

Intergovernmental Oceanographic Commission

Workshop Report No. 221



Surface Ocean CO₂ Atlas Project Pacific Regional Workshop

Tsukuba, Japan
18-20 March, 2009

IOCCP Report Number 12

UNESCO

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Abstract:

The SOCAT Pacific Regional Group met at the National Institute for Environmental Studies in Tsukuba, Japan from 18-20 March 2009. The workshop was co-chaired by Yukihiro Nojiri and Steve Hankin and attended by twenty scientists from seven different countries. The Pacific regional group met with the developers of the Live-Access Server tools to learn how LAS can be used in the QC effort for SOCAT. The participants installed the tools and software on their computers, downloaded the data files for their regions, set up the shared QC environment, and worked through several exercises to demonstrate the system. The groups began working through the data sets for their region (flagging, determining which 2nd level QC tests may be applied, testing those, etc.)

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BACKGROUND

At the “Surface Ocean CO₂ Variability and Vulnerability” (SOCOVV) workshop in April 2007, co-sponsored by IOCCP, SOLAS, IMBER, and the Global Carbon Project, participants agreed to establish a global surface CO₂ data set that would bring together, in a common format, all publicly available surface fCO₂ data for the surface oceans. This activity has been requested by many international groups for many years, and has now become a priority activity for the marine carbon community. This data set will serve as a foundation upon which the community will continue to build in the future, based on agreed data and metadata formats and standard 1st-level quality-control procedures, building on earlier agreements established at the 2004 Tsukuba workshop on “Ocean Surface pCO₂ Data Integration and Database Development”. This activity also supports the SOLAS and IMBER science plans and joint carbon implementation plan.

This data set is meant to serve a wide range of user communities and it is envisaged that, in the future, 2 distinct SOCAT data products will be made available:

- a 2nd-level quality controlled, global surface ocean fCO₂ (fugacity of CO₂) data set following agreed procedures and regional review, and
- a gridded SOCAT product of monthly surface water fCO₂ means on a 1° x 1° grid with no temporal or spatial interpolation.

An extended 1st-level quality-controlled data set has been developed as part of the EU CARBOOCEAN project, where Benjamin Pfeil and Are Olsen (Bjerknes Centre for Climate Research) have compiled the publicly available surface CO₂ data held at CDIAC (Carbon Dioxide Information Analysis Center) and other public data into a common format, 1st level quality-controlled, database based on the IOCCP-recommended formats for metadata and data reporting. The first SOCAT data compilation (version 1.1), available in May 2008 to SOCAT participants, already includes data from over 10 countries, producing an initial database composed of more than 1250 cruises from 1972 to 2007 with measurements of various carbon parameters.

A small technical meeting was held in Bremen, Germany, on 5 December 2007 (associated with the 3rd CARBOOCEAN Annual Meeting) to agree on 1st-level QC for the data set and to decide on a way forward for the 2nd-level QC issues.

The IOCCP, along with CARBOOCEAN and the SOLAS-IMBER Joint Carbon Group, held a 2nd technical workshop (SOCAT-2 meeting) at UNESCO, Paris, on 16-17 June 2008 to develop internationally agreed 2nd-level quality-control procedures and to discuss the coordination of regional scientific groups to conduct the 2nd-level quality control analyses. Refer to the background document SOCAT-II Report for more information.

http://ioc3.unesco.org/ioccp/Docs/SOCAT2_Final2.pdf

The SOCAT dataset now contains over 2,100 cruises from 1968-2007. Benjamin Pfeil and Steve Hankin have agreed that the best way to access the dataset is to keep each cruise as an individual file and to use the LAS system to serve all the data. The regional groups will use LAS to download data, based on definitions of regional boundaries.

Regional groups were tasked with identifying missing datasets from SOCAT version 1.1. The identified regional groups and chairs are:

- Atlantic and Arctic Ocean – Schuster, Lefèvre
- Indian Ocean – VVSS Sarma
- Pacific Ocean – Feely, Nojiri
- Southern Ocean – Tilbrook, Metzl
- Coastal seas – Borges, Chen.
- Global group – Bakker, Olsen, Sabine, Pfeil, Metzl

SOCAT QC-II Definitions of Regional Boundaries as of June 2009

1. **Tropical Pacific** -- Between 30°S, 30°N, North America and Asia. The boundary between the Indian and the Pacific is Malaysia, Sumatra, Java, and Timor and a line at 130°E to Australia through the Timor Sea.
2. **North Pacific** -- North of 30°N and between North America and Asia, including cruises that go north of Alaska into the Arctic Ocean.
3. **Southern Ocean** -- Everything south of 30°S
4. **Indian Ocean** -- North of 30°S, bounded on the east by the line described above, and on the west by Africa and the Suez Canal.
5. **Atlantic Ocean** -- North of 30°S including the Mediterranean, Black Sea, Barents Sea, and Labrador Sea.
6. **Coastal (a.k.a. "continental margins")** -- All ocean surface within 400 km of land* excluding the Southern Ocean Region.

