopy (CRDS) has become available for surface water CO_2 measurements (Friedrichs et al., 2010; Becker et al., 2012). The quality control criteria in SOCAT are deemed adequate for the measurements by CRDS. Measurements made by CRDS will be included in future SOCAT versions, provided calibrations have been carried out at least daily (SOCAT, 2012b).

The quality control criteria need revision for fCO_2 values from sensors on surface moorings and drifters (SOCAT, 2012b). These measurements do not follow all the standard operation procedures and at-sea calibration of such fCO_2 measurements is often infrequent or non-existent. Also the sensors tend to use fewer gas standards than on ships, due to logistical and power constraints. A working group on alternative sensors (Table 3) has developed a vision on how to include such fCO_2 values, as measured for example by infrared analysis and spectrometry, in future SOCAT versions (Wanninkhof et al., 2013a). The working group has recommended which quality control criteria should apply to these data.

4.3 Automation

The large effort for data entry and quality control is a major obstacle for regular and prompt SOCAT updates, especially with more data becoming available each year. The need for automating SOCAT was formally recognised in September 2011 (SOCAT, 2011) and an automation team was created (Table 3). The automation vision was accepted by regional and global group leads (SOCAT, 2012a, b). The automation system will allow the data provider to upload, review and submit data and metadata. It will calculate surface water fCO_2. The automation system will provide a single portal for data providers, data managers and quality controllers. Manual data entry by the SOCAT data managers will be reduced. Regular, prompt releases of SOCAT will be more straightforward, once the automation system is fully operational. The automation system is expected to become the primary mode of data submission from version 4 onwards.

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5 Scientific applications of SOCAT

Several scientific studies have already used SOCAT data products. The global synthesis product is the most commonly used SOCAT product in scientific publications. Files in zipped text format (Lourantou and Metzl, 2011; Tjiputra et al., 2012; Nakaoka et al., 2013; Rödenbeck et al., 2013a, b; Wanninkhof et al., 2013b) and the Ocean Data View collection (Chierici et al., 2012) are most commonly used for data access. Two studies use the global gridded products (Landschützer et al., 2013; Schuster et al., 2013).

Scientific applications of SOCAT include:

- Visualisation of surface ocean fCO_2 data coverage (Chierici et al., 2012) and data requirements (Wanninkhof et al., 2013b);
- Use of the SOCAT continental margin mask (Evans and Mathis, 2013);
- Process studies (Lourantou and Metzl, 2011);
- Creation and validation of surface water fCO_2 and CO_2 air-sea flux maps by a variety of techniques, including multiple linear regression (Schuster et al., 2013), neural network approaches (Landschützer et al., 2013; Nakaoka et al., 2013) and an ocean mixed layer model (Rödenbeck et al., 2013a, b);
- Quantification of the annual mean ocean carbon sink (Schuster et al., 2013);
- Studies of variation in the ocean carbon sink on seasonal (Rödenbeck et al,. 2013a), year-to-year (Rödenbeck et al., 2013b) and decadal time-scales (Lourantou and Metzl, 2011);
- Initialisation and validation fields for ocean carbon cycle models (Tjiputra et al., 2012).

These applications highlight the utility of SOCAT for regional and global air-sea CO_2 flux assessments, process studies and ocean carbon modelling.

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6 Conclusions

SOCAT version 2 represents a 44 yr record of surface water fCO_2 values from 1968 to 2011 for the global oceans and coastal seas (Figs. 1 and 2). Version 2 extends version 1 by four years to 2011, while also adding more fCO_2 values for the years 2006 and 2007. The data are in a uniform format and have been subject to fully documented quality control. The quality of data and of data reporting has improved in version 2 relative to version 1. The temporal data distribution at least partly reflects activities in large international research programmes. Over time, data coverage in all ocean regions has increased, with the exception of the Indian Ocean north of 20° S. Data coverage has increased four-fold from the 1990s to the 2000s, thus providing much better seasonal and spatial coverage for large parts of the northern hemisphere oceans and coastal seas. Data coverage remains sparse in large parts of the Southern Hemisphere and the Indian Ocean.

The international importance of SOCAT is evident from recent scientific articles using SOCAT data products for quantification of the ocean carbon sink, process studies and ocean carbon modelling. Regular updates to SOCAT will extend the SOCAT data record and ensure that new data are promptly made available for flux assessments and modelling. Future plans include automation and a revision of the quality control criteria for fCO_2 values from alternative sensors.

