

pCO₂ from Niskin bottle samples from NOAA Ship Ronald H. Brown cruise RB-08-02 in the Southwest Atlantic sector of the Southern Ocean near South Georgia Island in 2008 (SO_GasEx project)

Website: <https://www.bco-dmo.org/dataset/3148>

Version: 09 Sept 2009

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Project

» [Southern Ocean Gas Exchange Experiment](#) (SO_GasEx)

Programs

» [Ocean Carbon and Biogeochemistry](#) (OCB)

» [United States Surface Ocean Lower Atmosphere Study](#) (U.S. SOLAS)

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Dataset Description

SO-GasEx Discrete analysis of pCO₂ on CTD casts

Methods & Sampling

Sampling times and locations:

Samples were drawn on all CTD casts. At least 80% of unique depths were sampled at each station. At least one pair of duplicates from the same Niskin bottle was drawn at each station. See CTD cast log sheets for further details.

Overall sampling strategy:

While the MapCO₂ buoy was deployed, samples were always drawn from depths corresponding to the depths of the SAMI sensors on the buoy.

Operation Log:

No events of note - the system performed well.

Data Processing Description

Readme: Data reduction discrete pCO₂ for the Southern Ocean Gas Exchange study

Date of submission: April 26, 2009

Ship: Ronald H. Brown

Dates: March 7, 2008 to April 5, 2008

Study: A Lagrangian study focused on air-sea gas exchange

Study Area: 50 S, 38W about 200 miles North of South Georgia island.

Analyst: Robert Castle

Data Reduction: Rik Wanninkhof & Robert Castle

Analyses details:

Analyses were done by equilibrating water samples in 500-ml glass volumetric flasks at a fixed temperature of 20 °C. Headspace gas of known concentration was bubbled through the water and circulated through a LiCor 6252 infrared analyzer (IR). Details of the analysis and instrumental setup can be found in Wanninkhof and Thoning (1993). The analysis was done shipboard in the main laboratory that had poor temperature control which is believed to contribute to the variability in results.

A typical sampling sequence involves running six compressed gas standards, 8 samples, and ending with six more standards. The standards were run in following sequence:

Standard 1378.71 ppm

Standard 2792.51 ppm

Standard 31036.95 ppm

Standard 41533.7 ppm

Standard 5593.64 ppm

Standard 6205.7 ppm

Several times during the cruise the zero and span on the LiCor IR analyzer were set using nitrogen and the 1533.7-ppm CO₂ standard, respectively, such that the instrument output was close to standard values.

However, the sample concentrations were determined from the standard values run directly before and after the sample sequence.

Data reduction details:

A new data reduction program was created as an Excel macro to replace the GW-Basic program used from 1991- 2007. The program was set up to take the output from the IR (ppm CO₂, dry and with band broadening correction applied). To calculate the fCO₂ the following steps were applied by the macro:

- The XCO₂ in the headspace was calculated from a linear interpolation with time of the two bracketing standards. This assumes that instrument drift is linear between standard runs.
- From the XCO₂ in headspace after equilibration and the XCO₂ in headspace before equilibration along with water and headspace volumes the small change in DIC of water is calculated
- The fCO₂ is calculated in the headspace from the XCO₂ accounting for pressure and non-ideality of CO₂
- From the DIC and fCO₂ after equilibration the TALK of the water is calculated
- Since the TALK does not change during equilibration, the TALK and DIC before equilibration (obtained from the group analyzing DIC) are used to calculate fCO₂ in water before equilibration.
- A small correction is applied to normalize data to 20°C if the bath temperature differed from 20 °C. The maximum deviation from 20 °C during the study was less than 0.02 °C which corresponds to a correction in fCO₂ of less than 0.1 %.

The constants of Mehrbach as refit by Dickson and Millero (1987), along with other constants referenced therein are used in the calculations using the code based on Lewis and Wallace (1998) as ported to Excel by Pierrot. Silicate and phosphate values as provided by the nutrient group were used to determine the alkalinity. The final fCO₂ values are not sensitive to the range of reported errors in DIC, SiO₂ or PO₄ that are used as input to calculate the fCO₂ values.