* The intent of the various working groups was to exclude the margins around small, isolated islands, so the Distance-To-Land variable is calculated from a 20-minute resolution land mask that was altered (through guidance from Burke Hales) to eliminate such islands. The altered land mask retains New Zealand, Iceland, and Madagascar as 'land' and Caribbean islands that show up at the 20 minute resolution, as well as other islands like Tasmania, Sri Lanka, Japan, etc. The following islands were explicitly masked out: Reunion/Mauritius, New Caledonia, Vanuatu, Solomon Islands, Manus Island (N of New Guinea), Galapagos, Smith Island (Indian Ocean; Bay of Bengal), Hawaii, Azores, South Georgia, Macquarie (south of NZ), French Southern and Antarctic Lands.

The various regional groups have started meeting to evaluate the initial data quality, learn to use the LAS tools for conducting 2nd level quality control, and determine a course of action for performing the 2nd level QC checks. The Coastal group meeting was held in Kiel in January 2009 with financial support assembled by the SOLAS International Project Office from various sources including the European COST Action 735. The Pacific regional group met in March 2009 at the Tsukuba, Japan funded by the National Institute for Environmental Studies Institute and SCOR. The Atlantic, Indian, and Southern Ocean regional groups will meet in June at the University of East Anglia supported by COST (SOLAS) and SCOR (IOCCP and IMBER).

INTRODUCTION TO THE WORKSHOP

SOCAT Pacific Regional Workshop
March 18-20, 2009
National Institute for Environmental Studies
Tsukuba, Japan

The SOCAT Pacific Regional Group met at the National Institute for Environmental Studies in Tsukuba, Japan from 18-20 March 2009. The workshop was co-chaired by Yukihiro Nojiri and Steve Hankin and attended by twenty scientists from seven different countries (Appendix 1).

At the SOCAT-II technical meeting in Paris (June 2008), participants agreed that the next steps in the development of the SOCAT data set were to have the regional groups meet to identify missing data sets, review the quality of the data, determine which 2nd level quality-control checks may be performed, and begin testing them.

The Pacific regional group met with the developers of the Live-Access Server tools to learn how LAS can be used in the QC effort for SOCAT. The participants installed the tools and software on their computers, downloaded the data files for their regions, set up the shared QC environment, and worked through several exercises to demonstrate the system. The groups began working through the data sets for their region (flagging, determining which 2nd level QC tests may be applied, testing those, etc.)

Tuesday 17 March

An executive session was held on Tuesday 17 March, prior to the first day of the workshop, to finalize the agenda (Appendix 2).

Wednesday 18 March

The first day included a review of SOCAT II, status and overview of the SOCAT data set, and an overview of LAS. This was followed by presentations of Pacific data in SOCAT groups. Summaries of their presentations are found below.

REVIEW OF SOCAT II- BENJAMIN PFEIL, University of Bergen, Norway

“Input Database for SOCAT”

SOCAT is based on a surface fCO₂ database developed at the Bjerknes Centre for Climate Research (Bergen, Norway). The historical development of SOCAT, including goals and the outcome of previous SOCAT related meetings, was presented. The current database holds data from data centers (CDIAC, WDC-MARE), project and institute webpages. SOCAT version 1.2 holds data between the years 1968-2007 with approx. 7 million surface CO₂ measurements divided over 2150 cruises. All input data has been re-calculated to the same standards, metadata was standardized and essential missing variables were added from global data collections (WOA 2005, NCEP-NCAR). The scripts used for recalculations are documented and available to the community. At the end were the changes made since the SOCAT 2nd technical meeting presented.

OVERVIEW OF LAS – STEVE HANKIN, Pacific Marine Environmental Laboratory,
National Oceanic and Atmospheric Administration, Seattle, WA, USA

“The SOCAT QC2 effort- Overview of the problem, Description of on-line tools & How to use them”

This talk began with an overview of the nature of the SOCAT QC challenge -- a community of investigators, working independently to evaluate over 2000 carbon cruise files. It emphasized how performing QC by regions increases the likelihood of conflicts between reviewers, since most cruises pass through multiple regions. The talk outlined the use of a version control system, "SubVersion", to address this problem and to guarantee that there is a complete audit trail of all QC evaluations. The steps necessary between the release of new versions of the SOCAT collection were discussed. The QC flags from the June SOCAT-II meeting were reviewed and it was pointed out that another class of flag(s) is needed to indicate that a cruise should be removed outright or suspended until level-1 QC problems of the data were addressed.

A tutorial overview of LAS was provided covering how to constrain data requests; map the data; make property-property plots; access metadata documents; download full cruises or constrained subsets; examine QC flags and conflicts between scientists over QC evaluations. A couple of example scenarios were shown on how to track down specific quality problems in the data. A quick vision was presented of future capabilities that could be offered for a gridded outlook on the data.

QUALITY CONTROL COLLABORATION – JEREMY MALCZYK, Pacific Marine
Environmental Laboratory, National Oceanic and Atmospheric Administration,
Seattle, WA, USA

“Quality control using Subversion (SVN) and Live Access Server (LAS)”

This talk presented how version control software like Subversion can be used for scientific data management and collaboration, and how Live Access Server can be used in parallel as a data visualization tool.

