Workshop report:

pCO₂ on Ship of Opportunity (SOOP-CO2) Operations meeting

Location: AOML/Miami
Start: Thursday January 21, 2016, 9 AM
End: Friday January 22, 2016, 4 PM

Purpose:
The SOOP-CO2 operations meeting is focused on training in system hardware and software, and data reduction procedures of the Underway pCO2 systems. The venue also served for information exchange between the different groups.

Desired outcomes:
Improved knowledge of system operations and increased collaborations between the groups involved in SOOP-CO2

Attendees Underway pCO2 workshop

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Ryan Woosley	rwoosley@rsmas.miami.edu	U. Miami
Regis Cooke	RegisC@general oceanics.com	GO*
Victor Bersok	VictorB@general oceanics.com	GO
Alejandro Rodriguez		GO
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*Participants from General Oceanics (GO) (Jan 21. Only)

Agenda
Thursday January 21
9:00 to 9:15: Introductions (interactive, informal,) [Wanninkhof]
9:15 to 9:30: Discuss workshop scope "what participants want out of it" adjust agenda if desired [Wanninkhof]
9:30 to 10: Discussion of hardware and documentation (including differences and possible improvements in documentation) [Pierrot/Sullivan]
10-12: System operation [Sullivan/Pierrot]
12- 1:30: Lunch
1:30 -2:00: Ship installation issues including writing IOCCP whitepaper [Pierrot/Sullivan]
2:00- 3:30: System software operation [Pierrot/Sullivan]
3:30-4:00: Break
4:00-5:30: Data reduction software [Pierrot/Sullivan]

Friday January 22
9:00 to 10:30: Data QC procedures (both built –in software and SOCAT platform [Cosca/Pierrot]
11:00 to 12:00: Submission to SOCAT, CDIAC,NCEI ,Takahashi climatology [Wanninkhof]
12:00 to 1:30: Lunch
1:30 to 1:45: CO2 in air measurements [Dave Munro]
1:45 to 3:00: Other sensors [Cosca/Wanninkhof]
3:00- 4:00: Discussion of improved coordination, needs, future directions, outreach, ship recruitment [Wanninkhof]

Action items:
1. Conformity of analyses
-Decide if we use time of water intake or equilibration
-Formalize standards ranges that will be used
- All groups use same analysis sequence
-Document routine maintenance and replacement schedules
- Set protocol for air sampling and air QC
- Decide if we should submit data with bad/no fCO_{2w} but good SSS and SST

2. Improve documentation of procedures
-Document procedures for checking SST and SSS Wanninkhof
-Produce video of startup
-Produce video on use of data reduction software
- Finish installation manual

3. Increase communication and recommendations with manufacturer of systems
- Advise GO on Hardware modification (e.g. ability to adapt cable and tubing runs into dry box by installing mounting plates)
- Go over GO FAQ list, and suggest additions and corrections
- Improve understanding of issues and expectations that operators have

4. Work with IOCCP to have a follow-up meeting for the global community
Wanninkhof

Recommendations:
1. Hardware improvements for GO system
- Find better flow meter, (note, vent flow can be a good indicator of leaks)
- Ability to include a remote monitor
2. Specific documentation of GO system
- Improved documentation of GO system changes
- Diagram of terminal strip with labels
3. Specific documentation on operation
- Start-up procedure sheet that can be placed by computer [laminated, inside dry box ?]
- Shut down procedure sheet that can be placed by system [laminated, inside dry box ?]
- Provide ranges for settings and expected output values

4. Provide general user information on trouble shooting and things to watch (sharing of expertise)
- Document weak links system – flow meters, chiller, pumps, EPSCO valve (pump cleaning protocol, PC interface, and how these can be fixed

5. Outreach materials

- Ship recruitment/interactions with crew (U. Shuster is working on such a document
-Reach out to ICOS (Oceans) can assist with how to videos
- Provide a "how to" manual for UW pCO2 reduction and use of data reduction software.

