INSTRUCTIONS for the '***pCO_2 Data Reduction'***
Matlab Program

Program written by:

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Matlab Version: R2018b for Mac

Latest Revision: April 27, 2020

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Installing the program

The program is available as a Matlab '.m' file or as a compiled application, one for PCs and one for MACs.

Matlab® '.m' file

Some version of Matlab is necessary to run this program. It was written in version 8.2 (R2013b) but might work in other versions.

The files needed and their organization is described below.

The program requires several files:

1. 9 main program files :

"*pCO2_Sys_vxxx.m*"	"*merge.m"*	*"Edit_xml.m"*
"*pCO2_Sys_vxxx.fig*"	"*merge.fig"*	*"Edit_xml.fig"*
"*pCO2_Sys_vxxx.ini*"	"*savef_v2.m"*	*"findjobj.m"*
	"*savef_v2.fig"*	

2. At least 2 configuration files. 2 files are provided to the user to get started:

   - "*Initial Data Config.csv*" and
   - "*Initial System Config.ini*".

   The user can then edit them through the user interface. To edit the csv file, assign data columns to the variables AFTER loading data, then save the configuration in a new file. To edit the system configuration, edit the parameters on the bottom right of the interface and save the configuration in a new ini file. It is suggested to save all configuration files under the same folder so that the user doesn't have to browse through his whole hard drive to find the right configuration.

3. In addition, information pertaining to the metadata can be stored in a file used during the creation of the metadata xml file (see "Create xml" section). Use Excel to edit this file and save as a Text file.

   - "*xml.tsv.txt*"

4. The program also uses the ‘Statistics’ and ‘Map’ toolboxes from MathWorks® . As an alternative to the ‘Map’ toolbox, a few files can be used and are provided with the program.

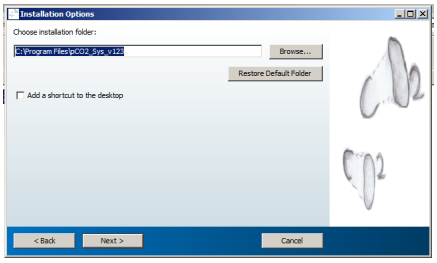
gshhs_l.b *gshhs_h.b* *gshhs_f.b*

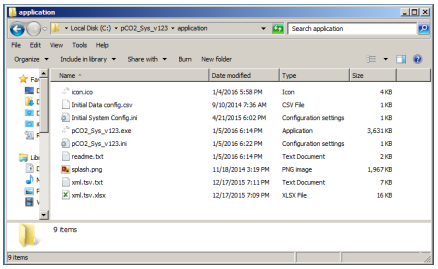
Compiled Application (PC and MAC)

A package can be provided, which contains all the files needed to run the program. The package will be different whether for PC or MAC but is deployed the same way.

On a Windows Machine:

1. Copy the executable (.exe) file to your computer. The file name is ‘*pCO2_Sys_Installer_web.exe*’
2. Double click the file:
3. It will download and install the Matlab Compiler Runtime (MCR) Engine automatically. (you need to be connected to internet)
4. The default installation location is ‘C:\Program Files\pCO2_Sys_v123\’. CHOOSE A LOCATION WHERE YOU HAVE WRITING PRIVILEGES. Usually, the ‘Program Files’ folder is protected and it is best to install it somewhere else like your documents or your desktop.
5. The application (pCO2_Sys_vxxx.exe) will be located under the ‘\pCO2_Sys_vxxx\application\’ folder, along with the 2 initial configuration files and the ‘xml.tsv.txt’ file needed to generate the metadata xml file. The ‘xml.tsv.xlsx’ file is the Excel version of the text file and is convenient to modify the text file.

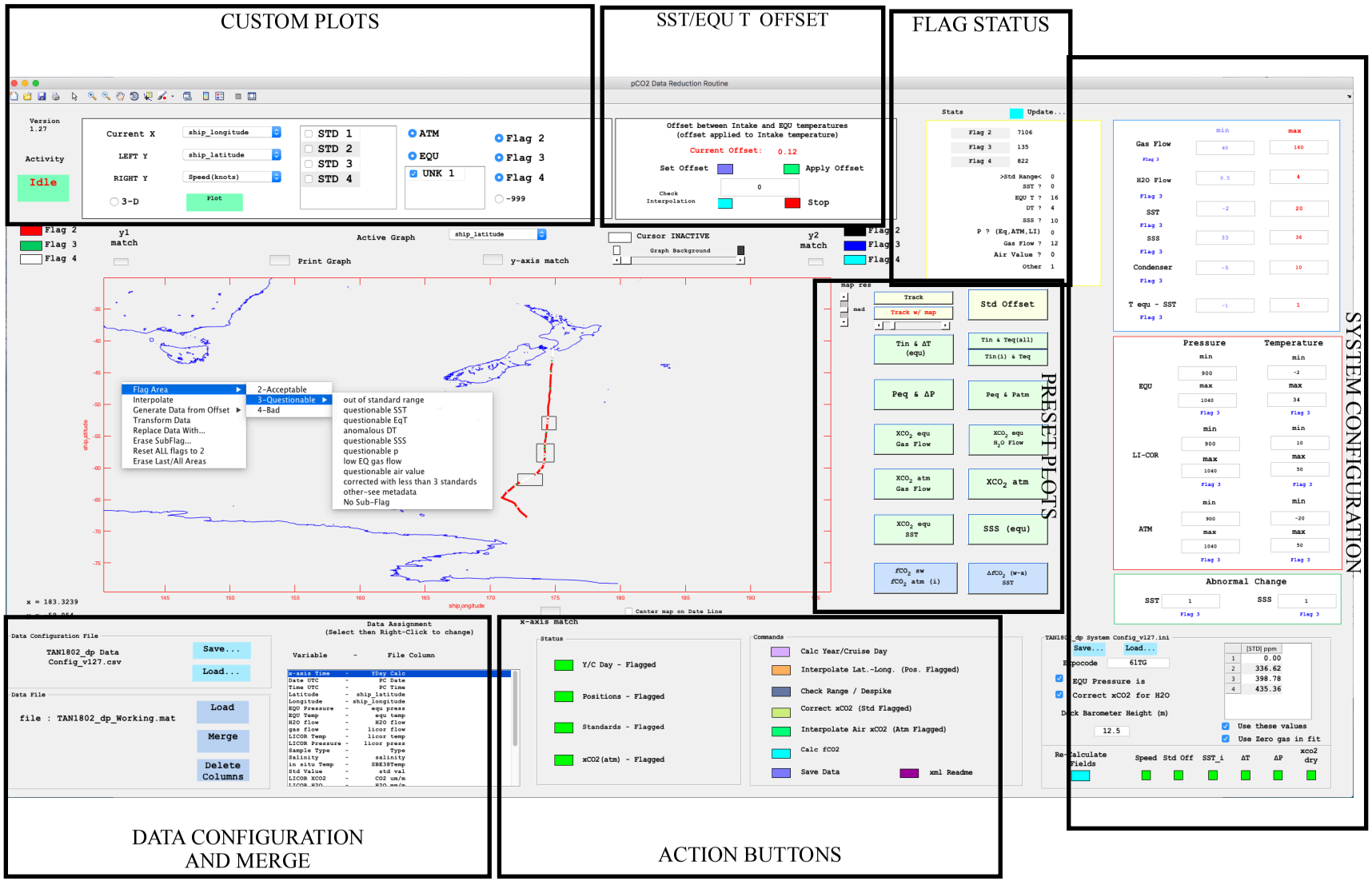




On a Macintosh Machine: (Not tested)

1. Copy the package (.pkg) file to your computer. The file name is ‘*pCO2 Sys vxxx exe MAC_pk.zip*’ for MAC and ‘*pCO2_Sys_vxxx_exe_PC_pkg.exe*’ for PC.
2. Double click the package:
3. On PC, it will install the Matlab Compiler Runtime (MCR) Engine (version 7.13) automatically. Just follow the prompts to install.
4. On MAC, the package will be expanded in the same directory and all the files copied there. The MCR Engine is contained in the MCRInstaller.dmg file. Open it and Double click the MCRInstaller.pkg file inside. Just follow the prompts to install.

5. The m_map files needed will not be visible on either platform but will be installed by the application itself at runtime.
6. Some instruction files will be included in the package. Be aware that these might not be the latest versions as the manual is a bit of a work in progress. Please contact Denis Pierrot for an updated version.


CUSTOM PLOTS
SST/EQU T OFFSET
FLAG STATUS
SYSTEM CONFIGURATION
PRESET PLOTS
DATA CONFIGURATION AND MERGE
ACTION BUTTONS
pCO2 Data Reduction Routine
Current X
LEFT Y
RIGHT Y
Activity
Idle
Plot
Offset between Intake and EQU temperatures
(offset applied to Intake temperature)
Current Offset: 0.12
Set Offset
Apply Offset
Stop
Stats
Update...
Flag 2
Flag 3
Flag 4
Active Graph
Print Graph
y-axis match
Cursor INACTIVE
Graph Background
Flag Area
Interpolate
Generate Data from Offset
Transform Data
Replace Data With...
Erase SubFlag...
Reset ALL flags to 2
Erase Last/All Areas
2-Acceptable
3-Questionable
4-Bad
out of standard range
questionable SST
questionable EqT
anomalous DT
questionable SSS
questionable p
low EQ gas flow
questionable air value
corrected with less than 3 standards
other-see metadata
No Sub-Flag
Std Offset
Tin & ΔT (equ)
Tin & Teq(all)
Tin(i) & Teq
Peq & ΔP
Peq & Patm
XCO2 equ Gas Flow
XCO2 equ H2O Flow
XCO2 atm Gas Flow
XCO2 atm
XCO2 equ SST
SSS (equ)
fCO2 sw fCO2 atm (i)
ΔfCO2 (w-a) SST
Gas Flow
H2O Flow
SST
SSS
Condenser
T equ - SST
Pressure
Temperature
EQU
LI-COR
ATM
Abnormal Change
Data Configuration File
TAN1802_dp Data Config_v127.csv
Save...
Load...
Data File
file : TAN1802_dp_Working.mat
Load
Merge
Delete Columns
Data Assignment
(Select then Right-Click to change)
Variable
File Column
x-axis match
Status
Y/C Day - Flagged
Positions - Flagged
Standards - Flagged
xCO2(atm) - Flagged
Commands
Calc Year/Cruise Day
Interpolate Lat.-Long. (Pos. Flagged)
Check Range / Despike
Correct xCO2 (Std Flagged)
Interpolate Air xCO2 (Atm Flagged)
Calc fCO2
Save Data
xml Readme
Epocode
61TG
EQU Pressure is
Correct xCO2 for H2O
Dock Barometer Height (m)
12.5
Use these values
Use Zero gas in fit
Re-calculate Fields
Speed
Std Off
SST_i
ΔT
ΔP
xco2 dry

First Time Use.

When the program starts, it automatically loads the 'Data Config File' and the 'System Config File' which were used last (unless a .mat file was loaded last). On the first run of the program, it will look into the '\System Configurations\' folder for the 'initial' config files. These only contain default values to feed to the program. They will need to be changed later.
If these 'initial' config files cannot be found, nothing will be loaded.