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Table 1. Key differences between SOCAT versions 1 (released as versions 1.4 and 1.5) and 2.

	Version 1	Version 2
Description	Pfeil et al. (2013); Sabine et al. (2013)	This study
Data coverage	1968 to 2007, 6.3 million surface water fCO_2 values, 1853 cruises	1968 to 2011, 10.1 million surface water fCO_2 values, 2660 cruises
Time stamp	The time stamp did not contain seconds. Some multiple entries for the same time stamp were reported in individual cruise files (version 1.4), but were averaged in the synthesis files (version 1.5).	The time stamp includes seconds for all new and updated cruises. Seconds were added artificially to time stamps for most version 1 cruises to avoid multiple entries. Artificial times with tenths and hundreds of a second have been generated for historical data reported at midnight or with insufficient decimals in the time stamp.
Version numbers	Two version numbers, version 1.4 and 1.5, highlighted the different treatment of multiple entries for the same time stamp.	Version 2 only.
Expocode	Expocodes were not used for moored and drifting buoys.	Expocodes have been used for moored and drifting buoys.
Arctic region	Arctic data were included under the North Atlantic, North Pacific and coastal regions.	An Arctic region has been defined as all open ocean and coastal waters north of 70° N for 100° W to 43° E, elsewhere north of 66° N.
WOCE flags	WOCE flags 3 and 4 were reset unintentionally to flag 2. Most fCO_2 values were reported with a flag of 2 (good), including 0.2 % of data initially given a flag of 3 (questionable) or 4 (bad).	The fCO_2 values have been assigned WOCE flags of 2 (good), 3 (questionable) and 4 (bad). Flags of 3 and 4 given during version 1 quality control have been reinstated. Individual cruise files contain all fCO_2 values with flags of 2, 3 and 4. Synthesis files only contain fCO_2 values with a flag of 2.
Output format	Atmospheric CO_2 mole fractions were from GLOBALVIEW-CO2 2008.	Atmospheric CO_2 mole fractions are from GLOBALVIEW-CO2 2012. New parameters are the data set quality control flags A to D and distance to a major land mass.

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Table 2. Key characteristics of the three SOCAT data products for surface ocean fCO_2 values in version 2, as described in Sect. 2.4. All data products can be accessed via the SOCAT website (http://www.socat.info).

	Key characteristics	Available formats
Individual cruise files	The cruise files contain all fCO_2 values with flags of 2, 3 and 4 and the original CO_2 measurements for data sets with flags of A, B, C or D (Table 6).	Text files[1].
Global and regional synthesis files	The synthesis files contain fCO_2 values with a flag of 2 (Table 6). The global synthesis file has been created by merging the individual cruise files. Regional files contain data from a specific region.	Zipped text files[2], in Ocean Data View format[3], and via the Cruise Data Viewer[4].
Gridded files	Gridded means of fCO_2 values on a 1° × 1° grid with minimal interpolation. Means are per year, monthly per year, monthly per decade and per climatological month from 1970 to 2011. A monthly 0.25° × 0.25° data set is available for coastal regions.	NetCDF files[5], in Ocean Data View format[6], and via the Gridded Data Viewer[7].

[1] http://doi.pangaea.de/10.1594/PANGAEA.811776
[2] http://cdiac.ornl.gov/ftp/oceans/SOCATv2/
[3] http://odv.awi.de/en/data/ocean/socat_fCO2_data
[4] http://ferret.pmel.noaa.gov/SOCAT2_Cruise_Viewer/
[5] http://dx.doi.org/10.3334/CDIAC/OTG.SOCAT_V2_GRID,
http://cdiac.ornl.gov/ftp/oceans/SOCATv2/SOCATv2_Gridded_Dat/
[6] http://odv.awi.de/en/data/ocean/socat_fCO2_data
[7] http://ferret.pmel.noaa.gov/SOCAT_gridded_viewer/

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Table 3. Activities and key participants in SOCAT versions 2 and 3. Regional group leads are in Table 4.