Data reduction issues:

The IR setup was incorrect for this cruise in that the values reported by the IR and logged by the computer were not corrected for water vapor but they did have the pressure broadening correction applied. A second issue was that the standard appeared noisier than in the past. This is attributed, in part, to fluctuating laboratory temperatures. The standards were dry but after running samples, the first two standards had appreciable water vapor in them from flowing through tubing that is used for circulating the moist headspace. Therefore a linear regression was created for all standard sequences using standards 3-6 that were dry and from this linear relationship the corresponding (dry) standards were calculated. The linear regressions though the 4 standards always had a correlation coefficient (r^2) of 0.99998 or better.

Since the water vapor channel was not spanned, we used the calculated water vapor value at 20°C (the temperature at which the samples were run) to correct the sample concentrations in the following manner:

$XCO_2(\text{dry}) = XCO_2 \text{ measured} (1 + pH_2O)$ where

pH_2O is the water vapor at 20°C of 0.0226 atm

Using the recalculated standards and the recalculated sample values the data reduction procedure listed above was executed.

Precision:

Precision of analyses was evaluated from the duplicates that were run every cast. Of the 46 duplicates the average precision was 0.3 % with a standard deviation of 0.2 % where the average precision is $(ABS((\text{sample1} - \text{sample2})^2 / ((\text{sample1} + \text{sample2})) * 100))$. The duplicate values plotted against station are shown in Figure 1.

(BCO-DMO Note: Figure 1 Not Included)

Quality checks:

After data reduction fCO_2 values at all stations were plotted versus depth and versus DIC to flag outliers that were assigned a quality control flag of 3 (questionable). The quality control flags of 3 (questionable) and 4 (bad) applied during analysis were retained. Values flagged as bad are not reported. In a few cases there were obvious input errors of sample number that were corrected. A multi-linear regression (MLR) was performed between $fCO_2(20)$ and DIC, T, and S. The resulting r^2 was 0.98 and the RMS error in calculated $fCO_2(20)$ was 30. The large rms error precluded the use of this MLR for QC purposes.

Values reported:

A total of 629 values were reported from 51 stations. 554 were (single) good values; 47 were averages of duplicate (good) values; 11 were deemed questionable, and 17 values were bad and assigned a default value of -999

The data is reported with following columns:

JD= year day of analysis (UTC time)

Station=

Sample ID = Station # * 10000+ cast # * 100 + sample #

Depth (m)

$fCO_2(20)$ = fugacity of CO_2 at 20 °C (\approx analysis temperature)

fCO_2 (situ) = fugacity of CO_2 at in situ temperature. This is a calculated value and dependent on dissociation constants or empirical equation used

QC= quality control flag; 2= good; 3= questionable; 4= bad (and not reported); 6 = duplicate

Talk(fCO_2 ,DIC) = Calculated alkalinity based on fCO_2 and DIC using the dissociation constants presented in Dickson and Millero (1987)

References:

Dickson, A. G., and F. J. Millero (1987), A comparison of the equilibrium constants for the dissociation of carbonic acid in seawater media, *Deep-Sea Res.*, 34, 1733-1743.

Lewis, E., and D. W. R. Wallace (1998), Program developed for CO_2 system calculations, Oak Ridge National Laboratory, Oak Ridge. <http://cdiac.ornl.gov/oceans/co2rppt.html>

Wanninkhof, R., and K. Thoning (1993), Measurement of fugacity of CO_2 in surface water using continuous and discrete sampling methods, *Mar. Chem.*, 44, 189-205.