1. Load a data file: (see Data Import)

   Readable file extensions are: txt, csv, xls, xlsx, mat

   After loading the data, the program calculates 'Fields' which are ΔT, ΔP, Speed…etc. Since the program does not know which column represents what, a few error messages should appear. This is normal. Just click 'OK' to close them.

2. SETUP DATA ASSIGNMENT

   - Assign Data columns to Variables (see Data Assignment)

   - Save Data Assignment by clicking the blue 'Save' button. The data assignment will be saved and automatically loaded next time the program is started.

3. SETUP SYSTEM CONFIGURATION

   - Enter the range checking values appropriate for the system which generated the data

   - Enter the standard values, type of equilibrator pressure transducer…etc.

   - Save the configuration by clicking the 'Save…' button. It will be loaded automatically the next time the program is started.

4. Go to step 3 of 'Suggested Reduction Sequence' on the next page.

Suggested Reduction Sequence.

If this is the first time you are using the program, see First Time Use above.

1. CHECK CONFIG FILES: Check 'Data Config' and 'System Config' files loaded. If not correct, either manually correct values or load appropriate files.

2. LOAD DATA FILE: (see Data Import)

   Readable file extensions are: txt, csv, xls, xlsx, mat

   After loading the data, the program calculated 'Fields' which are ΔT, ΔP, Speed…etc. Since the program does not know which column represents what, a few error messages should appear. This is normal. Just click 'OK' to close them.

3. CALCULATE YEAR DAY: Has to be calculated (see 'Calc Year\Cruise Day'), unless you import your own. Then click 'Y/C Day OK'

4. IMPORT EXTERNAL DATA:

   - If necessary, import external data such as ship's data (SST, salinity, winds…) or any other data by clicking the 'Merge' button.

   - Assign imported data to appropriate variable.

5. UPDATE 'FIELDS' by clicking the 'Re-Calculate Fields' button (bottom right interface).

6. CHECK POSITIONS:

   - Plot latitude vs longitude. Make sure values plotted are reasonable. Corrupted values need to be flagged 4.
   -
   - If the cruise crosses the International Date Line, data plotted versus longitude will not display properly unless you click the radio button 'Center map on Date Line' which is located below the x-axis of the graph (only visible when plotting longitude data)

   - When positions are flagged properly, click 'Positions –not flagged', which will enable the 'Interpolate Lat./Long.' button.

   - if necessary, interpolate flagged 4 positions (see Interpolate Lat./Long.)

7. CHECK TEMPERATURE, PRESSURE AND SALINITY DATA. Interpolate if necessary by right clicking on the graph (see Data Interpolations.).

8. CORRECT FOR TIME OFFSET between SST and EquT (see Offset between In situ T and EQU T.) (It is highly recommended to save your progress at this stage)

9. RANGE CHECK:

   - Check the values of the ranges on the right side of the interface

   - click on the "Check Range/Despike" button (see Range Checking).

10. FLAG STANDARD OFFSETS (see Standard Interpolation.). Click 'Standards – not flagged'.

11. CORRECT xCO_2 VALUES ('Correct xCO_2' button).

    - Check standard interpolation on the Popup that appears.

    - When done, close popup graphs of standard interpolation.

    The out-of-range xCO_2 values are flagged at this stage.

12. FLAG DATA MANUALLY (see Flagging Data) using Preset Plots or user-defined plots

13. FLAG ATM XCO_2 values. Click 'xCO_2 (atm) OK'

14. INTERPOLATE ATM xCO_2 values to water measurements

15. CALCULATE fCO_2

16. PLOT 'XCO_2 corrected', fCO_2 and ΔfCO_2. Look for flyers and correct if necessary.

17. SAVE DATA.

18. GENERATE XML. This is the metadata file.

Initial Program Parameters

The *pCO2_Sys_vxxx.ini* text file contains information about the files that are loaded automatically when the program starts. The content of the file is updated by the program and the user should not need to edit it. The information contained is the following:

Default Data File Path:

First directory displayed when the grey "Load…" button is pressed.

Default Header File Path:

First directory displayed when the grey "Change…" button is pressed.

Default Header File:

File containing organization information in the data file and which gets loaded when the program starts (see Data Assignment) .

Default System Configuration File Path

First directory displayed when the yellow "Load…" button is pressed.

Default System Configuration File

File containing hardware information about the system that measured the data and which gets loaded when the program starts (see Initial System Parameters).

Data Configuration

The arrangement of the Data Columns in the data file can be saved in a ".csv" file. The first line should have exactly the following, in order:

1. x-axis Time
2. Date UTC
3. Time UTC
4. Latitude
5. Longitude
6. EQU Pressure
7. EQU Temp
8. H2O flow
9. gas flow
10. LICOR Temp
11. LICOR Pressure
12. Sample Type
13. Salinity
14. in situ Temp
15. Std Value
16. LICOR XCO2
17. LICOR H2O
18. ATM Pressure
19. cpu Temp
20. Deck Box T
21. Deck Box P
22. Condenser T

The second line should contain the headers of the data file corresponding to the variable in the first line (See below for example)

		A	B	C	D	E	F
Line 1 **Variable →**	**1**	x-axis Time	Date UTC	Time UTC	Latitude	Longitude	EQU Pressure
Line 2 **Data Header →**	**2**	none	Date	PC Time	latitude	longitude	CO2 equ press

The program will assign data columns to the variables according to the configuration file. If no configuration file is selected, all variables will be assigned to "None". It will be up to the user to assign the data columns (see "Data Assignment"). Once the assignment is done, the configuration can be saved by clicking on the button "Save". In addition to the columns imported, the program will create 3 extra ones ("QC", "SubFlag" and "SubFlag-User). QC flags information will automatically be saved in these columns unless the user imported a file already containing the information, in which case these 3 variables will have to be manually assigned to the imported columns.

Initial System Parameters

This section contains information about the pCO_2 system that generates the data. That information is stored in a *system config.ini* file and is comprised of the following:

Expocode

This is a 4-character code which uniquely designate the platform. For ships, if they exist, they can be found on NOAA's NCEI website (formerly NODC) at: *https://www.nodc.noaa.gov/General/NODC-Archive/platformlist.txt*

Group

Name of the group doing the measurement (e.g. AOML)

Ship

Name of the Ship

Cruise ID

ID of the cruise when the measurements were done (e.g. RB2005)

Barometer Height (m)

The height in meters at which the atm pressure is measured (Deck height).
The ATM pressure will be corrected for the height of the transducer before being added to the EQU pressure according to the equation:

$$P(sw\ level) = P(height) + \varrho(air)\ g\ h$$

Where ϱ(air) = Air Density, g = Gravity acceleration = 9.8 m s^{-2} and h = height in meters.

The air density is given by:

$$\varrho(air) = P(height)\frac{M}{RT}$$

Which gives:

$$P(sw\ level) = P(height)\left[1+\frac{M}{RT}g\ h\right]$$

M is the molar mass of air (0.02897 kg/mol), R=8.314 $J.K^{-1}.mol^{-1}$ and T (K), the air temperature, is approximated by the sea surface temperature.

The gravity acceleration is approximated by 9.8 m s^{-2} and the height is in meters
P(height) can be expressed in any pressure unit. P(sw level) will have the same unit.

Check: for P(height)=1013.25 mbar, T = 298.15K and Height = 10m, ϱ(air) g h = 1.16 mbar

Pressure Correction Errors:

Parameter	Error in parameter	Error in Pressure (mbars) = Error in pCO_2 (µatm)
Gravity Acceleration (m/s^2)	0.1	0.01
Air Density(kg/m^3)	0.001	0.1
Height(m)	1	0.1

EQU Pressure Differential(1-Yes 0-No)

The type of pressure transducer in the equilibrator (differential or not). If the pressure transducer is differential, the data column associated with LICOR pressure will be added to the EQU pressure (all pressures are assumed to be in mbars).

Standard Values (1,2,3,..)

They are the standards' known concentrations. These will be used only if the 'Use these values' box is checked (see below). The number of values entered here will determine the number of standards used for the system.

Use these Values(1-Yes 0-No)

If yes, the standard offset will be calculated with respect to these values. If no, the program will use the values from the data file to calculate the offset (see field calculations) and correct the LICOR xCO_2 values (see fCO2 calculations). If the user wish to revert back to the values from the file, uncheck the box mentioned above and press the 'Calculate Std Offset' button.

Use Zero Std in fit(1-Yes 0-No)

The user has the option to use the zero standard in the linear fits to correct the LICOR xCO_2 output.

Values for Range Check.

Some of these values are system dependent such as condenser temperature, ΔT…etc, so they are saved in this file associated with the system.
The file contains the limits used to range check the data. These are minimum and maximum values for:

- gas flow (ml/min), water flow (l/min), SST (^oC), SSS ($^o/_{oo}$), condenser temperature (^oC), T_{in}-T_{eq} (ΔT) (^oC)
- Pressures (mbar) and temperatures (^oC) in the system
- Abnormal changes in SST (^oC) and SSS ($^o/_{oo}$)

It also has the flag values if the data is out of range (Range Check Flags) and the offset, in minutes, between insitu and equilibrator temperature (see Offset between In situ T and EQU T)

Correct xCO_2 for H_2O.

Two of the three LICOR models (LI-840 and LI-7000) do not take into account the dilution effect of the water vapor. The correction on xCO_2 is given by : $xCO_2dry=xCO_2wet/(1-xH_2O/1000)$. If the option is selected, the program will apply the correction. This information is saved in the System Configuration file

PI Names for this data

Names of the PIs associated with this data set. The format is "LastName, F. ; LastName2, T.". The different names should be separated by a semi-colon.

Example of a '.ini' file:

```
Expocode
33RO
Group
AOML
Ship
RV Brown
Cruise ID
RB2005
Barometer Height (m)
5
```

```
EQU Pressure Differential(1-Yes 0-No)
1
Standard Values (1,2,3,..)
      0       281.16   522.31   358.87
Use these Values(1-Yes 0-No)
1
Use Zero Std in fit(1-Yes 0-No)
1
min-max for gas flow, water flow, sst, sss, condsr, dt
  40    200    0.3     5        -2       32       0.1      45       0        7        -0.5     1
p min-max and t min-max for equ, licor, deck box
 900   1040    -2       34     900    1040     10       55     900    1040    -20      50
Abnormal values for sst and sss
1           1
Range Check Flags
3    3    3    3    3    3    3    3    3    3    3    3    3    3
Insitu Temperature Offset(minutes)
3.34
Correct xCO2 for water(1-Yes 0-No)
0
PI Names for this data
Dupont, D. ; Dupond, T.
Save Options (1-Yes 0-No)(Expocode as col, Group as col, Ship as col, Save flags 4, Exclude ATMs)
1           1           0           0           0
```

Data Import

Data can be imported 3 ways:

from a SINGLE ".csv", ".xls" or ".xlsx" (after Matlab 2012) file

The user can combine the data into one CSV file and import it directly into the program. It is STRONGLY suggested to replace any empty cell by '-999' before importing the file. To do this, open the file in Excel®, click one cell containing data then press 'Ctrl+A'. Go to 'Edit→Replace…' (Ctrl+H), leave the 'Find what' field empty and put '-999' in the 'Replace with' field. Then click 'Replace All'. Save the file you're done.
If Excel is not installed, only Excel 1997-2003 documents will work(.xls).

from MULTIPLE "dat.txt" files

The user can select multiple files (from the same cruise, for example) to import. The program will remove all the SLEEP, SHUTDOWN, FILTER…lines , combine all the remaining data into ONE FILE and import it into the program. The user will be asked if he wants to "delete the combined data file". If "no" is selected, the file will be saved in the directory indicated under the name "TempX.csv", where X is a number automatically incremented by the program.
If the user selects several files to load, the program will tell the user that only the files with "dat.txt" extension will be loaded.

from a SINGLE ".mat" file

All the data (original and calculated) can be saved in a ".mat" file with the "Save Data" button and can be re-loaded at a later time. This allows the user to save the data before it is fully

reduced and continue the work later. All the progress of the data reduction is saved in the .mat file so that the user can pick up where he left off.