Activity	Key Participants
Global group for coordination	Bakker (chair), Hankin, Kozyr, Metzl, Olsen, Pfeil, Pierrot, Telszewski
Data retrieval, data entry, recalculation of fCO_2	Pfeil, Olsen
Quality control	Alin, Bakker, Barbero, Castle, Cosca, Evans, Hales, Harasawa, Hoppema, Huang, Hunt, Huss, Park, Paterson, Pierrot, Schuster, Skjelvan, Steinhoff, Suzuki, Tilbrook, Van Heuven, Vlahos, Wada, Wanninkhof
Live Access Server	Hankin, O'Brien, Smith
Cruise files, synthesis products and gridded products	Pfeil, Smith, Manke, Hankin
Ocean Data View	Schlitzer
Matlab files	Pierrot, Landschützer
SOCAT website	Pfeil
Data archiving and online access	Pfeil, Sieger, Kozyr, Smith, Manke, Hankin
Meetings	Alin, Bakker, Hales, Hankin, Nojiri, Telszewski
Automation (version 3)	Hankin, S. Jones, Kozyr, O'Brien, Pfeil, Smith, Bakker, Olsen, Schweitzer
Alternative sensors (version 3)	Wanninkhof, Steinhoff, Bakker, Bates, Olsen, Sutton

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Table 4. Regions and regional group leads in SOCAT version 2 (Fig. 5).

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 to 70° N	Schuster
Tropical Atlantic	30° N to 30° S	Lefèvre
North Pacific	30 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

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Table 5. Meetings for SOCAT versions 2 and 3 to date.

Timing	Meeting description	Location	Reference
09/2011	Public release of version 1. Session on future SOCAT.	UNESCO, Paris, France	SOCAT (2011)
05/2012	Automation planning meeting	NOAA-PMEL, Seattle, USA	SOCAT (2012a)
07/2012	SOCAT progress meeting	Epochal Centre, Tsukuba, Japan	SOCAT (2012b)
10/2012	Coastal and Arctic SOCAT quality control workshop	NOAA-PMEL, Seattle, USA	IOCCP (2012)
06/2013	SOCAT side event at the 9th International Carbon Dioxide Conference. Public release of version 2.	Beijing International Convention Center, Beijing, China	SOCAT (2013b)

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Table 6. Content of the individual cruise files and the synthesis files in SOCAT version 2.

Individual	Synthesis	Unit	Description
–	Expocode	–	12-character expocode
–	SOCAT_DOI	–	Digital object identifier for the individual cruise and metadata
–	QC_ID	–	Data set quality control flag with 11 for A, 12 for B, 13 for C and 14 for D
Date/Time	–	–	yyyy-mm-dd/hh:mm:ss (ISO8859)
–	yr	Year	Year (UTC)*
–	mon	Month	Month (UTC)*
–	day	Day	Day (UTC)*
–	hh	Hour	Hour (UTC)*
–	mm	Minute	Minute (UTC)*
–	ss	Seconds	Seconds (may include decimals)*
Longitude	longitude	°E	Longitude (0 to 360)*
Latitude	latitude	°N, °S	Latitude (−90 to 90)*
Depth water	sample_depth	m	Water sampling depth*[1]
Sal	sal	–	Salinity on Practical Salinity Scale*
Temp	SST	°C	Sea surface temperature*
Tequ	Tequ	°C	Equilibrator chamber temperature*
PPPP	PPPP	hPa	Atmospheric pressure*
Pequ	Pequ	hPa	Equilibrator chamber pressure*
Sal interp	WOA-SSS	–	Salinity from WOA (2005)[2]
PPPP interp	NCEP_SLP	hPa	NCEP Atmospheric pressure[3]
Bathy depth interp	ETOPO2_depth	m	ETOPO2 Bathymetry[4]
Distance	d2l	km	Distance to major land mass
xCO2air_interp	GVCO2	μmol mol^{-1}	Atmospheric xCO_2 from GLOBALVIEW-CO2 (2012)
xCO2water_equ_dry	–	µmol/mol	xCO_2 (water) at equilibrator temperature (dry air)*
fCO2water_SST_wet	–	µatm	fCO_2 (water) at sea surface temperature (wet air)*
pCO2water_SST_wet	–	µatm	pCO_2 (water) at sea surface temperature (wet air)*
xCO2water_SST_dry	–	μmol mol^{-1}	xCO_2 (water) at sea surface temperature (dry air)*
fCO2water_equ_wet	–	µatm	fCO_2 (water) at equilibrator temperature (wet air)*
pCO2water_equ_wet	–	µatm	pCO_2 (water) at equilibrator temperature (wet air)*
fCO2water_SST_wet	fCO2rec	µatm	Recommended fCO_2 calculated following the SOCAT protocol
Algorithm	fCO2rec_src	–	Algorithm for calculating fCO_2_rec (0: not generated; index 1–14 in Table 3 in Pfeil et al., 2013)
Flag	fCO2rec_flag	–	WOCE flag for fCO_2_rec (2: good, 3: questionable, 4: bad)[5]

* Refers to data reported by the data originator; [1] If the intake depth has not been reported by the data originator, an intake depth of 5 m has been assumed; [2] Sea surface salinity on the Practical Salinity Scale interpolated from the World Ocean Atlas (WOA) 2005 (Antonov et al., 2006), available at: http://www.nodc.noaa.gov/OC5/WOA05/pr_woa05.html (last access: 1 May 2013); [3] Atmospheric pressure interpolated from the NCEP/NCAR (National Centers for Environmental Prediction/ National Center for Atmospheric Research) 40 yr Reanalysis Project on a 6-hourly, global, 2.5° latitude by 2.5° longitude grid (Kalnay et al., 1996), available at: http://www.esrl.noaa.gov/psd/data/gridded/data.ncep.reanalysis.surface.html (last access: 1 May 2013); [4] Bathymetry interpolated from ETOPO2 (2006) 2 min Gridded Global Relief Data, available at: http://www.ngdc.noaa.gov/mgg/global/etopo2.html (last access: 1 May 2013); [5] Individual cruise files contain all fCO_2_rec data. Synthesis files only contain fCO_2_rec data with a WOCE flag 2.

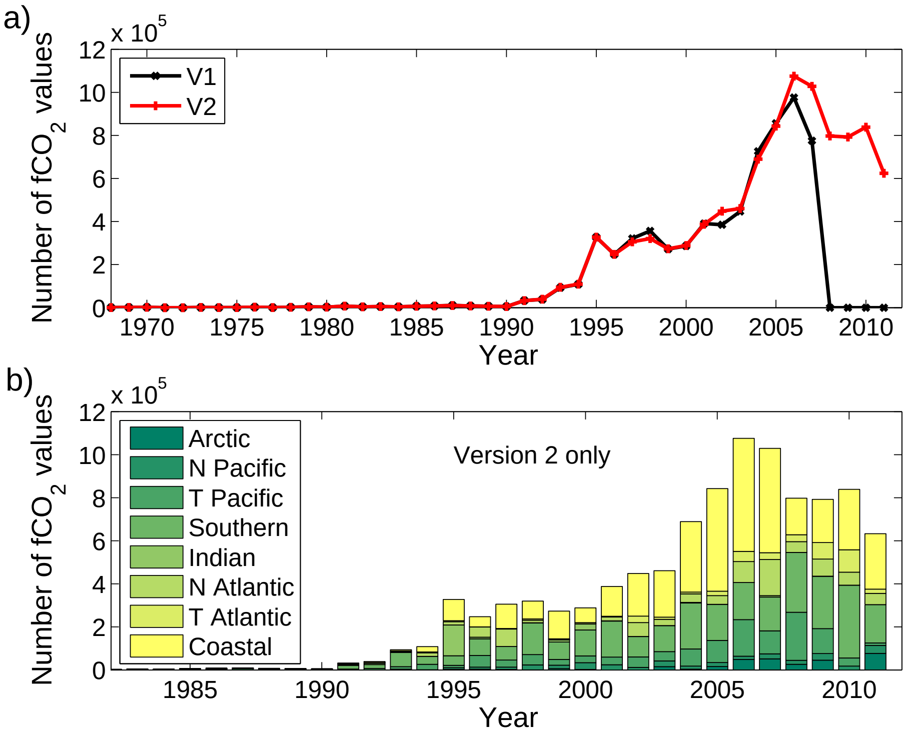

Fig. 1. (a) The number of surface water fCO_2 values per year in SOCAT versions 1 and 2 and **(b)** per region per year in version 2. The SOCAT regions are the Arctic Ocean, the North Pacific Ocean, the Tropical Pacific Ocean, the Southern Ocean, the Indian Ocean, the North Atlantic Ocean, the Tropical Atlantic Ocean and the Coastal seas (Fig. 5, Table 4). These data points originate from data sets with flags of A, B, C or D and have a WOCE flag of 2. The subsequent figures only show fCO_2 values with these characteristics.