OVERVIEW OF PACIFIC DATA IN SOCAT- Presentation by groups

- a) Alex Kozyr, Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, USA (CDIAC)

“Review of CDIAC”

CDIAC provides data management support for the underway (surface) measurements of CO₂-related parameters since 1993. All data from the research vessels are stored cruise-by-cruise at CDIAC and accessible through internet via Mercury meta-data search engine (<http://mercdev3.ornl.gov/ocean/>) and as a Global Surface pCO₂ (LDEO) Database through WAVES (<http://cdiac3.ornl.gov/waves/>) system. CDIAC plans to publish the final version of SOCAT database as a Numeric Data Package (NDP) and open the database to public through separate version of WAVES_SOCAT. CDIAC will also host the SOCAT version of LAS that will be open to public.

b) Chihiro Miyazaki, National Institute for Environmental Studies, Tsukuba, Japan

“The Composition of NIES Underway Measurement Data and its QA/QC”

NIES Ocean pCO₂ measurement of VOS has been performed by the three VOS (Skaugran, Alligator Hope and now Pyxis) over the Northern Pacific since March 1995 and by another ship (Trans Future 5) over the Western Pacific since June 2006.

The sequence of NIES oceanic pCO₂ observation system is followed as below; 1) SST measurement using two Pt-100 thermometers is performed at the fore-location of the water pump to avoid heating. 2) Salinity is measured using two thermosalinographs made by Seabird Electronics (SBE). 3) The CO₂ mole fraction of seawater-equilibrated air is measured every 10-second by a Tandem-type gas-liquid equilibrator, with the calibration using 5 standard gases (0ppm, 260ppm, 330ppm, 390ppm and 450ppm) twice a day. 4) The water temperature in the equilibrator (EqT) is also observed by a Pt-100 sensor. 5) To check the performance of NDIR measurement quickly, pH sensor and Chlorophyll fluorescence sensor are installed. 6) Atmospheric CO₂ is also observed by an independent CO₂ system installed in the atmospheric observation room. Hence, we can calculate delta pCO₂.

For the accuracy of water temperature measurement, the SBE thermometers in our system are calibrated by the manufacturer once per a couple of years. Their departures from the manufacturer standard temperature are generally within 0.002 degree C. Using these fairly accurate SBE thermometers, we check and calibrate Pt-100 thermometers for SST and EqT once per 6 months and result in the uncertainty generally within 0.02 degree C.

For the accuracy of pCO₂ system, Murphy et al. (2001) showed that Tandem-type Equilibrator was faster response and more stable compared with Shower-type Equilibrator. During Alligator Hope era, we installed double p CO₂ systems on board and get averaged difference of the two systems generally less than 1 ppm. The present logging interval of the pCO₂ system with tandem-type equilibrator is 10-second.

Our QA/QC process of VOS measurement data are summarized briefly as below; 1) 3 automatically sampled parameters are calibrated using the manually sampled data; Ambient pressure are calibrated based on the reading value from meteorological agency calibrated barometer by the seaman. On salinity, the data of SBE are calibrated against daily sampled bottle salinity. Calibration of Pt-100 thermometers for SST and EqT as above mentioned. 2) The every 10-second values of xCO₂, pCO₂ and fCO₂ are calculated with the warming correction of Weiss et al. (1982). 4) Finally, average and standard deviation of 60 data within 10 minutes are calculated. 5) On salinity, air bubble contamination occurred in the case of bad weather is flagged.

Since VOS have observed pCO₂ data frequently, we can show the seasonal cycle of delta pCO₂ over the North Pacific and the Western Pacific.

c) Yoshiyuki Nakano and Akihiko Murata, Japan Agency for Marine-Earth Science and Technology, Yokosuka, Kanagawa, Japan (JAMSTEC)

“Atmospheric and surface seawater pCO₂ measurements by the R/V Mirai”

Continuous measurements of atmospheric and surface seawater pCO₂ are made with the CO₂ measuring system (Nippon ANS, Ltd) installed in the R/V *Mirai* of JAMSTEC. The system comprises of a non-dispersive infrared gas analyzer (NDIR; BINOS[®] model 4.1, Fisher-Rosemount), an air-circulation module and a showerhead-type equilibrator. To measure

concentrations (mole fraction) of CO₂ in dry air (xCO_{2a}), air sampled from the bow of the ship (approx. 30 m above the sea level) is introduced into the NDIR through a dehydrating route with an electric dehumidifier (kept at ~2 °C), a Perma Pure dryer (GL Sciences Inc.), and a chemical desiccant (Mg(ClO₄)₂). The flow rate of the air is 500 ml min⁻¹. To measure surface seawater concentrations of CO₂ in dry air (xCO_{2s}), the air equilibrated with seawater within the equilibrator is introduced into the NDIR through the same flow route as the dehydrated air used in measuring xCO_{2a}. The flow rate of the equilibrated air is 600 – 800 ml min⁻¹. The seawater is taken by a pump from the intake placed at the approx. 4.5 m below the sea surface. The flow rate of seawater in the equilibrator is 500 – 800 ml min⁻¹.