Meeting summary:
Hardware
Most groups in the NOAA SOOP-CO2 effort use GO underway pCO_2 systems. The systems have undergone changes in hardware and operating systems over time that hampers interoperability and assistance in troubleshooting. Several systems have customized add-ons to address unique custom features and interfaces. R. Cook (GO) mentioned that interface issues are the #1 challenge that customers have. Major changes in hardware have been adding Fluke temperature sensors, additional/better pressure sensors, and upgrades to the GO board controlling chiller and pumps. Different groups use different LI-COR CO2 analyzers. The LI-6262 is the unit of choice but is not made anymore. The LI-7000 shows very good performance in shore-based laboratories but experiences increased noise due to motion, and it does not have option to include external pressure sensor. The LI-840 is a low cost unit that works well but needs an independent pressure sensor as the internal sensor does not meet specifications for accurate data.

While units overall function well at sea there are several parts that have been problematic. The following issues were mentioned by participants: The EPSCO water distribution valve is prone to leak due to the large orifices needed for the high flow through system. The flow meter on the secondary equilibrator vent is prone to failure, likely due to moisture. The chiller can fail possibly due to moisture entering the Peltier unit. It was recommended to improve ease of replacement through better access and wiring connectors.

The deck box containing barometric pressure sensor and iridium transmission is not used on many ships, instead the ship provided data transmission and pressure sensors are used. The ship's pressure gauges are often calibrated as part of WMO-VOS operations. The Iridium transmitter has been problematic. A new unit with smaller form factor and better transmitter has been produced at AOML.
It was decided at the meeting that routine maintenance and replacement schedules need to be instituted for:
-Replacing internal and external desiccant (magnesium perchlorate) and CO_2 scrubber Malcosorb® [sodium/calcium hydroxide] in the IR analyzers
-Replacing Nafion® drying tube tubes
-Replacing Acrodisc® filters
-Replacing or cleaning and drying Airline
- Cleaning underway water line. The was some discussion of the merit of this

Product support by GO is found lacking by several investigators. Moreover, replacement parts are deemed expensive or not compatible with the system

operated due to changes in OEM parts such as pumps, flowmeters and valves. Gas flowmeters in particular appear susceptible to moisture and failure prone (e.g. the flowmeter on between secondary and primary equilibrator indicating amount of air drawn into the system). The air pumps to recirculate headspace and draw bow air are custom ordered from KNF and are expensive ($\approx$ \$620). Pump failure often is attributed to salt buildup on diaphragms and can be dealt with by cleaning with fresh water. The GO FAQ manual should include these procedures.

Several of the GO units are at the end of their lifespan (estimated at 5-years of continuous use) and GO is being asked by users regarding refurbishing systems. GO is set up to do so but at a relatively high price.

GO also has a record of all the actual software installations for the pCO$_2$ including the latest versions of the "uw_pco2.exe" and "edit_config.exe" programs. Craig Neil (CCN) acts as a consultant to GO and makes most of the software modifications for the GO system.

Table 1 Major changes to GO Instrument operation software versions[1]

Beta[2] 2 V 6[3]: system can output line of data to port
V8: system can use Druck in dry box to set P of LI_COR for xCO2 mess.
V8: GPS COM port re-initialized after 10 attempts when sleep/wake positions used
V8: daily zipped files (7zip) + zipped on shut-down + run STDs on shut-down
V8.1 (06.2012): Chiller turned off when selecting Cancel from startup screen
V8.4 (08.2012): Generic serial data: LAST full data string taken, not first.
Also, Interval mode and "ms delay"=0, Serial buffer not flushed before read.
V9 (01.2014) pump speeds stays within 0-255
+ Druck code = reduced dropped lines
+ LabVIEWZIP functions (7zip not needed anymore)
+ Picarro CRDS detectors support
V10.2 (09.2015) - Just cosmetic changes

[1] For full list see appendix A
[2] Beta= one-off version to accommodate a specific sensor
[3] V = version

Software:
Three software packages were discussed:
-Data acquisition and control,
-Data reduction
-Data submission (SOCAT).

Data acquisition and control: This LabVIEW VI (virtual instrument) based software runs the GO system and acquires the data. The different versions are listed in Table 1 and detailed in Appendix A. No significant issues have been encountered other than that software appears to be customized for each unit because of different user demands. The software operates as a stand-alone application (executable), but

this precludes the ability to modify the software in the LabVIEW environment in case other data streams or sensors need to be included. The newer software versions have the ability to output all data in real time which was viewed as desirable by survey technicians on ships to monitor the GO system from their work stations. No software has been written to display data through a graphical interface, though.