Field Calculations

Once the data is imported in the program, some fields are calculated, if possible. These are:

- Interpolated SST. Using the offset between Tin and Teq, it interpolates Tin to find its value at the EQU measurements.

- Standard Offset

  XCO_2(std)[LICOR] – XCO_2(std)[KNOWN]
  Where XCO_2(std)[KNOWN] is either from the file or from the '.ini' file.

- ΔT
  (Teq-Tin)

- ΔP
  (EQU P – ATM P)
  where EQU P is added to the LICOR P if the EQU pressure transducer is differential.

- Ship speed
  It uses the x-axis Time variable (YDay or Cruise Day) and Position

NOTES:

- Fields will not be calculated if the needed data is absent or not assigned. When the problem is corrected, one needs to re-calculate the fields by clicking on the appropriate button on the interface.
- When loading data (except .mat files), the number of STDs used in the file is compared to the number displayed on the interface. When different, the user is notified and given the option to fix the issue manually or have the program fix it automatically (only the number of STDs on the interface will be adjusted, not their concentration).
- The user can load a "working" file previously generated by the program. If "calculated fields" headers are detected, the user will be given the option to assign them to calculated variables.

Data Assignment

On a routine basis, data assignment is handled by the data configuration file. As the data files are loaded, the columns are assigned to variables according to what is in that data configuration file.
If it is lacking, the user can assign the data columns by the following procedure.

1) In the text box, each variable is associated either with a column from the data file or no column ("None"). Click on the variable to select it (the corresponding line becomes shaded or highlighted).
2) Right-Click (Control+Click on MAC) on the box (anywhere, as long as the correct variable has been selected). A menu will appear containing all the column headers from the data file. "File Columns…" contains the column headers from the data file. "From Calculated Fields…" contains the calculated columns such as ΔT, ΔP…(see Field Calculations above) as well as YDay Calc, Cruise Day, the corrected mole fractions and the fugacities.
3) Select the column to assign to the variable.

NOTES:
Once the user is satisfied with the assignment, the configuration can be saved by clicking on the "Save" button.

Number of STDs, UNKs

The number of standard and unknown types is handled similarly by the program, except for their initialization.

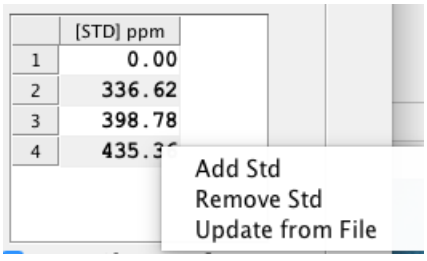
Initial State

The number of standards and their nominal values are stored in the System Configuration file and displayed on the interface when the configuration file (or .mat file) is loaded.

The number of UNK types is determined from the data file when it is loaded and then displayed on the interface.

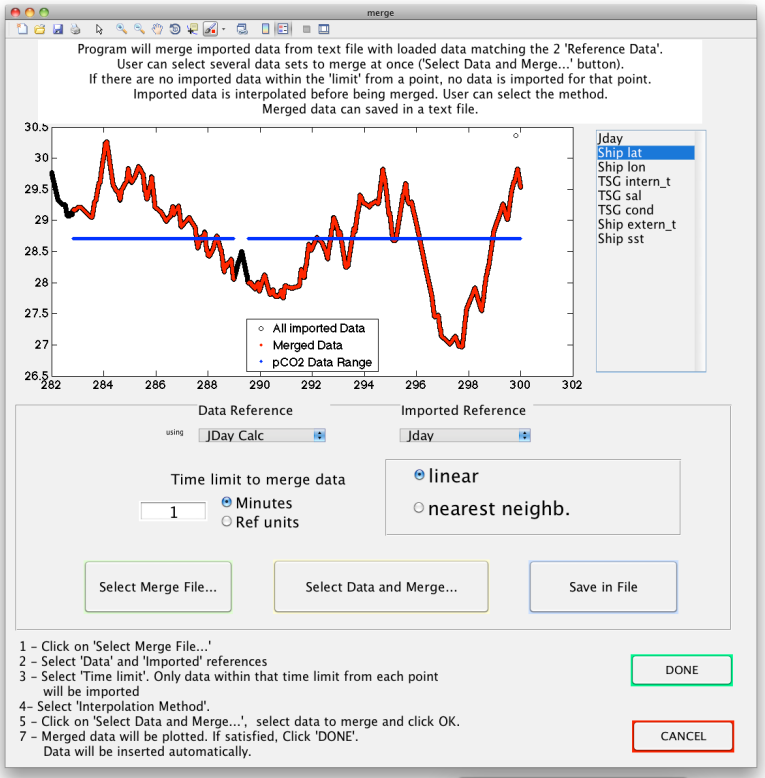
Modifying

Both are displayed in small tables on the interface. Right-clicking on these tables brings up a menu allowing the user to Add, Remove or Update the numbers from the data or configuration file .



Data Merging

The program allows the user to merge other data sets with the pCO2 data. The user selects a "key" (usually Year Day) to co-locate the two data sets. The resulting co-located data can also be saved in a separate data file if desired.



1. Click on the "Merge..." button on the bottom left side of the main panel. A new panel will appear.

2. Follow the instructions written at the bottom of the panel.

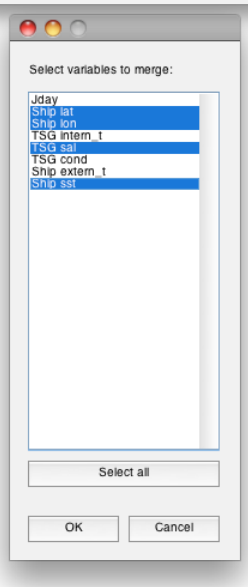
Time Limit to merge data:

For each pCO2 data point, if no data was found within that time limit, no data point will be imported.
When "Minutes" is selected, the "Data Reference" unit is assumed to be a fraction of year (like YDay). If "Ref units" is selected, it will use whatever units the "Data Reference" is in.

Interpolation Method:

If "linear" is selected, the merged data will be estimated by linear interpolation of the 2 data points surrounding the pCO2 data point on the time scale of the "Data Reference".

If "nearest neighbor" is selected, the point closest to the pCO2 data point will be merged in.



3. On step 5, after clicking "Select Data and Merge", a list of data column headers appears. Select the columns to merge (Ctrl-Click if selections are not adjacent) and click "OK".

4. The columns selected will appear on the right side of the graph in the previous panel. Clicking on each column there will plot the data:
   - IN BLACK: the data in the file
   - IN BLUE: the pCO2 data range on the "Key" scale.
   - IN RED: the data in the file corresponding to the pCO2 data range. That's the data that will be merged in.

For example, say YDay is the "Key" and the data to merge span YDay 1 to 200. If the pCO2 data covers YDay 50 to 100, a blue line will be plotted from 50 to 100. The red data will be the black data for YDay 50 to 100.

Graph

THE GRAPH IS A SUPERPOSITION OF 2 GRAPHS, EACH WITH ITS OWN X AND Y AXES.

Data Plotted.

The type of data in the graph depends on the button pressed. The name of the button that was pressed will show IN RED. For example, if the track is plotted, the first of the preset plot buttons will have its label red.

Active Graph

The active graph on which the user operates is selected by the "Active Graph" control. This is important to remember when zooming, viewing the x, y data or flagging the data.

Zooming

Zooming on the data is useful in order to pinpoint which data point is bad. The user can zoom on the plots by clicking on the zoom button. Zoom will only be effective on the active graph. Since only one of the graph's x axis is visible, zooming on the other one will not change the visible x axis scale, which will therefore not reflect the scale of the data.

NOTES:

- Plotting data will reset the axes scales to view the full range of data, and therefore undo any zooming action.
- When the zoom or pan (the hand) buttons are active, the flagging functions (drawing a box, access to the flagging menu) will be disabled. To re-enable them, click on the same tool button you are using again to de-activate it.

Displaying x, y Data

The user had the option to view the coordinates of the data points on the graph itself. In the bottom left corner of the graph is displayed the cursor position on the active graph scale. When selected, the "Active Cursor" button will allow displaying the x and y values of the data point in a yellow box next to the cursor when the cursor is placed on a single data point (within $1/100^{th}$ of each of the axes' scale). If more than one point is under the cursor, the program will display the number of points that the cursor covers. The user can then either flag all the data points covered by the cursor, or zoom in to separate them.

NOTES:

- In addition to the x and y data, the subflags (if any) will also be displayed when only one data point is selected. The subflags displayed are actually slightly different from the ones saved in the final data file – some have been defined to explain instances of "Other – see metadata" flags. These extra "user" subflags are: "LICOR t", "Water flow", "Deck box t", "Deck box p", "Condenser t" and "Interpolated position".
- Activating the cursor will hide the zooming and panning tools. They will re-appear when the cursor is de-activated.

Resize Axes

It is sometimes convenient to be able to rescale the axes to be able to compare the data plotted on each graph. Four (4) buttons perform the following tasks:

- Rescale the Y-axis BELOW to have the same scale as the OPPOSITE one.(see the "y1 match" and "y2 match" buttons).
- Rescale BOTH Y-axes to the same scale to view all the data (see the "y-axis match" button).
- Rescale INACTIVE X-axis to the same scale as the ACTIVE one (see the "x-axis match" button).

Flagging Data

See Flagging Data below

Interpolating Data

See Data interpolations and Temperature Inference. below

Correcting Offset between in situ and EQU Temperatures

See Offset between In situ T and EQU T below

Preset Plots

These 'Quality Control' plots were agreed upon during a workshop on pCO_2 data reduction held in Miami, FL in October 2005. The user can only control the FLAG NUMBER (2,3,4) of the data plotted and NOT THE TYPE (STD, ATM, EQU). The type is pre-selected, depending on the plot, as follows:

1)- "XCO2 equ, SST"	EQU
2)- "Tin, DT"	EQU
3)- "P, DP'	EQU

4)- “XCO2equ - Gas Flow” EQU
5)- “XCO2atm - ATM Flow” ATM
6)- “Std Offset” All STDs
7)- “SSS” EQU

Other preset plots have been added, namely;

8) Track ALL
9) Track with map ALL
10) Tin, Teq (all) ALL
11) Tin(i), Teq EQU
12) xCO2 atm ATM
13) xCO2eq – H2O Flow EQU

These plots should help the user spot the flyers relatively easily.