The CO₂ measuring system is set to repeat the measurement cycle such as 4 kinds of CO₂ standard gases, xCO_{2a} (twice), xCO_{2s} (7 times). This measuring system is run automatically throughout the cruise by a PC control.

In actual shipboard observations, the signals of NDIR usually reveal a trend. The trends are adjusted linearly using the signals of the standard gases analyzed before and after the sample measurements. Effects of water temperature rises between the inlet of surface seawater and the equilibrator on xCO_{2s} are adjusted, although the temperature rises are slight, being ~ 0.3 °C.

On land, we check values of xCO_{2a} and xCO_{2s} by examining signals of the NDIR on recorder charts, and by plotting the xCO_{2a} and xCO_{2s} as a function of sequential day, longitude, sea surface temperature and sea surface salinity.

- d) Tsuneo Ono, Hokkaido National Fisheries Research Institute,
Fisheries Research Agency, Kushiro, Japan (FRA)

“Oceanic pCO₂ survey around Japan”

FRA has occupied oceanic pCO₂ survey in the around-Japan coastal area in the western North Pacific from 1996 to 2001. The semipermeable tube-type equilibrator system connected with NDIR [Saito et al., 1996] was installed in two observation ships, and 3-5 pCO₂ survey cruise was operated a year for each ship. Mainly, these cruises were made on a set of repeat hydrography section in the Oyashio and Kuroshio extension domains, but sometimes cruise track was extended to subtropical gyre domain south of Kuroshio Current. Routine calibration was done by using gas standard made by Taiyo-Nissan Inc. Performance of pCO₂ system we used was also repeatedly assessed by inter-comparison works organized as PICES working Group 13 activities. The results of inter-comparison showed that our data are correctly reported with the accuracy of ~3 ppm. After 2001, we suspended pCO₂ survey mainly due to the manpower problem, but very recently we resumed this activity on the repeat hydrography line in the Oyashio region (A-line).

Part of the data 1996-2001 can be obtained via the WDCGG CO₂ database:
http://gaw.kishou.go.jp/wdcgg/products/cd-rom/cd_14/A/metadata/co2/station/200612120155.html.

- e) Masao Ishii- Geochemical Research Department, Meteorological Research
Institute, Japan Meteorological Agency, Tsukuba, Japan (MRI)

“Quality of shipboard xCO₂ measurements: Underway measurements of pCO₂ in surface water and in marine boundary air”

Geochemical Research Department of MRI has made underway measurements of $p\text{CO}_2$ during 55 cruises since 1968 mainly in the North Pacific and in the equatorial Pacific, and in several cruises in the South Pacific and in the Australian sector of the Southern Ocean. Global Environment and Marine Department of JMA has also started $p\text{CO}_2$ measurements in 1989 and collected data from 128 cruises until April 2008 mainly in the western North Pacific including those on the repeat lines along 137°E and 165°E.

Underway measurements of $p\text{CO}_{2\text{sw}}$ in near-surface water has been made using shipboard pumping systems that continuously pumped seawater from the ship's sea chest and gas equilibration methods with shower-head type equilibrators equipped with a non-dispersive infrared gas analyzer (Inoue, 2000). The system uses four CO_2 -in-air reference gases that have undergone pre- and post-cruise calibration against standards traceable to the primary standards of the World Meteorological Organization.

Comparability of data obtained by this system with those obtained by other systems has been examined during an intercomparison exercise made in the North Atlantic on board the RV Meteor (Körtzinger et al., 1999). Since June 2003, the internal consistency among $p\text{CO}_{2\text{sw}}$, DIC and pH (total) has been examined for the data along 137°E using the dissociation constants of carbonic acid given by Lueker et al. (2002). The pH calculated from $p\text{CO}_{2\text{sw}}$ and DIC are in good agreement with the pH analysed by spectrophotometry {pH(calculated) – pH(analysed) = +0.003 ± 0.005}. All data of $x\text{CO}_2$ in dry, $p\text{CO}_2$ in wet at SST and ancillary data are available from WDCGG (<http://gaw.kishou.go.jp/cgi-bin/wdcgg/catalogue.cgi>).

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f) Gen Hashida, National Institute of Polar Research, Tokyo, Japan (NIPR)

“Underway $p\text{CO}_2$ measurements in the Indian sector of the Southern Ocean”

Underway $p\text{CO}_2$ has been carried out on board Icebreaker *Shirase* every Antarctic summer since 1987 by JARE (Japanese Antarctic Research Expedition). In collaboration between NIPR, Tokyo University of Marine Science and Technology, and NIES, UW $p\text{CO}_2$ has been carried out on board R/V *Umitaka Maru* of Tokyo Uni. Marine Sci. & Tech. in 2002, 2003, 2006, 2008, 2009. Data obtained above could be possibly registered SOCAT and/or CDIAC database after appropriate preparation.

g) Sophie Johannessen, Institute of Ocean Sciences, Fisheries and Oceans, Canada

(IOS)