Data reduction: A comprehensive data reduction and QC software has been developed by D. Pierrot (AOML) that is optimized for reducing data from the GO system.   There is also a utility produced in Excel that can correct for negative water vapor values which occur if the reference channel contains water vapor (e.g. if external or internal desiccant in LI-COR has saturated).   Several group members are starting to use the data reduction software that uses visualization and graphical user interfaces for quality control. While the software can ingest and merge the daily files from the GO system, and additional data streams (e.g. shipboard TSG), many groups still do the initial checks and merging in Excel, and import the resulting .CSV file into the data reduction and QC software. A screen grab of the visual interface of the software is shown in Figure 1. The data reduction software is used by several participants and others users worldwide. Improved documentation will facilitate broader use of this excellent utility.   One useful feature is the ability to overlay plots of SST versus time and Equilibrator Temperature versus time and align them to determine and correct for offsets caused by the transit times from the seawater intake to the equilibrator. Currently adjustments are made to align with time of analysis (rather than time when water passed by the SST probe).
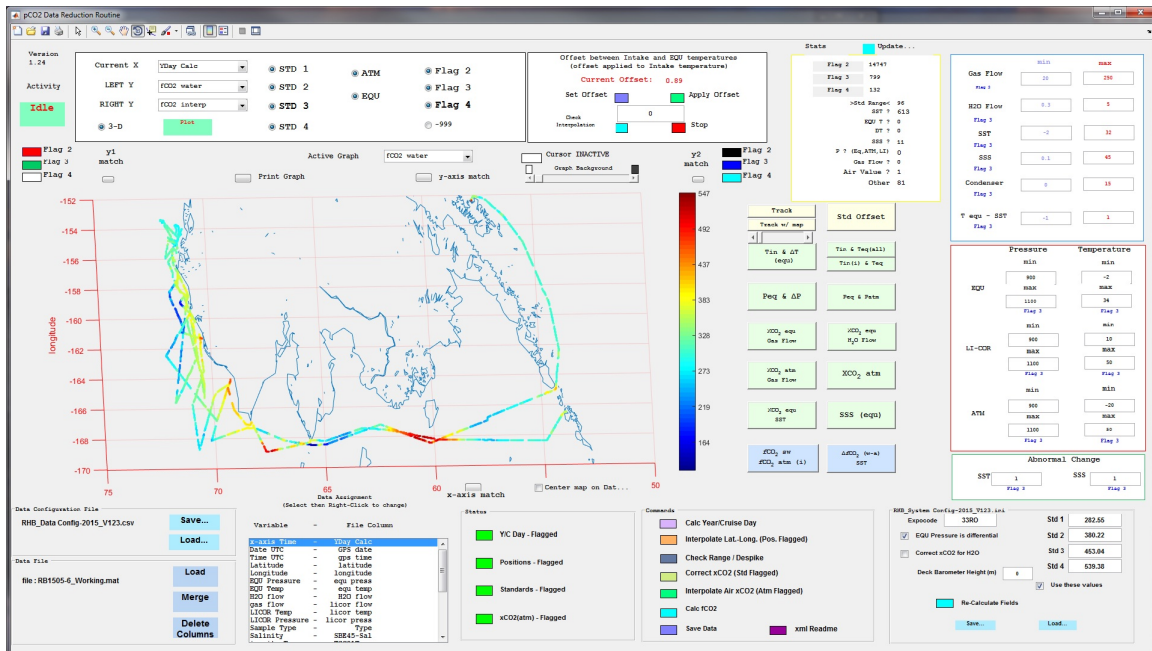
Figure 1. Screen grab of the display of the data reduction program

Data submission (SOCAT): All data from participants have to be submitted to a data center for public dissemination. Depending on funding source (NOAA/CPO/COD-ocean carbon or NOAA/OAR/OA) this is either CDIAC or the NCEI-OA project. Most data are now submitted though the SOCAT automated data ingester (www.socat.info). Metadata can be submitted in XLM format and datacenters (CDIAC and NCEI) are working on uniformity of tags and submission requirements. Issues with style sheets to display the data are being worked out.