Notes:

- A slider control appears below the ‘Track w/ map’ button’ when it is clicked. It allows the user to zoom out.
- When plotting data versus longitude, plotting the track or plotting in 3D, a radio control (“Center map on Date Line”) appears below the graph allowing the user to plot data across the dateline.
- A button labeled ‘Flag Quest. Air values’ appears only when the preset ‘XCO2 atm’ is selected. It is a shortcut to flag selected data as “Questionable air value”.
- Tin(i) stands for interpolated SST. When an offset between SST and EQU temperature has been applied, it is the adjusted (interpolated) SST that will be plotted. The preset plot 10 (Tin, Teq (all)) allows to plot the original SST data.

Range Check and De-Spiking

The range checking of the data consists in determining “valid data ranges” for certain measurements like flows, pressure…etc… and assigning a FLAG 3 or 4 to the data that fall outside these ranges. The ranges are user-definable, although some recommendations were made during the workshop. The recommendations were the following:

Parameter	Range	Type applicable	SubFlag
Gas Flow	40 to 200 ml/min	ALL	Low LICOR gas flow
Water Flow	0.3 to 5 L/min	EQU	Other, see metadata
SST	-2 to 32 ^{o}C	EQU	Questionable/Interpolated SST
SSS	0 to 45	EQU	Questionable/Interpolated SSS

Teq – SST	-0.5 to 1 °C	EQU	Anomalous DT
EQU Pressure	900 to 1040 mbar	EQU	Questionable Pressure
LICOR Pressure	900 to 1040 mbar	ALL	Questionable/Interpolated Pressure
ATM Pressure	900 to 1040 mbar	EQU	Questionable/Interpolated Pressure
EQU Temperature	-2 to 34 °C	EQU	Questionable/Interpolated EQU Temp
Condenser Temperature	0 to 7 °C	EQU, ATM	Other, see metadata
LICOR Temperature	10 to 50 °C	ALL	Other, see metadata
Abnormal Teq change	± 1 °C	EQU	Questionable/Interpolated EQU Temp
Abnormal SST change	± 1 °C	EQU	Questionable/Interpolated SST
Abnormal SSS change	± 1 unit	EQU	Questionable/Interpolated SSS
Deck Box Pressure	900 to 1040 mbar	EQU	Other, see metadata
Deck Box Temperature	-20 to 50 °C	EQU	Other, see metadata

De-spiking values and SubFlags:

The flag assigned to out-of-range data is user selectable by clicking on the string (e.g. “flag 3”) below each parameter to toggle the value of the flag between 3 and 4.
These selections get saved in the System Config.ini file

Note: if a parameter (e.g. Deck Box T) is assigned to ‘none’ in the Data Assignment panel, it will not be used to do the range check.

Sub-flags .

Sub-flags are a description of why data was flagged 3. These sub-flags will be reported in the final data file. The different sub-flags applicable are:

1. *'out of standard range'*
2. *'questionable/interpolated SST'*
3. *'questionable/interpolated EqT'*
4. *'anomalous DT'*
5. *'questionable/interpolated SSS'*
6. *'questionable/interpolated p'*
7. *'low LICOR gas flow'*
8. *'questionable air value'*
9. *'corrected with less than 3 standards'*
10. *'other-see metadata'*

Not all sub-flags can be applied to all measurement types. The table below describes which sub-flag can be applied to which type.

SubFlag	Type applicable
• Out of Standard Range • Corrected with less than 3 standards	EQU, ATM
• Questionable/Interpolated SST , EQU T, SSS • Anomalous DT • No Subflag	EQU
Questionable Air Value	ATM
• Low LICOR gas flow • Questionable/Interpolated p • Other, see metadata • None	All

User Sub-flags

In addition to the "agreed upon" subflags mentioned above, several extra subflags (referred to as "user subflags") have been defined in order to explain the "Other, see metadata" flag and help identifying the origin of the automatic flagging. These are for the user only and will not appear in the final file. They are:

11. *'LICOR t'*
12. *'water flow'*
13. *'deck box t'*
14. *'deck box p'*
15. *'condenser t'*
16. *'interpolated position'*
17. *'interpolated using questionable SST'*

They are only set by the program during the automatic de-spiking routine. Users do not have access to them, except in some cases of manual flagging from popups.
Except for '*interpolated using questionable SST',* these sub-flags will NOT be reported in the final data file. They will only show as sub-flag 10. They will, however, be visible to the user with the active cursor on the interface.
For SST in the final file, flags "questionable/interpolated SST" will be removed (since the measured data is not reported) and '*interpolated using questionable SST'* flags will be reported instead.
When the data below is out of range or when they are interpolated, the following sub-flags will be assigned:

Parameter	Range	Type applicable	User SubFlag
LICOR t	10 to 50 ^{o}C	ALL	LICOR t
Water Flow	0.3 to 5 L/min	EQU	water flow
Deck Box Pressure*	0 to 45	EQU	deck box p
Deck Box Temperature*	-2 to 32 ^{o}C	EQU	deck box t

Condenser t	User Select	EQU-ATM	condenser t
Interpolated Position	N/A	ALL	interpolated position
Interpolated SST	N/A	ALL	interpolated using questionable SST

* These are no longer used starting in version 1.27

‘Status’ Section and ‘Commands’ Section

These sections allow the control of the data reduction in a sequential manner.

Calc Year/Cruise Day.

Most of the plots will use either Year Day or Cruise Day on the x-axis. It is also one of the data saved in the “FINAL” file. The first thing to do after the data is loaded and the variables are assigned to the file columns, is to calculate it from Date and Time using the button provided. Once the button is clicked, a popup panel asks the user to select the proper Date format (see NOTE below).
At the end of the calculation, the user is given the choice to assign either Year Day or Cruise Day to the x-axis Time . If the cruise spans 2 different years, Cruise Day will be preferable to Year Day since it will allow a sequential display of the data. Year Day, going from 365 to 1 over new year’s day, would not be a proper variable to display the data.
If the user had already assigned a data column to YDay, there will be a ‘No Change’ option. Following the calculations, the button “J/C Day - Not Flagged” will become visible.

NOTES:

- The Year Day here is defined as the Year Day, STARTING AT ONE.
  January 1 00:00:00 = 1
  January 1 18:00:00 = 1.75
  This is the same as the definition used in the program controlling the GO/Neill pCO_2 system.
- The Cruise Day is the day of the cruise, STARTING AT ONE AT MIDNIGHT OF THE FIRST DAY, even if the cruise did not start at midnight. This is done so that the fractional part of the Cruise Day indicates the same time of day as the Year Day (i.e. 18.5 means it’s at noon)
  Day 1 00:00:00 = 1
  Day 1 18:00:00 = 1.75
- The Cruise Day will only be available when the Year Day is calculated by the program from date and time columns, not when the user imports its own Year Day column.
- The GO/Neill pCO_2 System (dat.txt files) outputs the date in the European format (DD/MM/YY).

Y/C Day – Not Flagged

Setting Year(Y) or Cruise(C) Day to Flagged turns the "Positions - Flagged" button visible. The user can then check the lat. and long. data for misread values.

Positions – Not Flagged.

Any lat and long data flagged 4 will be interpolated.
The program will NOT interpolate position values of '-999' unless they are flagged 4 as well. To flag them , they need to be plotted by selecting the 'Missing values' control. Once the corrupted lat and long values are flagged, click on the "Positions – Not Flagged" button and the "Interpolate Lat.-Long." button will become visible. Clicking on it will replace corrupted positions (flagged 4) with interpolated lat. and/or long. (see below).

Interpolate Lat. Long. button.

This routine takes all the data that is flagged 4 and interpolates them using the good data (non-missing, non-flag 4 data). It interpolates Latitude data, then Longitude data, consecutively. A plot of the good and interpolated data appears at the end of the routine. The user has the choice to accept or not the interpolated values. If the values are accepted, they are used to replace the bad data. The interpolated data is then flagged 3 with a sub-flag of "Other – see metada". In the program itself, a "user subflag" is set to "Interpolated position". The subflag can be viewed by the user when the mouse cursor is activated (see Displaying x, y Data) and put over the points on the graph.
NOTE: Interpolating position assumes the ship was sailing in a straight line at the time of interpolation…This could lead to errors.

Check Range/Despike button.

This button becomes available when both "Year Day – Not Flagged" and "Positions – Not Flagged" have been pressed. Pressing this button will flag data which are out of range, according to the min and max values specified in the controls on the top right side of the interface. It will also find outliers in temperature and salinity data but it will not range check xCO2 values since they have not been corrected yet. This will be done when xCO2 values are corrected (see Correct xCO2) (See also Range Check and De-Spiking). The small red button which appears to the left of the "Check Range" button after pressing it allows the user to restore the flags to what they were before pressing the "Check Range" button. Once the red button pressed, it will disappear. It will only restore the flags and subflags, not data values.

Standards – Not Flagged.

When satisfied that the data has been properly range checked, the standards offsets need to be checked and bad values flagged before xCO_2 values can be corrected. Standard offsets can be viewed by pressing the 'Std Offset' button. (see Correct xCO2). Press the 'Standards – Not Flagged' button when standards have been flagged properly. This will activate the "Correct xCO_2" button.

Correct xCO2

This button is active when the range check has been done and standards have been flagged. The standards will be interpolated and used to correct xCO_2 values for EQU and ATM (see Standard Interpolation.). Plots of interpolated standards will be shown. This graph can be closed at any time.
The "xCO_2(atm) – Not Flagged" button will appear.

xCO2 (atm) – Not Flagged.

The user should then check the xCO_2 (atm) values for any outliers. This step determines which air values will be used for interpolation to seawater measurements.
Bad air measurements need to be flagged "questionable air value". When plotting the xCO2atm values, a button appears on the left side of the graph. Clicking this button is equivalent to flagging the selected data as "questionable air value".
Only flag 2 and 3 ATM measurements will be used for the interpolation, EXCEPT the flagged 3 data which has been subflagged "questionable air value".
When satisfied with the air values for xCO_2 , the user should click on the "XCO2 (atm) – Not Flagged" button

NOTE: When plotting ATM xCO2 values, it is not possible to distinguish the 'questionable air value' points from the other flag 3 points. All flag 3s will be the same color, yet only the former will be excluded from the interpolation. The user needs to try to keep track of which air value has been flagged questionable air value. After clicking the 'Interpolate Air xCO2' button will appear a plot of all air values, averaged good air values and interpolated values. The user can then double check that all bad values have been flagged properly by visually checking that the averaged and interpolated values look reasonable.

Interpolate Air xCO2

When BOTH the "xCO_2 (atm) Flagged" and "xCO_2 Range - Flagged" buttons are green, the user will be allowed to interpolate the xCO_2 (atm) values to the seawater measurement times by clicking on the "Interpolate air xCO2 " button. For each EQU measurement, an xCO_2 (atm) values will be calculated from LINEAR INTERPOLATION between the ATM measurements (see previous section). Before interpolation, the sets composed of successive good ATM measurements are AVERAGED. Interpolation occurs between averaged values.

Calc fCO2

For details on the calculations, see the section on fCO2 calculations.

Save Data

The "Save Data" allows the user to save his work. Five files will be saved in this subroutine:

- The '_FINAL' csv file that will be reported to the scientific community. It will have 4 "pre-headers" lines of metadata in order to be easily uploaded to the SOCAT v4.0 dashboard. These lines are:

  Expocode: XXXXyyyymmdd
  Ship: Gordon Gunter
  Group: AOML
  Investigators: Dupont, D. ; Dupond, T.