“Time series of pCO₂ at Station P and along Line P, 1973-present”

The partial pressure of carbon dioxide has been measured at station P and along line P about 3 times a year since 1973, in a programme instigated by Dr. C.S. Wong at the Institute of Ocean Sciences (Fisheries and Oceans Canada). Both the analytical methods and the quality of measurements have varied over time. Data from 90 cruises have been recovered, of which those from about 60 cruises are likely to be usable. There were numerous methodological problems with the measurements from 1997 to 2008, but these have recently been corrected, and the new data will be usable, beginning with the January 2009 cruise. Data will undergo primary quality control this year and should be ready to submit to the CDIAC and SOCAT data collections by October 2009. A data report and a journal publication are in progress.

h) Bronte Tilbrook, CSIRO Marine and Atmospheric Division, Hobart, Tasmania (CSIRO)

“Australian surface fCO₂ measurements”

Surface fCO₂ measurements are now made using General Oceanics (GO) 8050 Neill CO₂ systems. The standard output of the GO systems is logged with ship position, meteorological and thermosalinograph data. The newest installation on the RV Southern Surveyor is supported through Australia's Integrated Marine Observing System (IMOS) program. The system uses four CO₂-in-air standards calibrated at CSIRO on the WMO-X2007 mole fraction scale. Sensors for temperature are calibrated at the beginning and end of the field season at a CSIRO NATA test facility and salinity is calibrated against discrete samples collected from the ships underway seawater line. Pressure sensors are checked by comparison against barometric sensors on the ship and in the laboratory and have been found to be stable. If any problems arise with the pressure sensors, they are calibrated by the Australian Bureau of Meteorology.

For normal operating, a limited data set is emailed from the ship every 6 hours and is used as a rapid check of the system. These data are displayed on a public web site

(<http://www.marine.csiro.au/mapserver/cgi-bin/underway/underway>). Every 24 hours the complete data set is sent from the ship and all variables logged by the system are checked visually. At the end of the cruise, the daily data files are combined and any calibrations updated for the various sensors. Data exceeding normal operating ranges and outliers are identified and the causes investigated. The data are flagged as good, suspicious or bad. Data collected in 2008 and current cruises are available through the IMOS data centre from June 29, 2009 (http://imos.org.au/emii_data.html).

i) Don Jing Kang, Seoul National University, Korea (SNU)

“Oceanic pCO₂ Measurement in Korea”

Oceanic pCO₂ measurement in Korea has been carried out since 1995. The first part was supported by CREAMS (Circulation Research of East Asian Marginal Sea) until 1999. Since 2006, EAST-1 (East Asian Seas Time-series I) has supported the underway pCO₂ measurement. This study is focused on the East(Japan) Sea.

Underway pCO₂ measurement in the Pacific was carried out in 2003 and 2004. In 2003, CO₂ of surface seawater and atmosphere were measured cross the

Pacific from Busan, Korea to Chile, and from Busan to Hawaii and Kamchka Peninsula in 2004, respectively.

Modified Weiss-type equilibrator is used for oceanic $p\text{CO}_2$ measurement whose volume is 24 liters (15 liters of seawater and 9 liters of air). Usually the seawater flow rate is around 20 liters per minute. The headspace gas is vented but fresh air supplies through 2nd stage equilibrator.

We use infra-red CO_2 analyzer (Li-6252) with totally dry gas by Nafion dryer. SST, SSS, and location are also measured at the same time. Usually atmospheric CO_2 is measured for 15 minute and surface seawater for 45 minute ever hour. Calibration is carried our every 12 or 24 hours with three different standard gases, and one working standard gas is run every 4 or 6 hours. The first 3 minute data are discarded and one minute average data are used.

We have a plan to submit the data we get in the Pacific to CDIAC as soon as possible. In 2010, a new ice breaker named Araon will begin to operate by KOPRI (Korea Polar Research Institute). Underway $p\text{CO}_2$ measurement system will be built in the ship. Their plan is Araon cross the Pacific once a year with underway measurement (Arctic-Korea-Equator-Antarctic). This will provide a very good surface oceanic $p\text{CO}_2$ data.

- j) Cathy Cosca, Pacific Marine Environmental Laboratory, National Oceanic and Atmospheric Administration, Seattle, WA, USA (PMEL)

“Underway $p\text{CO}_2$ QC Procedures”

The CO_2 group at NOAA/PMEL has been making underway $p\text{CO}_2$ measurements since 1982. We have data from 116 cruises files in the current SOCAT database, the majority of which was collected in the equatorial Pacific (104 cruises). As part of an ongoing collaboration of U.S. scientists involved in the shipboard measurements of underway $p\text{CO}_2$, a working group was formed in 2002 to design and implement $p\text{CO}_2$ instrumentation on VOS ships. The resulting criteria for such instrumentation includes: a compact design, $p\text{CO}_2$ measurements with 2 uatm, temperature measurements within 0.01 degree C, pressure measurement with 0.5 mB. The agreed upon design would also allow for the system to run fully automated, and would allow data transmission via satellite. A similar group met again in 2004 to agree upon data reduction and quality control procedures. At PMEL, data is transmitted daily via iridium or e-mail and is automatically plotted for quick verification that the system is running properly. After a cruise is completed, the data file is processed and QC'd following the protocols described in Pierrot, et al. Final data is submitted to CDIAC using the format suggested by CDIAC for CO_2 data submission and corresponding metafiles.