Only data with quality control flags 2 (good) and 3 (questionable) are submitted/retained by the data centers. At the meeting there was discussion on:

-Should data fields without good pCO$_2$ data be retained (in order the keep the T, & S data, and possibly other biogeochemical data). *The general feeling was not.*

-Currently the only value that is flagged is the calculated fCO$_2$ value. Should there be separate flags for T, S, and XCO$_2$? At this point we'll stick with just flagging fCO$_2$ (which means that if T and S are questionable but XCO$_2$ is good, the calculated fCO$_2$ will be flagged 3. Flagging is problematic with respect to SOCAT as SOCAT recalculates everything based on XCO2)

-Other biogeochemical parameters will be added to SOCAT but they will not undergo higher-level QC. At the meeting it was felt that including QC flags of other biogeochemical parameters from the submitter should be advocated.

- For GO-SHIP cruises the groups taking UWpCO2 measurements are also responsible for QC and submission of TSG data. Procedures of QCing TSG data, in particular adjusting the CTD data need to be worked out.

Additional biogeochemical parameters, notably O_2, NO_3, and pH are being taken on some ships but not being quality controlled. The group recommended that standard operating procedures (SOP) be developed for these parameters and guidance on means of standardization and quality control. An automated bottle filling system was considered a high priority for validation sampling on the unattended cruises.

Marine air is routinely measured from the bow but no formal procedure is in place to check quality and, in particular, to determine stack gas contamination. Often the standard deviation of 5 air samples taken at two-minute intervals right after a standard sequence are used to determine homogeneity of the air mass with large standard deviations being flagged. For calculations the Marine boundary reference values are commonly used. It was recommended that a formal operating and QC protocol is adapted and that air values are checked with independent measurements. C. Sweeney and D. Munro NOAA/ESRL/GMD have proposed to build and deploy an instrument dedicated to quality air measurements that can be used in round robin fashion on different ships for in situ validation of air measurements on SOOP-CO2.

Interactions

The workshop was the first formal interaction of the system operators and was deemed highly effective in exchanging knowledge and forging a common path ahead. It was recommended to have the meetings (at least) biennial and inviting all groups involved in SOOP-CO2 measurements, possibly seeking travel funds from the program office and IOCCP. Increased exchanges on operating issues and lessons learned were encouraged along with possibly trying a message board/blog post the share common issues in operation.

Appendix A. Documented revision history of LabVIEW VIs for GO pCO2 systems.

(adapted from file provided by Peter Quasada, GO)
Version names in blue are the text that appears in the icon in the upper right corner of the main program screen.

Version GO beta 2 V4 -8 October 2009:
Added support for Hart 1523 thermometer.
Check LI-COR gas flow reading before saving data, if less than 40 ml/min the value in the STD column will be -9 instead of the standard concentration. If it is a zero or span run, the program will not set the zero/span on the LI-COR.
Changed initial state of "read ok" variable from false to true (to avoid problems with chiller staying on).
Added switch in edit configuration (and indicator in config page of startup screen) to select whether the Valco valve should be stepped to stop flow for EQU runs or if a stop flow solenoid is installed.
Added switch in edit configuration (and indicator in configuration page of start-up screen) to select if there is a Druck barometer permanently installed in the dry box.*
Added an option, "Druck in dry box" to the menu of sensors that can be tested from the test panel page. This could be a permanently installed Druck or just connected temporarily for checking the LI-COR pressure sensor.*
* - In either case it is assumed that the Druck is connected to the same RS-485 port as the ADAM modules.
Added universal serial interface.
Added GPS date under header "GPS Date". The date is taken from the NMEA sentence $GPRMC. So now we are using $GPGGA and $GPRMC. We could live with $GPRMC alone if we give up the "# of sats" reading in the test panel, but that might have some use so for now it's using both (and the Garmin sends both by default).
Changed header "Date" to "PC Date".
For LI-840, changed headers "H2O mv" and "CO2 mv" to "H2O abs" and "CO2 abs".
For LI-7000, added channel A (ref cell) raw readings for CO2 and H2O. Also renamed headers for raw readings to match the labels used in the LI-COR itself: "CO2a W", "CO2b W", "H2Oa W" and "H2Ob W".
Fixed problem that in the fault conditions in the log file "sleep" was logged as "shut down" and vice verse. This did not affect how the system ran (if sleep was selected, it would go to sleep, it was just logged as "shut down" in the log file). They are now logged correctly. Users will have to be told that the first time they run the new program their "shut downs" will change to "sleeps" and vv.