BCO-DMO Processing Notes

- Generated from original file SOGasEx_fCO2disc_submitted.xls

BCO-DMO Edits

- event, station, date, time, lon, lat inserted from CTD headers file
- '-999' (No data flag in original) changed to 'nd'
- decimal places padded to 1 or 2 places as appropriate for consistency
- parameter names modified to conform to BCO-DMO convention

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Data Files

File
Disc_pCO2.csv (Comma Separated Values (.csv), 54.72 KB) MD5:375bb16e864ae680be9b40fe33e93778
Primary data file for dataset ID 3148

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Parameters

Parameter	Description	Units
event	Unique event number	YDAHMM
date	Date (UTC)	YYYYMMDD
time	Time (UTC)	HHMMSS
lon	longitude (West is negative)	decimal degrees
lat	latitude (South is negative)	decimal degrees
SampNum	Station # * 10000 + cast # * 100 + sample #	integer
station	Station Number	integer
JD	year day of analysis (UTC time)	YrDay.time
depth	Sample depth in meters	meters
Fugacity_at_20C	fugacity of CO2 at 20 °C (\approx analysis temperature)	uatm (??)
Fugacity_InSitu	fugacity of CO2 at in situ temperature. This is a calculated value and dependent on dissociation constants or empirical equation used	uatm (??)
QC	quality control flag; 2= good; 3= questionable; 4= bad (and not reported); 6 = duplicate	integer
TA_calc_fr_fCO2_20	Calculated alkalinity based on fCO2 and DIC using the dissociation constants presented in Dickson and Millero (1987)	uatm (??)

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Deployments

RB-08-02

Website	https://www.bco-dmo.org/deployment/57846
Platform	NOAA Ship Ronald H. Brown
Report	http://bcodata.whoi.edu/SO-GasEx/SO_GasEx_Cruise_Report.pdf
Start Date	2008-02-29
End Date	2008-04-12
Description	The Southern Ocean GasEx experiment was conducted aboard the NOAA ship Ronald H. Brown with 31 scientists representing 22 institutions, companies and government labs. The cruise departed Punta Arenas, Chile on 29 February, 2008 and transited approximately 5 days to the nominal study region at 50°S, 40°W in the Atlantic sector of the Southern Ocean. The scientific work concentrated on quantifying gas transfer velocities using deliberately injected tracers, measuring CO ₂ and DMS fluxes directly in the marine air boundary layer, and elucidating the physical, chemical, and biological processes controlling air-sea fluxes with measurements in the upper-ocean and marine air. The oceanic studies used a Lagrangian approach to study the evolution of chemical and biological properties over the course of the experiment using shipboard and autonomous drifting instruments. The first tracer patch was created and studied for approximately 6 days before the ship was diverted from the study site, 350 miles to the south, to wait near South Georgia Island for calmer seas. After more than 4 days away, we returned to the study area and managed to find some remnants of the tracer patch. After collecting one final set of water column samples and recovering the two drifting buoys deployed with the patch, we relocated to the northwest, closer to the area where the first patch was started. A second tracer patch was created and studied for approximately 15 days before we had to break off the experiment and transit to Montevideo, Uruguay for the completion of the cruise.

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Project Information

Southern Ocean Gas Exchange Experiment (SO_GasEx)

Website: <http://so-gasex.org/>

Coverage: Southwest Atlantic sector of the Southern Ocean (nominally at 50°S, 40°W, near South Georgia Island)

The Southern Ocean Gas Exchange Experiment (SO-GasEx; also known as GasEx III) took place in the Southwest Atlantic sector of the Southern Ocean (nominally at 50°S, 40°W, near South Georgia Island) in austral fall of 2008 (February 29-April 12, 2008) on the [NOAA ship Ronald H. Brown](#). SO-GasEX is funded by NOAA, NSF and NASA.

The research objectives for Southern Ocean GasEx are to answer the following questions:

- What are the gas transfer velocities at high winds?
- What is the effect of fetch on the gas transfer?
- How do other non-direct wind effects influence gas transfer?
- How do changing pCO₂ and DMS levels affect the air-sea CO₂ and DMS flux, respectively in the same locale?
- Are there better predictors of gas exchange in the Southern Ocean other than wind?
- What is the near surface horizontal and vertical variability in turbulence, pCO₂, and other relevant biochemical and physical parameters?
- How do biological processes influence pCO₂ and gas exchange?
- Do the different disparate estimates of fluxes agree, and if not why?
- With the results from Southern Ocean GasEx, can we reconcile the current discrepancy between model based CO₂ flux estimates and observation based estimates?

Related files

[SO-GasEx cruise report](#)
[SO-GasEx Science Plan](#)
[SO-GasEx Implementation Plan](#)

The SO-GasEx cruise report and Science and Implementation plans, may also be available at [the SO-GasEx science Web page](#).

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Program Information

Ocean Carbon and Biogeochemistry (OCB)

Website: <http://us-ocb.org/>

Coverage: Global

The Ocean Carbon and Biogeochemistry (OCB) program focuses on the ocean's role as a component of the global Earth system, bringing together research in geochemistry, ocean physics, and ecology that inform on and advance our understanding of ocean biogeochemistry. The overall program goals are to promote, plan, and coordinate collaborative, multidisciplinary research opportunities within the U.S. research community and with international partners. Important OCB-related activities currently include: the Ocean Carbon and Climate Change (OCCC) and the North American Carbon Program (NACP); U.S. contributions to IMBER, SOLAS, CARBOOCEAN; and numerous U.S. single-investigator and medium-size research projects funded by U.S. federal agencies including NASA, NOAA, and NSF.

The scientific mission of OCB is to study the evolving role of the ocean in the global carbon cycle, in the face of environmental variability and change through studies of marine biogeochemical cycles and associated ecosystems.

The overarching OCB science themes include improved understanding and prediction of: 1) oceanic uptake and release of atmospheric CO₂ and other greenhouse gases and 2) environmental sensitivities of biogeochemical cycles, marine ecosystems, and interactions between the two.

The OCB Research Priorities (updated January 2012) include: ocean acidification; terrestrial/coastal carbon fluxes and exchanges; climate sensitivities of and change in ecosystem structure and associated impacts on biogeochemical cycles; mesopelagic ecological and biogeochemical interactions; benthic-pelagic feedbacks on biogeochemical cycles; ocean carbon uptake and storage; and expanding low-oxygen conditions in the coastal and open oceans.

United States Surface Ocean Lower Atmosphere Study (U.S. SOLAS)

Website: <http://www.us-solas.org/>

Coverage: Global

The Surface Ocean Lower Atmosphere Study (SOLAS) program is designed to enable researchers from different disciplines to interact and investigate the multitude of processes and interactions between the coupled ocean and atmosphere.

Oceanographers and atmospheric scientists are working together to improve understanding of the fate, transport, and feedbacks of climate relevant compounds, and also weather and hazards that are affected by processes at the surface ocean.

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Physical, chemical, and biological research near the ocean-atmosphere interface must be performed in synergy to extend our current knowledge to adequately understand and forecast changes on short and long time frames and over local and global spatial scales.

The findings obtained from SOLAS are used to improve knowledge at process scale that will lead to better quantification of fluxes of climate relevant compounds such as CO₂, sulfur and nitrogen compounds, hydrocarbons and halocarbons, as well as dust, energy and momentum. This activity facilitates a fundamental understanding to assist the societal needs for climate change, environmental health, weather prediction, and national security.

The US SOLAS program is a component of the International SOLAS program where collaborations are forged with investigators around the world to examine SOLAS issues ubiquitous to the world's oceans and atmosphere.

[Â» International SOLAS Web site](#)

Science Implementation Strategy Reports

[US-SOLAS](#) (4 MB PDF file)

[Other SOLAS reports](#) are available for download from the US SOLAS Web site

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Funding

Funding Source	Award
National Oceanic and Atmospheric Administration (NOAA)	unknown SO_GasEx NOAA
National Aeronautics & Space Administration (NASA)	unknown SO_GasEx NASA
National Science Foundation (NSF)	unknown SO_GasEx NSF

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