  It will also contain the columns agreed upon in the Miami workshop. These are:

YD_UTC	TEMP_EQU_C
DATE_UTC__mmddyyyy	SST_C
TIME_UTC_hh:mm:ss	SAL_permil
LAT_dec_degree	fCO2_SW@SST_uatm
LONG_dec_degree	fCO2_ATM_interpolated_uatm
xCO2_EQU_ppm	dfCO2_uatm
xCO2_ATM_ppm	WOCE_QC_FLAG
xCO2_ATM_interpolated_ppm	QC_SUBFLAG
PRES_EQU_hPa	
PRES_ATM@SSP_hPa	

If an offset between SST and EQU temp has been determined as not 0, the flag 'quest./ interp. SST' will be removed since the original measured SST data is not reported. Instead, the flag 'interpolated using quest. SST' will be reported for the appropriate data points.

- A '_WORKING' csv file containing all the original data as well as all the calculated fields.

- A '_WORKING' ".mat" file containing all the reduced and calculated fields like the csv file mentioned above but also containing information on the reduction steps taken at the

time of save. This file can be re-imported so that data reduction can be stopped, saved and continued at a later time. The paths for the Data Configuration and System Configuration files are also stored so that the proper configuration can be loaded together with the data.

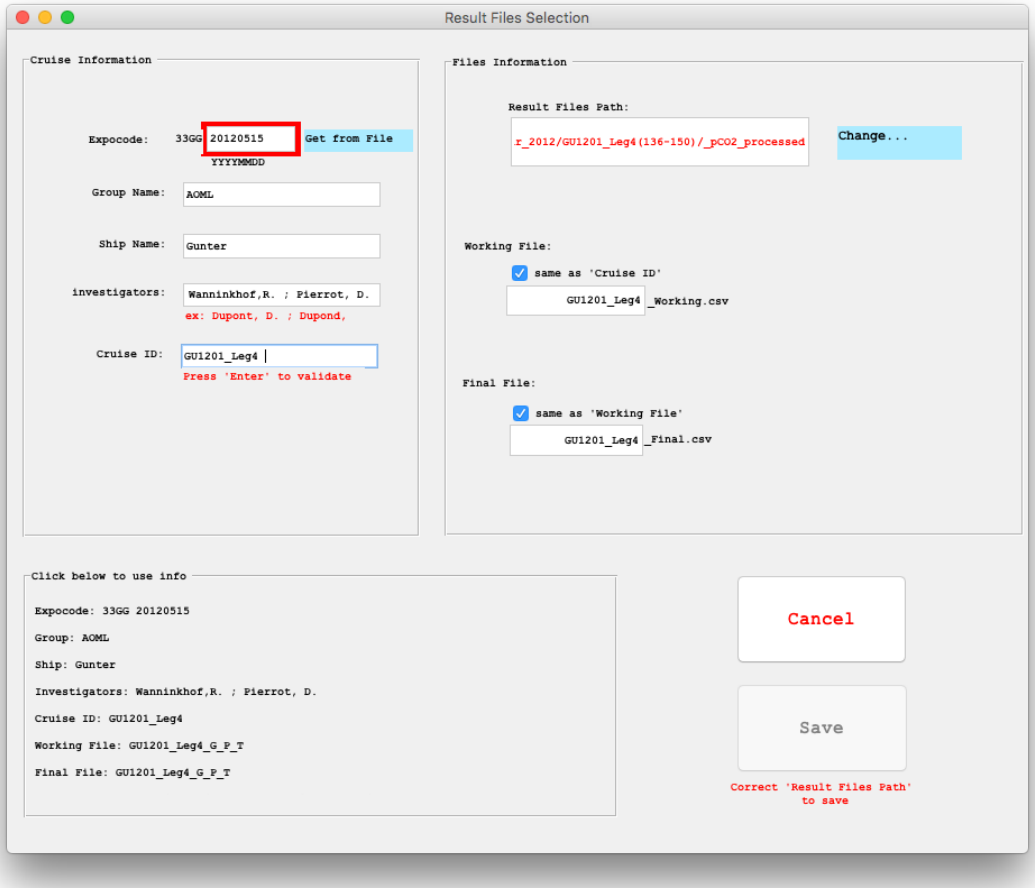
- In addition to the 3 data files mentioned above, the program will also save the configurations (data and system) used during the processing of the data. The file will be automatically saved in the same directory as the 3 data files with the following format:

  Cruise_ID Data Config_vxxx.csv and Cruise_ID System Config._vxxx.ini

  These file names will be saved in the .mat file as well and displayed on the main interface.

NOTES: For ATM measurements, Tequ, Pequ, Patm, SST and SSS are set to -999 in the FINAL file as they do not affect the xCO2(atm) measurements.

When the "Save" button is clicked, the following window will appear:



Features of the window:

- Expocode:

  The first good date is automatically taken to create the final Expocode. If that first date is not the first day of the cruise, then the date for that first day of the cruise should be manually input in the yyyymmdd format.

- Final Files Path

  Non existant paths will show in red.

  A path can be entered either manually or by clicking on the “Change…” button.

  Only when the path entered exists will the “Save” button be enabled.

- File Names (_Final and _Working):

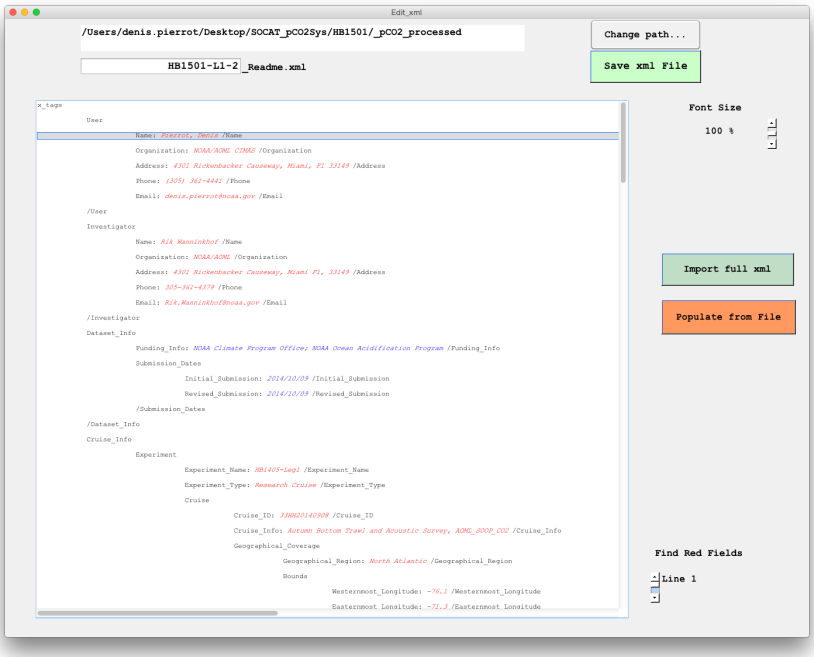
  Depending on which option is selected, the name can either use the Cruise ID field or not.

  One can double-click on the text of the extensions (“_Final.csv” and “_Working.csv”) to open a File Selection dialog window. The name of the selected file (minus the corresponding extension) will be placed in the text box next to it.

  When the path is correct, the program instantaneously checks if the file already exists in that path. If it does, the user must select “Overwrite” for the file to be saved. If the file does not exist, that choice will not be available.

- ‘Click below to use info…’

  The info in this text box might be different than the info in the controls of the window, especially when just loading a .mat file. To populate the controls of the window with the info contained in that box, just click on the box.



Create xml.

This interface allows the user to create an xml file with the tags or fields that were agreed upon by CDIAC and SOCAT. This process requires a 'template .xml' file (usually one per ship/ system), which is then modified by the program by extracting appropriate information from the data and populating the fields in the template.
.
The xml file is composed of fields the name of which are displayed in BLACK text and the value of these fields, which are displayed in BLUE text, on the interface.

All fields can be edited on the interface. The ones displayed in RED are the ones that usually vary from cruise to cruise and the user should pay close attention to them. The user can jump from red lines to red lines by using the "Find Red Fields" scroll bar at the bottom right corner of the interface.

Most of the information needed (about sensors, variables, etc…) can be stored in the template xml file that the user can create manually for each ship. For example, it could be created using the CDIAC"Metadata Creation Toolkit" (http://mercury-ops2.ornl.gov/OceanOME/editor.htm) and then saved locally.
This template can then be imported in this program using the "Import full xml" button.
After editing the fields, they can be saved as a new xml file.

Editing Fields:

- Manual Edits:

  Clicking on a line containing blue text will open a pop-up window which will allow the user to either edit the text directly or select from a list of choices. These lists are stored in the configuration file called "xml.tsv.txt" (see below).

- Automatic Edits: (Performed by clicking on "Populate from File" button)

  A few of these tags can be filled in automatically with information taken directly from the data and the configuration files. These are listed below:
  <Cruise_Info><Experiment><Experiment_Name> : set to Cruise ID from the "Save Data" window.
  <Cruise_Info><Experiment><Cruise><Cruise_ID>: set to the Expocode from the "Save Data" window.
  <Cruise_Info><Experiment><Cruise><Cruise_Info>: taken from the "Platform Info" list in the "xml.tsv.txt" file (see below) by matching the ship Expocode saved in the "System Config File.csv".
  <Cruise_Info><Experiment><Cruise><Geographical_Coverage><Bounds>: taken from data directly
  <Cruise_Info><Experiment><Cruise><Temporal_Coverage>: taken from data directly

<Cruise_Info><Vessel>: all info (Vessel_Name, Vessel_ID, Vessel_Owner) taken from the "Platform Info" list in the "xml.tsv.txt" file (see below) by matching the ship Expocode saved in the "System Config File.csv".
<Method_Description><CO2_Sensors><CO2_Sensor><Manufacturer_of_Calibration_gas>: taken from the "Standards Info" list in the "xml.tsv.txt" file (see below) by matching the standards concentrations saved in the "System Config File.csv".

- Special Edits:

<User> or <Investigator>.
There can only be one "User" whereas several "Investigators" can be selected.
Editing those fields require selecting a name (or several) from a list which also comes from the "xml.tsv.txt" file.
Selecting a name will replace all the fields (Name, Organization, Address, Phone, Email) at once.

<Cruise_Info><Experiment><Cruise><Ports_of_Call>
Several poc can be entered at once on separate lines. They will be displayed on the interface as separate.
To delete a poc, select it and delete its name on the pop-up, leaving the text field blank, before clicking OK.

"xml.tsv.txt" file:

There are 5 lists contained in this file. Each list has a header describing the informations needed for each list. Each item on the list needs to be TAB separated. The user can edit this file to input his/her own information.

Here is an example of "xml.tsv.txt"

"Standards Info (conc, tank num, owner)"
0.00 AOML
391.28 RSMAS
248.73 JA2280 AOML
282.59 CA4890 ESRL

"Platform Info (Expocode, Name, Owner, Experiment Type)"
33RO R/V Ronald H. Brown NOAA Research Cruise AOML_SOOP_CO2
74X1 M/V Las Cuevas Greenlight Transport S.A SOOP Line AOML_SOOP_CO2

"People Info (name, organization, address, phone, email)"
"Wanninkhof, Rik" NOAA/AOML "4301 Rickenbacker Causeway, Miami, Fl 33149" (305) 361-4379 rik.wanninkhof@noaa.gov
"Pierrot, Denis" NOAA/AOML CIMAS "4301 Rickenbacker Causeway, Miami, Fl 33149" (305) 361-4441denis.pierrot@noaa.gov

Region Info
North Atlantic
Caribbean Sea

Cruise Type Info
Reasearch Cruise
SOOP Line

User-Select Plots

- Select the X-Axis, Left Y-Axis and Right Y-Axis Data to be plotted. The accessible data is:

  All the columns in the data file
  All the calculated fields
  All the data calculated during the fCO_2 calculations (corrected XCO_2, fugacities and fCO2W-fCO2ATM.