Version GO beta 2 V4NF

Supports new firmware (fan control uses integers for temps) – UW   pCO2 init.

Version GO beta 2 V5
   4 sig figs on drip 2 voltage (UW pco2.vi and uw pco2 init.vi)

Version GO beta 2 V6
   visa write-read.vi, only read if bytes in buffer > 0
   GO board.vi, use "visa buffer flush" function for initial flush, in RD loop
   edit configuration.vi, add control for data out port
   Added "data out port" to allow data file lines to be sent out a com port.
   Fixed bug in display of LI-COR values in "set flow.vi" for LI-7000.

Version GO beta 2 V6NF
   Version supports new firmware (integer temperatures for fan control settings).

Version GO beta 2 V7
   Added support for new Valco actuator (automatic detection of which one is connected) -VVI and main VI.

Version GO beta 2 V7NF version supports new firmware

Version GO V8 – Jan/Feb 2012.
   Name change on icon to "GO V8" (uw pco2.vi)
   New GO board firmware supported by default (uw pco2 init.vi).
   Option for dry Druck to set LI-6262 pressure just before taking CO2 readings (druck dry.vi, edit configuration.vi, uw pco2 init.vi, uw pco2 init storage.vi). This allows use of LI-6262's without the internal pressure sensor option.
   Removed optode support (user specific data.vi, uw pCO2 init.vi, edit configuration.vi)
   Fixed bug in "generic serial data.vi" that caused data dropouts on strings sent at fixed intervals.
   Changed "hart 1521.vi" to make more reliable data return from Hart 1521 thermometer (check strings length in addition to search characters, more iterations of loop). Removed error code 128 for multiple iterations of loop.
   Changed gps.vi and sleep-wake.vi such that the GPS com port will be re-initialized after ten bad GPS readings (only when system is set to use position based sleep/wake).
   Removed explicit support for Turner fluorometer (uw pco2 init.vi, uw pco2 init storage.vi, edit configuration.vi, user specific data.vi).
   Changed compression format for .dat files from zlib functions to standard zip format. This requires that the files 7zip.exe and 7zip.dll are present in the same folder as the Vis or LabVIEW executable program (edits to pack and send.vi).

Added option to log diagnostic parameters for LI-7000 (uw pco2 init.vi, licor visa.vi, edit configuration.vi, uw pco2 init storage.vi).

Made data table in "uw pco2.vi" scroll to last line when the table tab is clicked.

Hide "drip 2 index" control on uw pco2 init.vi

Removed explicit support for 7 sensor module (uw pco2 init.vi, uw pco2 init storage.vi, edit configuration.vi, deleted 3 Vis).

Initialize fault and error string indicators with empty strings (uw pco2.vi).

Removed "get pump speed" option from test panel (GO board does not respond to this command).

Added second call of "pack and send.vi" in shutdown sequence in "uw pco2.vi" to send compressed files on shutdown.

Removed "incoming commands.vi" from "get next state.vi".

Cleaned up code in visa write-read.vi – removed support for Technman RS-485 converter.

Fixed display of LI-COR readings on LI-COR page of start-up screen (values for LI-7000 were displayed in the wrong fields).

Added ability to test auxiliary serial devices from test panel (uw pco2 init.vi).

Removed unused elements from arrays of com port numbers (uw pco2 init.vi, uw pco2 init storage.vi, edit configuration.vi, no send list.vi).

Removed explicit support for Hart thermometer at seawater intake.

Removed list of items to not send by iridium (may put it back if desired, but in a better way).