OVERVIEW OF NEURAL NETWORKS – MACIEJ TELSZEWSKI, University of East Anglia, Norwich, England

“Estimating the monthly $p\text{CO}_2$ distribution in the North Atlantic using a self-organizing neural network”

M. Telszewski, A.Chazottes, U.Schuster, A.J.Watson, C.Moulin,
D.C.E. Bakker, M.González-Dávila, T.Johannessen, A.Körtzinger,
H.Luger, A.Olsen, A.Omar, X.A.Padin, A.Ríos, T.Steinhof,
M.Santana-Casiano, D.W.R. Wallace, and R.Wanninkhof

Here we present monthly, basin-wide maps of the partial pressure of carbon dioxide

(pCO₂) for the North Atlantic on a 1° latitude by 1° longitude grid for years 2004 through 2006 inclusive, constructed using a neural network technique which reconstructs the non-linear relationships between 3 biogeochemical parameters and marine p CO₂. A self-organizing map (SOM) neural network has been trained using the SeaWiFS-MODIS chlorophyll *a* concentration, the NCEP/NCAR reanalysis sea surface temperature, and the FOAM mixed layer depth. 389,000 such triplets were used. The trained SOM was labelled with 137,000 underway pCO₂ measurements collected in situ during 2004, 2005 and 2006 in the North Atlantic, which span the range of 208 and 437 μatm. The root mean square (RMS) deviation of the neural network fits from the data is 11.55 μatm, which equals to just above 3 per cent of an average pCO₂ value in the in situ dataset. The seasonal pCO₂ cycle as well as the interannual variability estimates in the major biogeochemical provinces is presented and spatial and temporal variability of the estimated fields is discussed. High resolution combined with basin-wide cover makes the maps a useful tool for several applications such as monitoring of basin-wide air-sea CO₂ fluxes or improvement of seasonal and interannual marine CO₂ cycles in future model predictions. The method itself is a valuable alternative to traditional statistical modeling techniques used in geosciences.

INTERNATIONAL OCEAN PCO₂ INSTRUMENT INTER-COMPARISON USING INDOOR SEAWATER POOL-YUKIHIRO NOJIRI, National Institute for Environmental Studies, Tsukuba., Japan

An international ocean pCO₂ instrument inter-comparison including underway and autonomous buoy systems was held at National Research Institute of Fishery Engineering in Kamisu City, Ibaraki, Japan using the indoor seawater pool. The campaign was supported by pCO₂ buoy project by JAMSTEC/MEXT and pCO₂ data analysis project by NIES/MOE. Seven underway systems and seven buoy systems were gathered for the campaign.

List of underway systems

NIES Tandem equ. + LICOR 7000 (A1 and A2) by Kimoto Electric Co.
Down sized Tandem equ. + LICOR6262 (B) by Kimoto Electric Co.
NOAA Serial shower equ. + LICOR 7000 (C1) by General Oceanic Co.
NIO Serial shower equ. + LICOR 7000 (C2) by General Oceanic Co.
NIWA Shower equ. + LICOR 6251 (D), laboratory made
PML Beads equ. + LICOR 840 (E) by Dartcom Co.

List of buoy systems

NIES Goatex tube equ. + LICOR 840 (W1 and W2) by Kimoto Electric Co.
NOAA Bubbling equ. + LICOR 840, NOAA/PML MAPCO₂ System with MBARI
Montana Univ. SAMI colorimetry with tube equ. (Z1 and Z2) by Sunburst Sensors Co.
JAMSTEC Colorimetric detection with tube equ. (Y1 and Y2), laboratory made (equ.=equilibratoor)

The pool has a nominal volume of 170 m³ and is enable to be kept at a stable pCO₂ over night because of the small temperature change. The pool water was well circulated by submergible pumps. Main water line of 300 L/min flow rate was installed at the pool side and water is supplied for underway systems. Because the line water temperature was warmed by heat from the water line pump, underway pCO₂ result was critically corrected by the measured difference of line and pool waters. It was in between 0.04 to 0.06 degree C during the inter-comparison period.

Five overnight comparisons were run on Feb. 27, 28, Mar. 1, 2 and 3. First, second and third night runs were fixed pCO₂ comparison at 281, 437, and 357 ppm, respectively. In the fourth and fifth night runs, pCO₂ was abruptly changed at mid night by HCl or NaOH. NIES standard underway system (A1) and NOAA system (C1) were kept untouched during the inter-comparison and served for reference systems. The overall difference of the two systems was 0.22±0.19 ppm as dry equilibrated air xCO₂ scale. The difference was 0.40

ppm in the earlier 3 days but decreased to 0.09 ppm in the later 2 days, which would be an ultimate agreement for seawater pCO₂ systems. Other underway systems, two NIES, NIO and NIWA systems, showed reasonable agreement within the range from -0.67 to +0.37 ppm compared with NIES reference system, however, instrument problem in PML system made its critical comparison difficult.

NIES buoys showed great agreement with the reference underway systems of 0.33 and 0.24 ppm as the average difference during the comparison period. NOAA NDIR buoy also showed reasonable average agreement of 0.71 ppm. It was shown well designed NDIR buoy systems already obtained practical accuracy in the pCO₂ measurement. However, the technical barrier in colorimetric buoy systems might be higher than NDIR buoy systems. Montana University systems properly worked during the comparison period but the difference from the reference significantly fluctuated. Small drifting CO₂ buoy by JAMSTEC meet instrumental problem and gave only three night data for one system but the difference from the reference system was fluctuated.

The result of inter-comparison was very successful and we confirmed well designed NDIR pCO₂ systems will give very tight agreement for wide pCO₂ range even for underway and buoy application. Under way system agreement of three NIES, two NOAA/NIO and NIWA systems can be stated the range is generally within plus minus 0.5ppm in xCO₂ scale, and NIES and NOAA/MBARI buoys are generally within plus minus 1ppm compared with standard underway value. Colorimetric buoy has been improved and very stable operation for the whole comparison period was achieved for SAMI, however, situation of buoy pCO₂ system may be similar to the first international inter-comparison of pCO₂ system organized at Scripps Institute for Oceanography by in 1994, when some system worked stable but some not.

Thursday and Friday 19-20 March

The final two days of the meeting were spent on practical exercises with cruise data and 2nd level quality control, including downloading the data files, provisional flagging, and identification of possible crossovers. Specifically, breakout groups were given assignments to run 2nd level quality control on different cruises so that not everyone was using the same files at the same time. They found duplicate cruises and flagged data in the data set.

Following these exercises, the discussion revolved around flagging issues. The group felt the user should know which data have larger uncertainties and that this should be noted in the metadata. Steve Hankin proposed that a new flag "X", be applied in situations where there are problems with the dataset that can be resolved as opposed to an "F", which would indicate the entire data set is bad. The group concluded that the PI needs to be alerted to problems with their data set, whenever possible, and asked to correct it. However, this may delay the release or inclusion of their data. Benjamin agreed to notify the relevant PIs.

MEETING SUMMARY

At the end of the meeting, suggestions were solicited from the group on ways to improve the LAS system and the underlying database. Among the most important agreements was the consensus realization that level 1 QC issues remained to be corrected in the database. Benjamin agreed to issue a new version of the collection (v1.3) that would address the level 1 QC problems identified at the Tsukuba meeting. Steve and Jeremy agreed to add capabilities in the LAS system to facilitate a community process on rooting out level 1 QC problems, as well. Many of the suggestions were of a technical nature regarding enhancements to LAS. Steve and Benjamin agree to prioritize this list and complete as much of it as possible in time for the next (Norwich) meeting. The list will be reviewed and refined again at the Norwich meeting.

ACTION ITEMS

Major items

1. (*) Increase the speed of the system (remove X,Y,T constraints from SQL queries if full-range; better cache hit rates; 1 10-minute subsampling; ...)
2. Publish URL specification for LAS requests
3. Add an email-to button to help notify PIs who are responsible for cruise questions
 - * Is there a do-able way to generate the URL of a product so it can be sent in an email?
4. (*)add new QC flags. Propose: "RMVE" = remove (permanent); "SPND" = "suspended (temporary)"
5. (*) create a 10-minute subsampling resolution
6. (possibly) plot min/max within subsampled intervals
7. Allow entering a comment on a cruise with flag still set to null (e.g. "I've contacted Benjamin about this one")
8. In the Table of Cruises show at least one line for each relevant region
9. able to click-and-drag zoom on the property-property plots (mouse-over showing coordinates, too)
10. (Ansley) more digits of precision in the quick "Property-property Values" output
11. (?or something??) Data Downloads button should always give full resolution data
12. able to upload descriptive documents that explain why QC evaluations were made, along with the QC flags and short comments
13. Download the cruise data files as zip files
14. Community-edited FAQ: e.g. "How to evaluate QC when situation ZZZZ arises."
15. (*) On SOCAT-LAS home page put announcement that V1.2 will be updated to v1.3 shortly with many duplicates removed
16. (*) A visualization tool to locate where data are "missing"
17. (ignore?) A way to visualize cruises by name on the map (e.g. On the map plot the colored icons and plot legend that we see on the property-property plots.)
18. Offer Two side-by side prop-prop plots -- to help explore the relationship between three vars instead of just two. (dotted lines to help compare alignments of points)
19. Add delta-T ($\Delta T = \text{eqT} - \text{SST}$) variable to the database (note: can this be a prototype for computed expressions, generally? Add "delta-T" into the dataset config XML; then hack the Velocity template so it grabs eqT and SST; and hack the Ferret scripts to compute the quantity. The "Data Download" would remain as-is.)
20. Include Expocodes in Table of Cruises (Think of other ways to encourage a transition to Expocodes)
21. To make queries smaller/faster -- Add option to exclude missing values from queries.
22. Make it easy to download ODV-ready data subsets
23. Provide indications (of some kind) of what QC flags have been added recently.(include a date-of-QC field in the Table of Cruises, so it can be sorted on?)
24. Other variables to add? (?? worth having?? "FCO₂-range" and "SST-range" to show the data range in the subsampled interval)
25. Set up for QC of data records, too:
 1. Add per-data record flag onto database
 2. Add same fields to all of the data files
 3. decide on flags (see June report)
 4. set initial flag value to something like PA (Presumed "A").
 5. add a constraint on the map page