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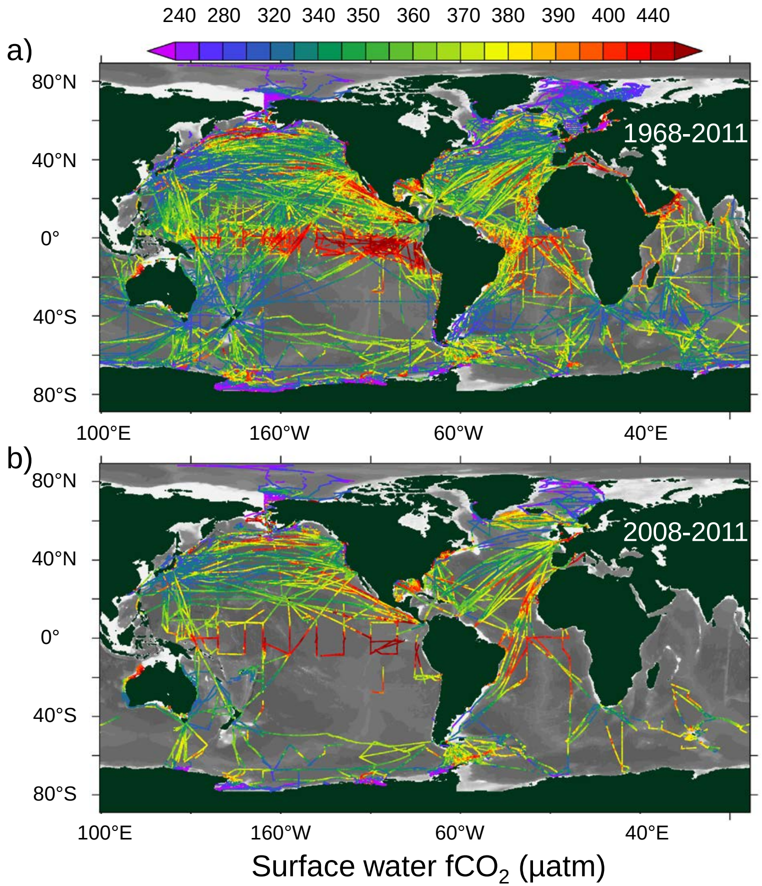

Fig. 2. The global distribution of surface water fCO_2 values in SOCAT version 2: **(a)** for 1968 to 2011 and **(b)** for 2008 to 2011.

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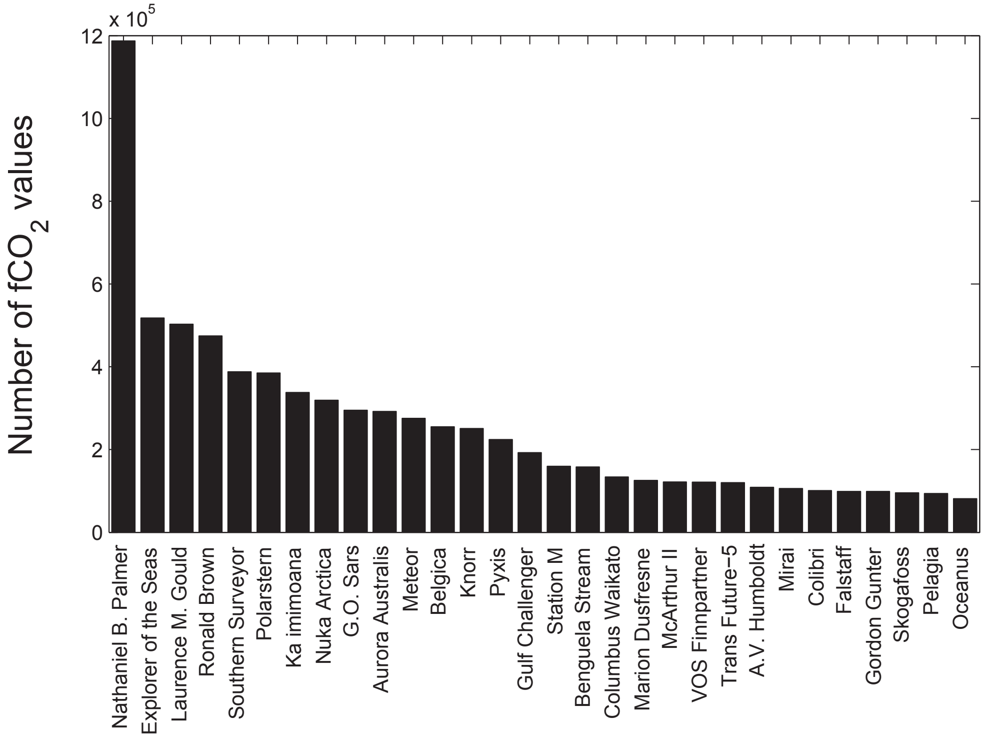

Fig. 3. The number of surface water fCO_2 values obtained on the 30 ships and time series hosting the most intense data collection effort in SOCAT version 2.