Made default plots EQU/CO2 and ALL/equil temp (uw pco2.vi)

Added year to data file names. File name is now:

sysID_YYYY-JD-HHMMdat.txt

(uw pco2 init.vi, save data.vi)

Added option to run standards on shut down. User is prompted with question when STOP button is pressed.   System will automatically run standards when going to sleep based on position or a fault condition

Added an indicator showing how many minutes until the next set of standards will start – so that a person looking after a system at sea will know exactly when the standards will start to know when to clean the filter. New vi "time till standards.vi" modified "uw pco2.vi", "uw pco2 init.vi" and "get next state.vi".

Version GO V8 changes done 15 March 2012 -

Fixed bug in druck dry.vi – command sent to LI-6262 to set barometric pressure should be *77.

Licor visa.vi – changed order of reading LI-COR and druck such that druck is first (so that the pressure setting in LI=-6262 is from now instead of the previous cycle).

Version 8.1 8 – June 2012

Added code to turn off chiller when exiting program by selecting "cancel" from the start-up screen.

Version 8.2 – 21 June 2012
Changed fan control commands to GO board in "uw pco2 init.vi" to be compatible with new (version 2 and later) GO board firmware. This was meant to be done already but the old code found it's way back into version 8.0
Changed default position of scroll bar on the big data table on the main VI – previously it was set to a low position.

Version 8.3 – 26 June 2012
Fixed problem with new valco valve actuator. As with the change in 8.2, this change has been done before but got lost. Changed main vi (icon only) and valco multi-pos serial visa.vi

Version 8.4 –17 August 2012
Changed code in "generic serial data.vi" and "generic serial data setup.vi" such that when reading data in interval mode, the program takes the LAST full data string (everything between the last two terminators) instead of the FIRST full data string. Also changed such that if in interval mode AND "ms delay" is set to zero, the program will not flush the serial buffer before the delay (none) and reading of it. This setting is useful for the SeapHox units – set the seaphox to one minute readings, GSD to interval mode and zero delay.

Version 8.5 – 1 November 2012
Generic serial data.vi
Init ports case – set "enable termination character" to False.

Version 8.5 – 30 April 2013
Edit configuration.vi
Fixed bug in case structure numbering (changed 8 to 4) so that the code for deleting an aux serial device from the configuration would actually execute. Changed text on the front panel icon to read "edit config v8.5" instead of "edit config v8". Until now there was only one edit configuaraion program for all v8 sub-versions, so v8.5 should work with any v8.x version of the main program.

Version 9 – 29 January 2014
Pump speed.vi – convert pump speed to V8 and back to DBL each time to force it to stay within 0-255.
Main VI – replace old (7.1 and 8.5) semaphore Vis with new versions (no difference to user, just modernizing code).
Druck.vi – changed so that expected 1st character for visa w/r call is 0 instead of nothing (should reduce number of missed pressure readings).
Druck dry.vi – same as above.
Pack and send.vi – change 7zip to LabVIEW zip functions. Eliminates the need to have the 7zip program and DLL on the PC.
Druck dry.vi – Made so it will not set the LI-6262 pressure if dry druck reading is outside the range of 925 – 1070 hPa. Prevents screwing up the calibration of

the LI-COR if the the program gets a bad reading from the Druck pressure sensor.

Version 10 –September 2015
Replace old semaphore Vis in flush licor.vi
Added explicit support for Sea Bird SBE-21 and SBE-45 thermosalinographs by adding in the sub VIs that were removed after version 7.
Added support for Picarro CRDS detectors. See the document "Picarro CRDS on General Oceanics pCO2 system".

Version 10.1 – 15 September 2015
Fixed plotting menu on main VI.

Version 10.2 – 25 September 2015
Arranged front panel controls for Arial 14 font. The following three lines should be included in the labview.ini or UW_pCO2_v10-2.ini file:
appFont="Arial" 14
dialogFont="Arial" 14
systemFont="Arial" 14

Version 10.3 – 15 December 2015-12-16
Added control to changed header for A/D channel 4 (formerly "drip 2") and calibration function in UW pco2 cals.dat (6th line).

Version 10.4 – 23 January 2016
Fixed bug in new SBE TSG feature that edit configuration.vi would erase the TSG from the log.dat file.
Fixed an old bug in edit configuration.vi where it would erase drip 1 or drip 2 entries from fault conditions.