Minor items

1. re-do the Southern Ocean and Coastal regional boundaries.
2. make sure that cache hits are working (especially on prop-prop plots, where the list of cruises is the only change)
 1. For Roland: Can LAS set properties that inform when results are based on cache hits?
3. Raise back to (say) 500K the limit of 120K points per plot that was imposed on the XTRA server
4. Incorporate the "intelligent" method (using Roland's new Java method) for anticipating the sizes of queries.
5. make the "MASTER" flags in the Table of Cruises stand out more. Make the MASTER QC documents stand out in SVN.
6. (Ansley) BUG -- full resolution, large prop-prop plots involving lat, lon, time sometimes crash with "TITLE=???" Ferret script error.
7. crashes can occur if QC update (which clears the cache) occurs simultaneous with product requests. Can Roland provide a method call to clear cache, where he makes sure to execute it between product requests?
8. Is there a way to get the batch responses to go into pop-up windows (or otherwise behave nicer
9. plot options? (contour levels? graticules?)

ANNEXES

ANNEX 1

PARTICIPANTS

Participants:

PACIFIC	DATA / TECHNICAL
Catherine E. Cosca (NOAA PMEL, USA)	Steven C. Hankin (NOAA PMEL, USA)
Gen Hashida (NPRI, Japan)	Alexander Kozyr (CDIAC, USA)
Masao Ishii (MRI, Japan)	Jeremy Malczyk (NOAA PMEL, USA)
Sophia C. Johannessen (IOS, Canada)	Benjamin Pfeil (Univ. Bergen, Norway)
Dong-Jin Kang (SNU, Korea)	Kathy Tedesco (IOCCP, France)
Chihiro Miyazaki (NIES, Japan)	
Akihiko Murata (JAMSTEC, Japan)	
Yoshiyuki Nakano (JAMSTEC, Japan)	
Shin-ichiro Nakaoka (NIES, Japan)	
Yukihiro Nojiri (NIES, Japan)	
Tsuneo Ono (FRA, Japan)	
Jeong Hee Shim (SNU, Korea)	
Toru Suzuki (MIRC, Japan)	
Maciej Telszewski (UEA, UK)	
Bronte Tilbrook (CSIRO, Australia)	

**ANNEX II
AGENDA**

Tuesday, 17 March – Technical Committee meeting and set-up (Nojiri, Hankin, Malczyk, Pfeil, Kozyr, Cosca, Tedesco, Nakaoka and Miyazaki).

DAY 1	Wednesday 18 March
Morning	<p>9:30- Welcome and Presentation of Goals for the meeting – Nojiri</p> <p>Self introduction of the participants</p> <p>Review of SOCAT-II – Pfeil</p> <p>Overview of LAS – Hankin</p>
Afternoon	<p>13:30- Quality Control Collaboration - Malczyk</p> <p>14:00- Overview of Pacific Data in SOCAT</p> <ul style="list-style-type: none"> • Review of primary QC methods carried out by each group before submission to SOCAT <ul style="list-style-type: none"> CDIAC – Kozyr NIES – Miyazaki JAMSTEC – Murata and Nakano FRA – Ono MRI – Ishii NIPR – Hashida IOS – Johannessen CSIRO – Tilbrook SNU – Kang NOAA – Cosca • Discussion and Review of Pacific data in SOCAT (anything missing?) – Pfeil + all. <p>16:40- Installation and set up of LAS on computers</p> <ul style="list-style-type: none"> • installing the necessary tools on laptops <p>18:30- Dinner (Kintaro-Sushi, near Hotel Epochal)</p>
DAY 2	Thursday, March 19
Morning	<p>9:30- Demonstration of SOCAT Data on LAS – Hankin and Malczyk</p> <p>Practical exercises with real cruise data that can be QCed, run through the steps of encountering and resolving QC conflicts, etc.</p> <ul style="list-style-type: none"> • download the data files, and begin flagging

	<ul style="list-style-type: none"> • identify possible cross-overs and other 2nd level consistency check
Afternoon	13:30- Continue with exercises... 16:00- Introduction about the results of February 2009 pCO ₂ inter-comparison in Hasaki, Japan – Nojiri
DAY 3	Friday, March 20
Morning	9:30- Open discussion in plenary – sharing problems, approaches, etc. 11:30- Overview of Neural Networks – Telszewski
Afternoon	13:40- Open discussion and summary – status of what’s been done to each region, plans for a way forward 15:00 Adjourn