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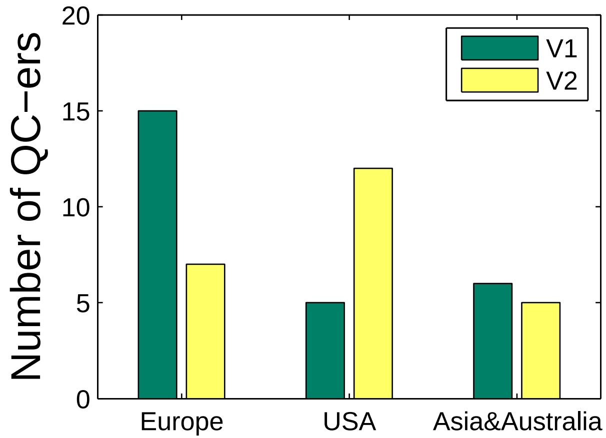

Fig. 4. The number of quality controllers in SOCAT versions 1 and 2 based in Europe, the US, Asia and Austria, respectively. The figure demonstrates the international character of the quality control effort in SOCAT.

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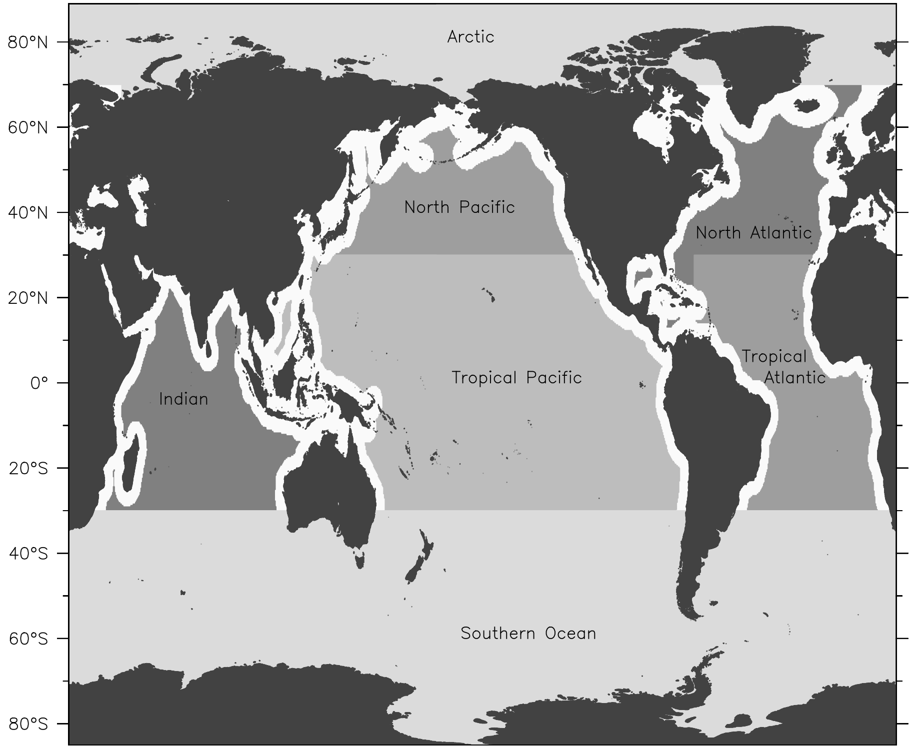

Fig. 5. Quality control regions for SOCAT version 2 (Table 4). White shading corresponds to the coastal region. All regions have been defined for operational reasons and do not necessarily reflect common oceanographic definitions.