- Select the TYPE of data to be plotted (STDs, ATM, EQU, UNK).

- Select the FLAG to be plotted (2, 3, 4).

- Click on the 'Plot' button. The text inside the button will turn red.

NOTE: XCO_2 (EQU) and XCO_2 (ATM) corrected (called XCO2W and XCO2A in the program) cannot be plotted. Instead, the user is told to select 'XCO_2 corr', which is the corrected mole fractions for both EQU and ATM and to select the type of sample to plot (EQU to plot XCO2W and ATM to plot XCO2A)

Flag Colors

The user can select a different color for each flag value on each graph. The flag colors on the right side of the panel refer to the data plotted on the right Y axis and vice-versa for the left side.

To change the color of a flag, simply click on the square in front of the flag number to which the color will apply. Select the new color on the palette that pops up and click OK.

To view the changes, the plot needs to be redone…simply click on one of the preset plot buttons or the 'Plot' button, whichever has a red label

Flagging Data

When the user detects bad points:

The user needs to draw one or more rectangle area enclosing all the data to be flagged. This is done by clicking and dragging the mouse cursor on the graph. More than one rectangle can be drawn by pressing either the “Shift”, “Alt” or “Control” key while dragging the mouse cursor.

Once the areas are done, right click anywhere on the graph and select ‘Flag Area’ in the menu that pops up (see the menu on the graph). Then select the flag number to be used.

NOTES:

- Drawing a rectangle erases all previous ones drawn, unless the “Shift”, “Alt” or “Control” key is pressed.
- Areas can be deleted by right-clicking on the graph and selecting “Erase All/Last Area”. The user will then have the option to erase either all or only the last rectangle drawn.
- Flags will be applied on the data from the ACTIVE GRAPH. The user needs to be aware of which graph is active.
- Not all flags can be applied to any data, For example, ATM pressure cannot be flagged if it belongs to an EQU measurement since it only affects ATM fugacities.. Flags can be applied as follows:

Quest. SST,Quest. EqT Quest. SSS, Quest. ΔT	EQU only
Quest. LICOR, EQU Pressures Outside STD range Less than 3 STDs used for correction Other-See metadata, No Flag	EQU and ATM
Quest. ATM Pressure, Quest. Air Value	ATM Only

* UNK types can only be flagged automatically and for LICOR issues (T, P, gas flow)

Flags Status

Detailed flag counts are given on the top portion of the interface. It is automatically updated only after clicking on the “Range Check” button. Click on the “Update…” button to refresh the information at other times. Only the subflags that are going to be reported are listed here. Other subflags such as “out-of-range deck box pressure, for example, will be given on individual points by the mouse cursor when it is activated (see Displaying x, y Data section).

Undoing a SubFlag

The user can select points and choose to remove a sub flag on these points. See the Erase SubFlag… section below.

Data Interpolations.

The program provides a simple way to LINEARLY interpolate data between two good points. Whether this is scientifically acceptable is left up to the user to assess.

- Draw one or more rectangle areas encompassing the data of the ACTIVE GRAPH to interpolate.
- Right click anywhere on the graph and select 'Interpolate'.
- THE ORIGINAL DATA WILL BE REPLACED BY THE INTERPOLATED ONE.
- After the interpolation, the user is asked whether the data should be flagged automatically or not.
- If the user selects to flag the data automatically and the data is assigned to either a Temperature, Pressure or Salinity, it will be flagged 3 with an appropriate subflag: 'Questionable/Interpolated' X where X can be either "SST", "EqT", "SSS", or "p".
- If the same column of data is assigned to more than one of the SSS, SST or EqT variables, the user will be asked which subflag to apply.
- If the user selects NOT to flag the data automatically or if the data is neither a temperature, pressure or salinity, IT WILL NOT BE FLAGGED AT ALL.
- One cannot interpolate calculated data. A message will pop up when that is the case and the user should interpolate the original data it is calculated from.
- Only the data shown on the graph is used for the interpolation.

It is strongly suggested to do the interpolation at the beginning of the data reduction, before doing the range check and despiking.

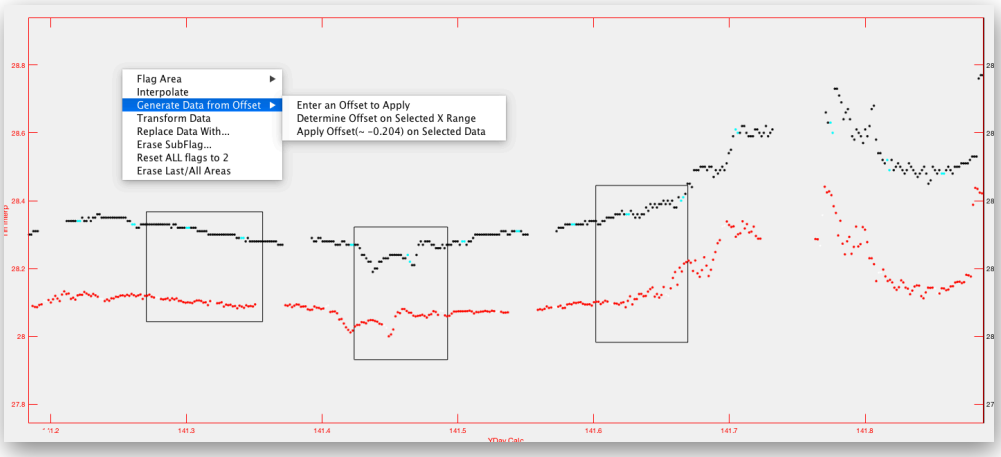
Data Inference.

It is sometimes desirable to be able to replace some bad data by applying an offset to some good data and using these values instead. For example, when a large chunk of temperature data is bad and interpolation is not an option, it is sometimes possible to estimate the values if one has another set of data that co-varies. Namely, one can estimate equilibrator temperatures that are bad if one has in situ temperatures that have a constant offset with the equilibrator.
This feature is accessed by right-clicking on the graph and selecting "Generate Data from Offset" when the proper data is plotted.

Two steps are involved:

1. *Determination of the offset between the 2 data sets.*

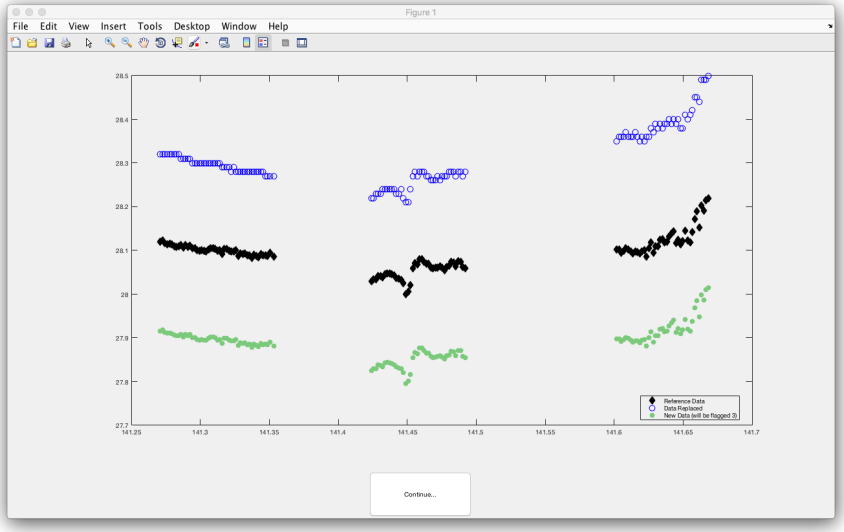
Select one or more areas where the offset seems constant, then right-click and select "Generate Data from Offset --> Determine Offset on Selected X Range"



The offset will be calculated by taking the average of the differences between the 2 data sets over the X range selected, using only FLAG 2 data.
Each data set is plotted on a different y-axis. The offset is the average of (RIGHT axis - LEFT axis).

2. *Generation of data by applying the calculated offset*

Once an offset is generated, it can be applied to any data, provided the following:
- The offset will be applied to the data on the ACTIVE graph.
- The data to be replaced has to be on the INACTIVE graph.



- Pay attention to the sign of the offset shown in the menu. It is opposite, wether you apply the offset on the LEFT axis data or the RIGHT axis data. In other words, the offset determined in step 1 is always added to the left-axis data and subtracted to the right-axis data.

Select the area containing the reference data
Select “Apply Offset (~ x.xxx) on Selected Data”.

Note: If the data plotted is not the same as that used to generated the offset, a warning will let the user know, but won't prevent the use of the offset.

A graph will pop up showing the reference data and the new data generated from it. Click "Continue..." and choose whether to accept or not the generated data with the pop-up dialog that follows.

NOTES:

- This features can work with the following variables:
  EQU pressure (measured, not calculated as when differential)
  EQU temperature, IN SITU temperature (measured AND interpolated)
  Latitude, Longitude
  Water flow, gas flow
  LICOR pressure, LICOR temperature
  LICOR xCO2, xH2O
  Salinity , ATM pressure
  cpu, Deck Box, and condensor temperatures.

- The generated data is flagged differently, depending on its kind:

Generated Data	Type flagged	Flag	Subflag
in situ temp* (meas. and interp.)	EQU only	3	"questionable/interpolated SST"
EQU temp	EQU only	3	"questionable/interpolated eqT"
LICOR P	EQU and ATM	3	"questionable/interpolated P"
ATM P	ATM only	3	"questionable/interpolated P"
Salinity	EQU only	user	"questionable/interpolated S"
other	EQU and ATM	3	"Other/see metadata"

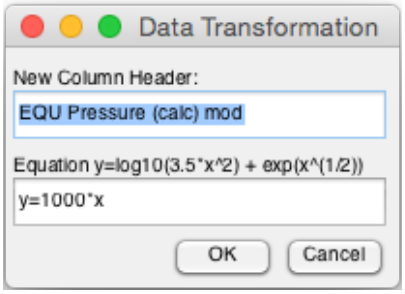
* see note below

- Issue with generating IN SITU temperature.

To account for the time it takes the seawater to reach the system, the measured SST values are offset in time and then interpolated to the time of the pCO2 measurements (see "Offset between In situ T and EQU T" section below). When estimating SST from another temperature, it is the interpolated values that should be generated. But these are calculated by the program from the SST measurements so ideally, one would like to generate SST measured values which, when offset and interpolated, would give the right temperatures. Since I didn't know how to do this programmatically, I just generate the SST values directly, taking the time offset into account. After doing that, the ΔT calculated is not exactly the offset that was applied to the other temperature record but it is close.

Data Transformation.

This refers to the process of applying an equation to a data column and thus generating a new column. This could be useful to change the units of the column, e.g. bar to mbar. The new column header will have " mod" added to it.