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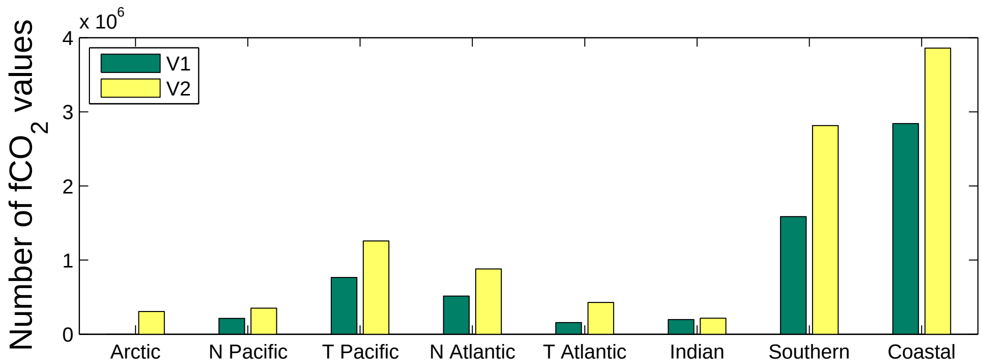

Fig. 6. The number of surface water fCO_2 values for each region in SOCAT versions 1 and 2. The regions are the Arctic Ocean, the North Pacific Ocean, the Tropical Pacific Ocean, the North Atlantic Ocean, the Tropical Atlantic Ocean, the Indian Ocean, the Southern Ocean and the coastal seas (Fig. 5, Table 4). In version 1, Arctic data were included in the North Pacific, North Atlantic and coastal regions.

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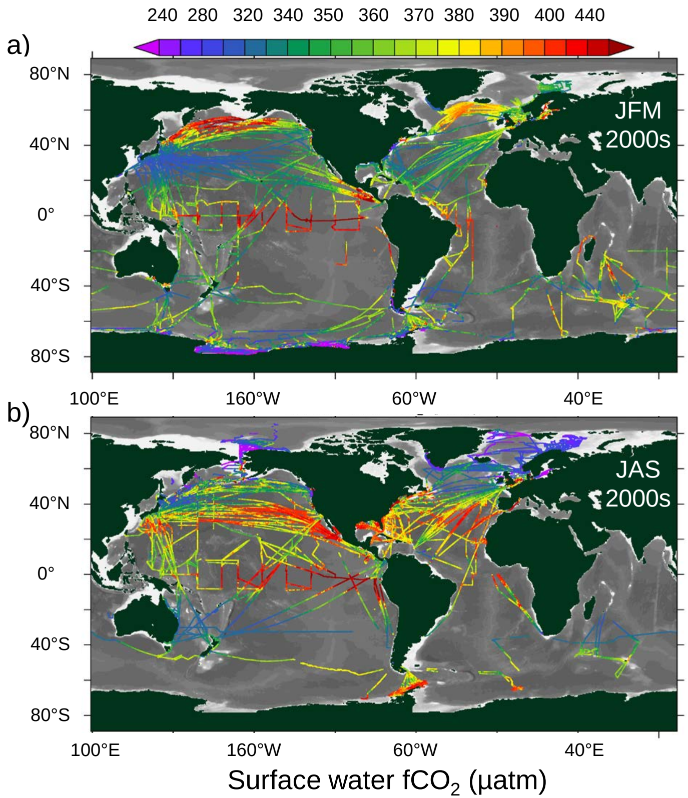

Fig. 7. Seasonal distribution of surface water fCO_2 for 2000 to 2009 in SOCAT version 2 for **(a)** January to March and **(b)** July to September.

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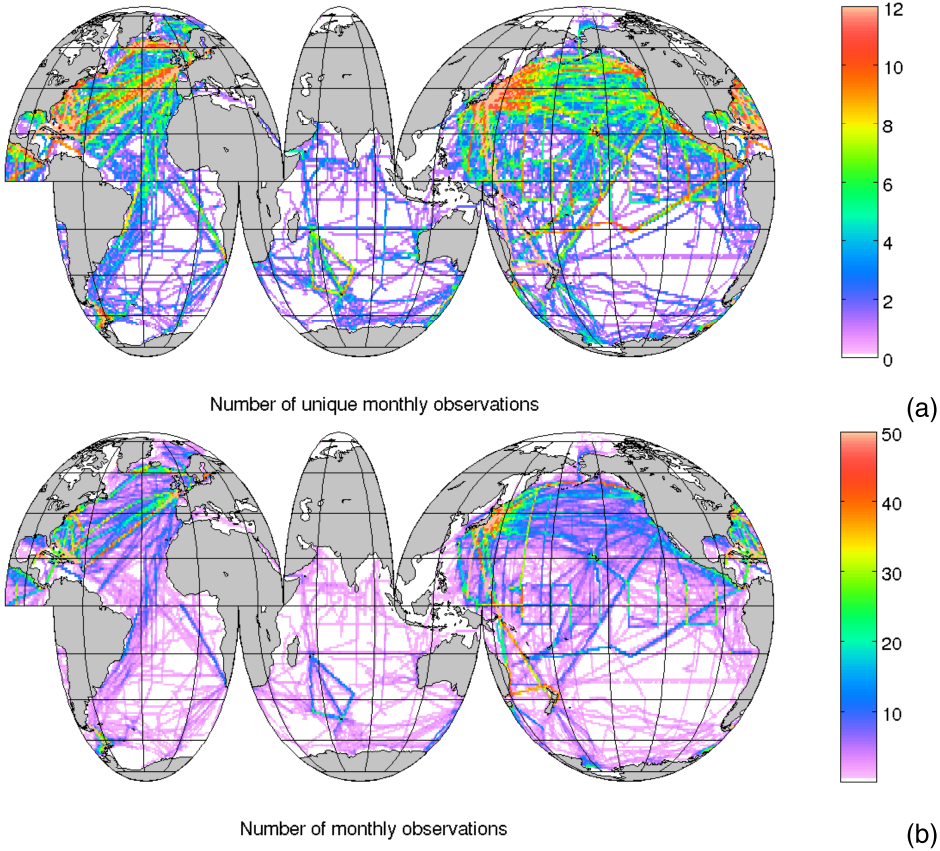

Fig. 8. The number of **(a)** months of the year and **(b)** total months with surface water fCO_2 values in each 1° latitude by 1° longitude grid cell from 1970 to 2011 in SOCAT version 2. **(a)** updates the figure for version 1 in Sabine et al. (2013, Figure 5).

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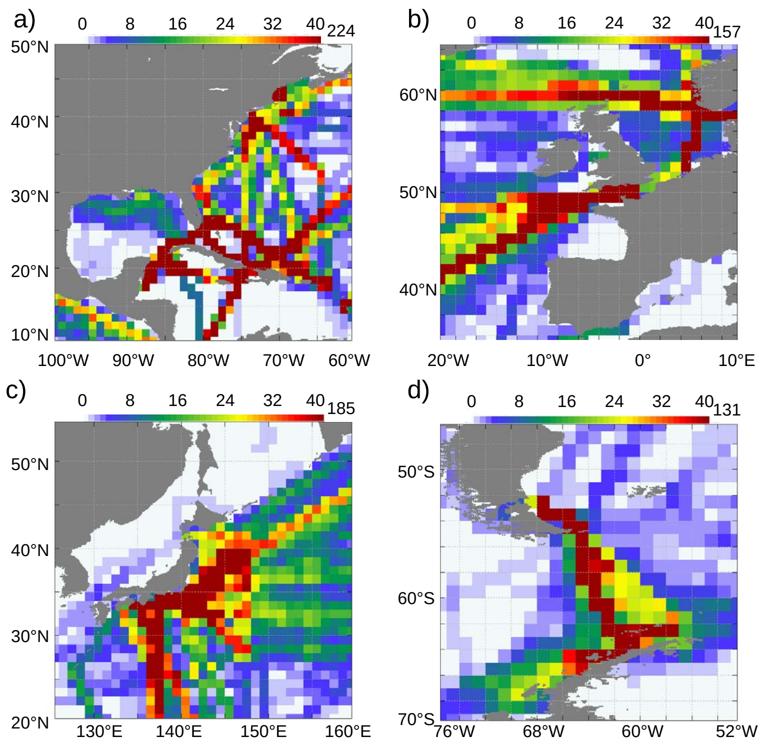

Fig. 9. Number of cruises (see colour bar on top of subplots) with surface water fCO_2 measurements per 1° latitude by 1° longitude grid cell for 2000 to 2009 for **(a)** the Northwest Atlantic Ocean and the Caribbean Sea, **(b)** the Northeast Atlantic Ocean and European shelf seas, **(c)** the Northwest Pacific Ocean and **(d)** Drake Passage in the Southern Ocean. Repeat observations made on voluntary observing ships and research supply ships are clearly visible, both for coastal seas and the open ocean.

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