Right-clicking on a graph will bring up a popup window asking the user to enter the new column header and the equation to apply.

The equation can be any expression that Matlab® understands:

- It should be written in the form y=f(x)
- It recognizes the regular operators: +, -, *, /, ^
- Some useful functions: log, log10, exp

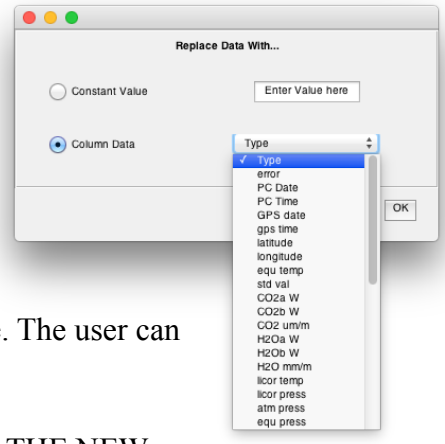
The equation will be applied to the ACTIVE GRAPH, as indicated by the suggested new column header which is derived from the data that will be used.

Data Replacement.

It is sometimes necessary to replace part of a data record (missing or problematic data) with data imported from another instrument or a constant value (as in the case of salinity for example).

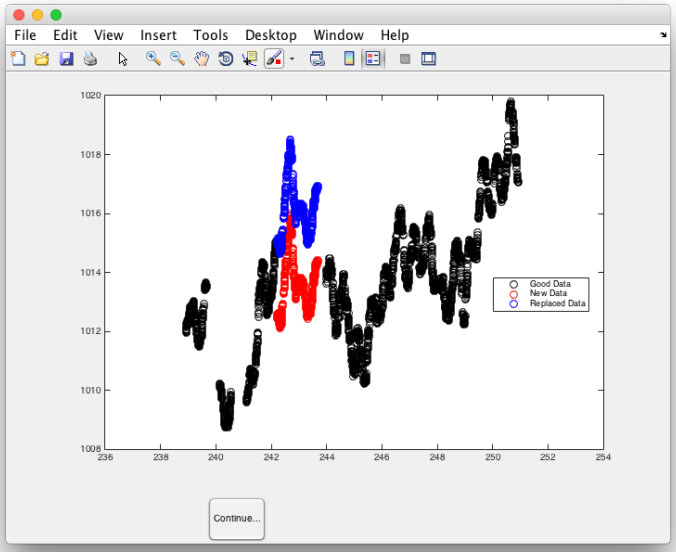
To do so:

- Draw a rectangle area encompassing the data of the ACTIVE GRAPH to replace.
- Right click anywhere on the graph and select 'Replace Data With…'.
- Select "Constant Value" or "Column Data" and either enter value or select the 'File Column' to use. Click OK.



- The program will plot the old and new data look like. The user can accept or reject the replacement.

- THE ORIGINAL DATA WILL BE REPLACED BY THE NEW ONE.



- After the replacement, the user is asked whether the data should be flagged automatically or not.
- If the user selects to flag the data automatically and the data is assigned to either a Temperature, Pressure or Salinity, it will be flagged 3 with an appropriate subflag: 'Questionable/Interpolated' X where X can be either "SST", "EqT", "SSS", or "p".
- If the same column of data is assigned to more than one of the SSS, SST or EqT variables, the user will be asked which subflag to apply.
- If the user selects NOT to flag the data automatically or if the data is neither a temperature, pressure or salinity, IT WILL NOT BE FLAGGED AT ALL.
- One cannot replace calculated data. A message will pop up when that is the case and the user should replace the original data it is calculated from.
- Only the data shown on the graph is used for the replacement.
- Some flags are only applied to some types (e.g. quest. SSS only applied to EQU) (See Flagging Data section)

It is strongly suggested to do the replacement at the beginning of the data reduction, before doing the range check and despiking.

Erase SubFlag…

The user can remove the sub flags on selected points.

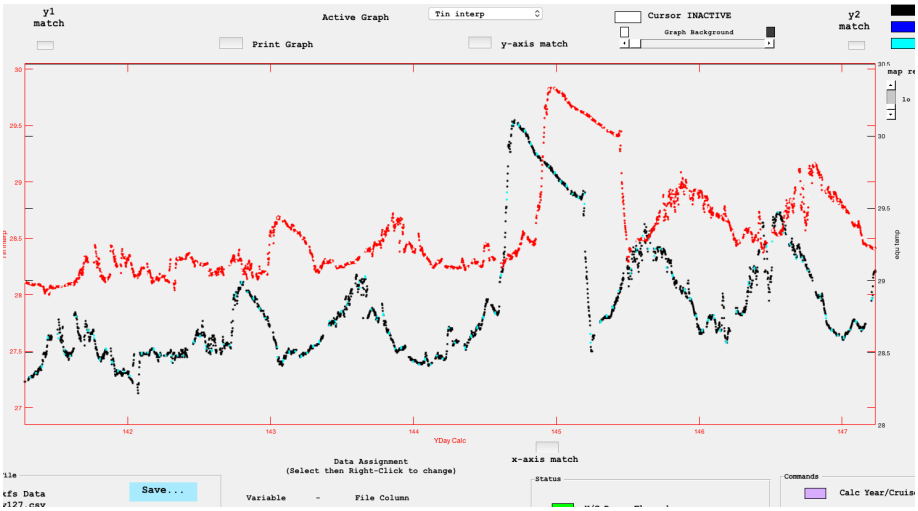
- First, the data needs to be selected by drawing one or more rectangles around it
- Right-Click anywhere on the graph and select 'Erase SubFlag…'

- Select Subflag to be removed from the control on the popup, then click OK.
- A popup will give the tally of sub flags changed as well as the number of points whose flag 3 had been changed back to 2 (see note below).

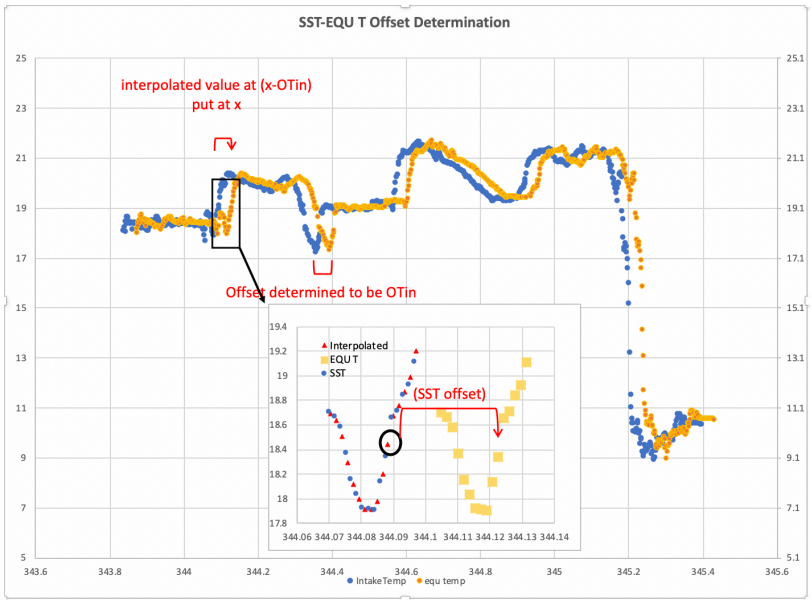
NOTE: Points can have several sub flags as they can be flagged for different reasons. If a point has its only sub flag removed, its flagged 3 will be changed to 2.

Offset between In situ T and EQU T.

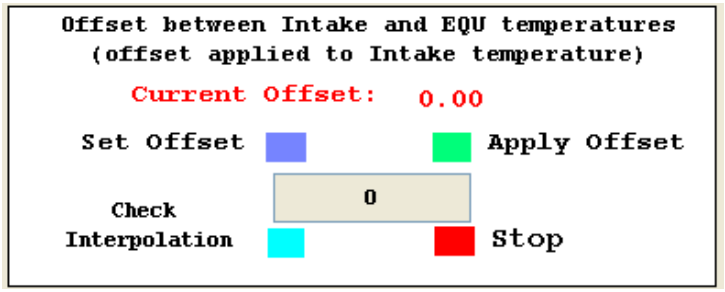
In most installations, the seawater flowing through the system needs to travel a while before reaching the system. At the time of measurement, the temperatures for the equilibrator and the in situ will refer to different waters and therefore could have different values, which could lead to unrealistic offsets between the two. A correct offset is important as it determines the temperature correction to apply to the fugacity. An example is shown below. The offset is evidenced by the peaks not matching.



The program can help the user evaluate the offset between the two.



The value of the offset, shown in MINUTES in the box, is applied to the IN SITU TEMPERATURE data. That data is then interpolated to calculate the in situ temperature at the time of the equilibrator measurement. The procedure is described below. The section of the interface (top right) used for the procedure is shown here:



1. Check Intake temperature set for bad data. Since the April 2020 version, measured SST data cannot be flagged 4 anymore, only 3. Before generating the interpolated SST data, the user should replace bad SST by "better"data like through interpolation or inference. Interpolated SST data using questionable measured SST data will automatically be flagged 3: 'interpolated using questionable SST' in the working file. In the "FINAL" file, data points will NOT be flagged for questionable measured SST, only for SST values interpolated using that questionable SST.
2. Plot the in situ temperature on the LEFT axis and the EQU temperature on the RIGHT axis. Alternatively, press the "Tin – Teq" preset button.
3. Zoom on a section of the graph which has peaks or features you can use to match the two temperatures. After each zooming, reset the x-axes of the two graphs to the same scale by clicking on the "x-axis match" button below the x-axis.
4. Click on the blue button "Set Offset". The measured SST graph will be shifted by the offset value entered in the numeric box. Using the "hand" tool (ghost toolbar top right of graph), move the in situ temperature graph to match the EQU temperature one. The offset will automatically be calculated and displayed in the numeric box.
5. When the two graphs match, click on the red "Stop" button.
6. The light blue "Check Interpolation" button allows the user to check the interpolated values that will be generated.
7. Click on the green "Apply Offset" button when satisfied with the matching. The offset will be applied to the Year Day values of the in situ temperatures. The temperatures will then be interpolated to the Year Day values for the EQU temperatures so as to have matching data. The new temperatures are saved in the variable called "Tin interp" which is the one used as the in situ Temperature.

NOTES:

- After a non-zero offset has been applied, the SST data used in the preset plots will be the interpolated values ("Tin interp" or Tin(i)). Since this is a calculated value, the manual interpolation of outliers won't be allowed. To access the original SST data, either use the "Plot" button or use the preset plot labeled "Tin & Teq", which will continue to plot the original SST data.
- When the offset is zero, the original SST data, which can be manually interpolated, is plotted in all cases.
- Data interpolated using questionable measured SST data points will be automatically flagged by the program as 'interpolated using questionable SST'. This subflag will be saved in the final file.

fCO_2 calculations

Standard Interpolation.

- The first step in these calculations is to interpolate the standards in order to calculate the value of each standard at the time of the EQU or ATM measurements by LINEARLY INTERPOLATING between two measurements of that standard as a function of Year Day. A graph containing the interpolation for each standard appears for the user to check. The values obtained ('stdx values'; x= 1, 2, 3,..) can also be plotted on the interface.
- The values before the first standard measurement are made equal to the first measurement. The values after the last standard measurement are made equal to the last measurement.
- If a standard value is missing or has been flagged 4, the interpolated standard values before and after the bad value, up to the next set of standards, will be flagged and will not be used to correct the xCO_2 data. If a Standard value is flagged 3, however, it will not affect the interpolated values which will be used to correct the xCO_2 data.
- At the time of the EQU or ATM measurement, the known values of the standards calculated are fitted to a LINEAR EQUATION with respect to the values of the standards interpolated, which is then used to correct the XCO_2 (water) values output by the LICOR.
- The same is done for **the interpolated XCO_2 (air)** values calculated previously.
- When a xCO_2 value is corrected using less than 3 standards, the corresponding xCO_2 corrected values will be flagged 3 and assigned a "corrected with less than 3 standards" subflag. Since xCO_2 cannot be corrected with only one standard, "less than 3" means "2".
- The interpolation of the standard values is **estimated to be good up to 100 ppm outside the range of the standards**. A measured xCO_2 value outside the standard range by more than 100 ppm will be flagged 3 "Out of Standard Range".

pCO_2 .

- For the seawater measurements, the EQU pressure is used, using the LI-COR pressure if the pressure transducer is differential.

- For the air measurements, the ATM pressure corrected for height is used but these values are not reported.

fCO_2 .

It is calculated according to Weiss, 1974.

$$fCO_2 = pCO_2 f$$

with:

$$pCO_2 = XCO_2 \ (p - pH_2O)$$

$$f = \exp (p (B + 2 \delta_{12})/ R T)$$

- B, first virial coefficient: (valid from 265 - 320 K (-8.15 - 46.85 °C))

$$B \ (cm^3 \ mol^{-1}) = -1636.75 + 12.0408 \ T - 3.27957 \ 10^{-2} \ T^2 + 3.16528 \ 10^{-5} \ T^3$$

- Cross virial coefficient δ_{12}: (valid from 273 – 313K (-0.15 - 39.85 °C))

$$\delta_{12} \ (cm^3 \ mol^{-1}) = 57.7 - 0.118 \ T$$

- R, Gas constant

$$R = 82.0578 \ cm^3 \ atm \ mol^{-1} \ K^{-1}$$

- pH_2O, vapor pressure of water (Weiss, 1980) (T=273 – 313K, S=0-40)

$$\ln pH_2O \ (atm) = 24.4543 - 67.4509 \ (100/T) - 4.8489 \ \ln (T/100) - 0.000544 \ S$$

Temperature Correction.

It is calculated according to Takahashi (1993).

$$\delta \ln (fCO_2) / \delta t = 0.0423 \pm 0.0002 \ °C$$

Saving the Data.

The data is saved by clicking the “save data” button. Details have been given earlier in the description of the “Save Data” button in the “Commands Section” on page 26 and can be reviewed here.

Hidden Functions:

Project and Working Directories.

By clicking on the version number (top left corner of the interface), one can display these two directories. It is useful when one searches for the pCO2_Sys_vx.xx.ini file, for example.

Display of DataA array.

By right-clicking on the "Data File" frame title, one can display the content of the DataA array in a new window. The DataA array is the one containing all the imported and calculated data. This is purely for debugging purposes and should not be used by regular users. Changes to that array can have unpredictable consequences. User discretion advised.

LI-7000 firmware 2.0 bug correction.

The LI-7000 firmware version 2.0 had a bug affecting the calculations of xCO2. Licor issued a set of equations to apply in order to correct the values. The program can calculate the new correct values from the old bad ones by plotting the xCO2 values that the LICOR output and selecting "Transform Data" on the Right-Click menu. Instead of typing an equation of the form "y=ax+b", typing "li7000" (not case sensitive) will generate a new data column with the corrected values (the user gets to choose the column header.).
If the transformation is attempted when the LICOR xCO2 values are not plotted, the program will warn the user that it will use the data assigned to the LICOR xCO2 to perform the calculations, if the user agrees.

NOTE: the correction equations are not defined for negative xCO2s so, if they exist, as can happen when measuring a zero gas, they will be replaced by 0. This also applies to Standards, which could then slightly affect the xCO2 correction.

Troubleshooting – Error Messages

- *'Cannot find 'pCO2_Sys_vxxx.ini' file in: yyy\zz\ Do you want to search for it? It will be copied over'*

  This file is needed at different levels. Browse for it or create you own using the template given in this manual (see Initial Program Parameters). It will be copied in the project directory once selected.

- *'First line different than expected. config. file possibly compromised. Need new configuration.'*

  The first line in the Configuration file is not what it supposed to be. Re-assign all the variables through the interface and click on the 'Save Config' button.

- *'Date seems to be in wrong FORMAT (Here is the first good date value: xx.xx.xx hh.mm.ss). Select proper format or correct in data file..'*

  An error occurred when trying to calculate the Year Day, most likely because it detected a month greater than 12. Dates can only be in one of 3 formats: mm/dd/yy (US), dd/mm/yy (Euro or a number ##### (Excel). Try another format when prompted or fix in the file . GO/Neill pCO_2 systems have the US format.

- *'No Date or Time column selected'*

  Year Day calculations need Date and Time data. This error comes up if those variables are not assigned to any column from the data file.

- *'Can't figure out Date format. YDay Calculation aborted!'*

  Dates in Excel can be based on either 1900 or 1904. The program will try both, asking the user if the dates look reasonable. If not, this message will appear.

- *'Data spans at least 2 different years. Data will be plotted versus cruise day'...*

  When the data crosses new year's day, the data plotted versus Year Day would not look right as adjacent records in time would go from YDay 365 to 1 and would show at both ends of a graph. When the data spans 2 different years, a 'Cruise Day" is calculated and used for plotting (see Calc Julian/Cruise Day above).

- *'No Area found'*

  Could not find a rectangle to delete. Probably due to a bug in the program.

- *'No points plotted yet!'*

  Occurs when trying to activate the cursor without any points on the graph. Create a plot first.

- *'No Flags selected'*

  The program needs at least one flag value to plot. Select a flag (2, 3 or 4) to plot at the top of the interface.

- *'No Data Selected'*

  The program cannot find any data to plot. Make sure you select a Type or Flag to plot.

- *'No Standards selected'*

  Error occurs when trying to plot Standard offsets without selecting any standard to plot. Select at least one standard to plot (STD1,STD2, STD3, …)

- *''xxx' cannot be plotted.'*

  Some variables cannot be plotted. These are the 'known values of the standards' and the 'Type' (EQU, ATM…)

- *'variable X cannot be plotted...Data not calculated yet. Use the 'Correct xCO2' button'*

  Variable X refers to:
  - Interpolated Standard values
  - Corrected XCO_2 values

- *'variable X cannot be plotted...Data not calculated yet. Use the 'Interpolated Air xCO2' button'*

  Variable X refers to:
  - Corrected interpolated Air XCO_2 values

- *'variable X cannot be plotted...Data not calculated yet. Use the 'Calc fCO2' button'*

  Variable X refers to:
  - Air and Water fugacities
  - Interpolated Air fugacities
  - Δ fCO_2 (water-air)

- *'No data plotted'*

  Error occurs when the user tries to flag data that is not plotted or tries to interpolate data that is not plotted

- *'No point selected' Or 'No area selected'*

  Error occurs when the user is trying to flag data but no data is in the selection (either under the cursor or in a rectangle area). Can also occur when trying to interpolate data without drawing a rectangle area. The program needs an area to interpolate on.

- *'No Data to interpolate. Check Data or Flags'*

  The interpolation process uses ‘Flag 2’ data. Make sure that the data you want to interpolate with has points that have a flag 2.

- *'Can only interpolate original Data. xxx is calculated. Action Cancelled'*

  The user is trying to interpolate data that has been calculated by the program from original data, such as ΔT or interpolated SST.

- *xxx is not assigned. Select column to assign.'*

  A variable needed for the operation was not assigned a data column.

- *'Problem with (lat./long.) Data. Check Data or Flags'*

  Occurs in the latitude and/or longitude interpolation. The program uses:
  - lat./long. data which is flagged 2 or 3
  - lat./long. data equal to ‘-999’ or ‘0’.

  It uses the former to do the interpolation and replaces the latter with the interpolated values. If no data correspond to either category, the error is displayed.

- *'Couldn’t find missing lat./long. data'*

  Similar to previous error. The program could not find any lat./long. data equal to ‘-999’ (missing data) or ‘0’.

- *'Couldn’t find good lat./long. data'*

  Similar to previous error. The program could not find any good lat./long. data (flagged 2 or 3) usable for interpolation.

- *'Error in STDx known values. Standard Deviation > 0.01. Check data!'*

When the program tries to use the known standard concentrations from the data file, it reads all the values in the data column associated with it corresponding to each Standard type, takes an average and standard deviation of the values for each Standard type. If the column is right, it should just be a repetition of the known standard concentrations and therefore, the sigma for the average value should be close to zero. If it is greater than 0.01, the program assumes that the data column associated with the standard known concentrations has a problem.

- *'Not enough data points for STDx. STD NOT INCLUDED!'*

  if one std has been measured less than 50% of the time of the other standards, it will not be used to correct the xCO_2. This could be the case of a standard only used for zero/span.

- *'Variable X not assigned to a column. fCO2 not calculated.'*

  fCO_2 calculation require values for EQU and ATM pressure, EQU temperature, SST and SSS. If any of these variables is not assigned the program cannot calculate the fugacities.

- *'Either no EQU or no ATM to interpolate from or to. Check your data.'*

  In interpolating air values, the program first selects the data needed:
  - EQU data with flag 2 or 3
  - ATM data with flag 2
  - ATM data with any flag

  This error occurs if no such data is found.

- *'Problem with Data. Interpolation uses only Flag 2" and "Flag 3" which are not a "Questionable Air Value". Check Data or Flags'*

  As a second step in the interpolation of air values, the program also needs the Year Days for EQU with flag 2 or 3. This error occurs if the program cannot find that data.

- *x EQU Points have already been flagged 3 (Other-see metadata) due to missing critical data.',*
  or x Points have already been flagged 4 due to missing position or YDay/Cruise Day data.'
  or 'number of skipped lines other than SHUTDOWN...etc: x

  When loading data, the program checks for missing "Critical Data" in the assigned columns of the following variables: Peq, Teq, Water flow, LICOR t and p, SSS, SST, xCO2, xH2O, Patm and Deck box p. Records with missing data are flagged 3.
  It also looks at the length of each line to determine if it is complete and skips it if it isn't. Lines containing the words "shutdown", "filter", "go to sleep" or "wakeup" (from the GO/Neill system) are skipped automatically.

- *x Points Were Outside the Range of Flag 2 Data and Were Not Extrapolated.'...*

Points to be interpolated need to have good points on both sides (before and after). This message comes up if it is not the case.

References:

"Underway pCO_2 Data Reduction Workshop for 'Neill' Systems". October 5-6, 2005. NOAA/AOML. Miami, Fl.

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Weiss, R.F., Price, B.A., 1980. Nitrous Oxide Solubility in Water and Seawater. Marine Chemistry, Vol. 8, pp. 347-359:

Takahashi, T., Olafsson, J., Goddard, J., Chipman, D.W., Sutherland, S.C., 1993. Seasonal Variation of CO_2 and Nutrients in the High-Latitude Surface Oceans: A Comparative Study. Global Biogeochemical Cycles, Vol. 7, p. 843-878: