CTD Data Processing

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This document discusses processing of the rosette CTD dataset from the 2018 Southampton Island Marine Ecosystem Project (SIMEP). The procedure is based on what Janine and Kate were taught by Pascal, and the SBE Data Processing Manual (https://www.seabird.com/asset-get.download.jsa?id=55174002258). Page 20 of the manual outlines the steps for processing data.

Instrument: SBE 19plus V2 SeaCAT Profiler CTD SN7798 in an SBE 32 Carousel Water Sampler SN32-1173 (Rosette CTD)

Vessel: RV *William Kennedy* and its small boats

Cruise date: August 10-22, 2018

Spatial region: Hudson Bay

Notes: NA

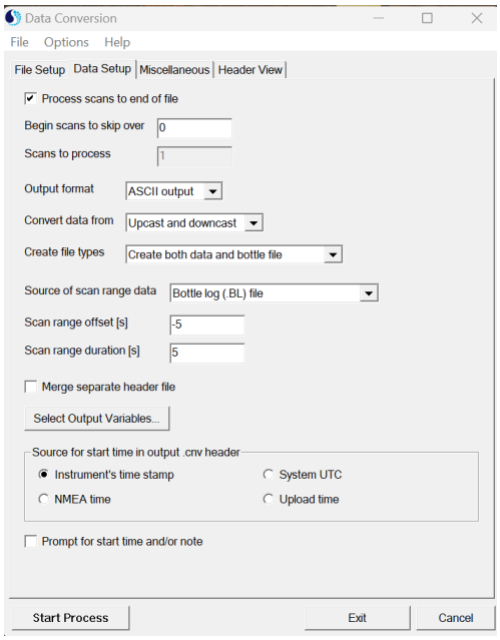
The following steps were taken to process the data:

1. Create the following folder structure:
    a. 2018_wk_ros_ctd_sn7798
        i. logbooks
        ii. originals
        iii. r_scripts
        iv. seabird_psa_and_xmlcon
        v. data
            1. 00_raw
            2. 01_datacnv
            3. 02_section
            4. 03_filter
            5. 04_align
            6. 05_ctmass
            7. 06_loopedit
            8. 07_derive
            9. 08_binavg
            10. 09_split
            11. 10_bottlesum
            12. 11_final
2. Into the logbooks folder, place the ship logbook.
3. Into the originals folder, place all original data from the field (data files, logbooks, calibration files, etc.); zipped to prevent accidental modification.
4. Ensure CTD files all follow the same naming structure, and that the casts correspond to entries in the digital logbook.

5. All .xmlcon files in the raw data were checked. There was a change in configuration after station 7. The .xmlcon files were identical for these stations-casts: 1-1, 1-2, 2-1, 3-1, 4-1, 5-1, 7-1. The .xmlcon files were identical for these stations-casts: 9-1, 10-1, 12-1, 12-2, 22-1, 25-1, 27-1, 27-2, 28-1, 28-2.
   The changes are summarized here:

Changed From	Changed To
SPAR Conversion Units: 5 (quanta/m2/sec) SPAR Conversion Factor: 6.0220e+017	SPAR Conversion Units: 1 (umol photons/m2/sec) SPAR Conversion Factor: 1.6140e+003

   The main .xmlcon file (non-cast specific) aligns with the "changed to" cast-specific .xmlcon files. The main .xmlcon file was checked against calibration documents (except SPAR calibration documents could not be found) to ensure all values were correct. For SPAR, the units, conversion factor, and ratio multiplier were compared against the 2023 .xmlcon file, and the values were very similar. The main .xmlcon file will be used to process the data instead of the cast-specific ones so that SPAR is processed the same way for all casts.
6. Convert raw .hex files to .cnv files, and .bl files to .ros files
   a. SBE Data processing → Run → Data Conversion (#1) → File Setup
      i. Open *01_DatCnv_SN7798_ROSCTD.psa* file from the seabird_psa folder
      ii. Under Instrument configuration file, load the .xmlcon file in the "seabird_psa_and_xmlcon" folder, uncheck "Match instrument configuration to input file"
      iii. Under Input directory, select all .hex files from "00_raw" folder
      iv. Under Output directory, select "01_datacnv" folder
   b. … → Data Setup. The chosen scan range offset and duration mean the software will extract scans from the 5 seconds before each bottle is fired.



      i. Click Select Output Variables…, and choose the following (note that NMEA was not connected this year, therefore coordinates will have to be obtained from the logbook):

a.

Seq. #	Variable Name [unit]
1	Scan Count
2	Descent Rate [m/s]
3	Pressure, Strain Gauge [db]
4	Depth [salt water, m]
5	Temperature [ITS-90, deg C]
6	Conductivity [mS/cm]
7	Salinity, Practical [PSU]
8	Oxygen raw, SBE 43 [V]
9	PAR/Irradiance, Biospherical/Licor [umol photons/m^2/sec]
10	Fluorescence, WET Labs CDOM [mg/m^3]
11	Fluorescence, WET Labs ECO-AFL/FL [mg/m^3]
12	Fluorescence, WET Labs ECO-AFL/FL, 2 [mg/m^3]
13	Voltage 0
14	Voltage 1
15	RS-232 WET Labs raw counts 0

b.

Seq. #	Variable Name [unit]
16	RS-232 WET Labs raw counts 1
17	RS-232 WET Labs raw counts 2
18	Frequency 0
19	Frequency 1
20	Frequency 2
21	Julian Days
22	SPAR, Biospherical/Licor [umol photons/m^2/sec]
23	CPAR/Corrected Irradiance [%]
24	Bottle Position in Carousel
25	Bottles Fired
26	
27	
28	
29	
30	

   c. Click Start Process
      i. Cast 2-1 had an empty .bl file, did not generate a .ros file.

7. Preparing an Excel sheet for taking notes
   a. Open the 01_datacnv folder
   b. Under Type, choose “CNV File” to display only the .cnv files
   c. Select all files (Ctrl+A)
   d. Right click, select copy as path
   e. Go to Excel and paste (Ctrl+V)
   f. Select column A, go to Find & Select -> Replace -> Type out the beginning of the paths in “find what”, and replace with blank. Type “.cnv” and replace with blank too.
   g. Add title row “cast id, start scan, end scan, notes”
   h. Save the file, titled “section.xlsx”, into the logbooks folder
8. Plotting casts

a. SBE Data Processing → Run → Sea Plot (#20) → File Setup
    i. For Program setup file, choose 02_SeaPlot_SN7798_ROSCTD.psa
    ii. For Input directory, select all files in 01_datacnv folder
    iii. For Output directory, select any folder (the plots do not get automatically saved)
b. → Plot Setup
    i. Title: datacnv
    ii. For variables, choose the following:
        1. y-axis: pressure
        2. x-axis 1: scan count
        3. hide other x-axes
c. Click Start Process
d. In the plot window select View → Show Cursor Position
e. Record scan # of beginning of downcast (when the CTD begins a descend after acclimating at ~1-5m depth for some time), and the end of the upcast (just before the CTD comes out of water at the end) for each cast in the Excel sheet you created in the previous step.
    i. Cast 2-1 is a failed cast, will not be proceeding with processing it

9. Cutting out soaking period (must go one file at a time)
    a. In SBE Data Processing: Run → Section (#16) → File Setup
        i. Program setup file: 03_Section_SN7798_ROSCTD.psa
        ii. Input: one cast at a time from 01_datacnv. (Definitely not the most time efficient method but the simplest at this point.)
        iii. Output: 02_section folder
    b. → Data Setup
        i. Section based on: scan count
        ii. Input minimum and maximum value for each cast and click Start Process, one cast at a time
10. Run the 01_section_check.R script to check that correct values were entered in the Section module and that none of the pressure/depth values ended up being negative (indicating measurements in the air).
11. Typically, a pump check R script would be run at this point to ensure that the pump started working before the downcast began (the pump typically only starts working once the minimum conductivity frequency is met and the pump delay elapses). However, there is no information in .hex or .hdr files regarding pump delay. Possibly there was no pump delay, and the pump started working immediately upon the SBE19Plus being turned on. This step is being skipped for this dataset. Only station-cast 28-2 did not have an equilibration period, all other casts had a good equilibration period.
12. Run the 02_sal_check.R to check the minimum conductivity measurements to ensure none of the samples were freshwater, as the processing steps are slightly different from seawater. SBE said in personal communication that the rough threshold for freshwater for data processing purposes is 0.6 S/m, i.e., 6 mS/cm.
    a. No casts were flagged.
13. Filtering

a. SBE Data processing → Run → Filter (#2) → File Setup
    i. Program setup file: 04_Filter_SN7798_ROSCTD.psa
    ii. Input directory: 02_section folder (all casts)
    iii. Output directory: 03_filter folder
b. → Data Setup
    i. Low pass filter A, time constant (s): 1.0
    ii. Low pass filter B, time constant (s): 0.5
    iii. Specify Filters…
        1. Clear all
        2. Pressure, Strain Gauge (db): Low pass filter A
        3. Temperature (ITS-90, deg C): Low pass filter B
        4. Conductivity (mS/cm): Low pass filter B
c. Click Start Process

14. Align CTD (advance parameters in time relative to pressure)
    a. SBE Data processing → Run → Align CTD (#3) → File Setup
        i. Program setup file: 05_Align_SN7798_ROSCTD.psa
        ii. Input directory: 03_filter folder (all casts)
        iii. Output directory: 04_align folder
    b. → Data Setup → Enter Advance Values
        i. Clear all
        ii. Temperature (ITS-90, deg C): +0.5 seconds
            1. This is the recommended value for SBE19plusV2 in the data processing manual
        iii. Conductivity (mS/cm): +0.5 seconds

            1. Note that the manual gives contradicting statements. First statement is: "For an SBE 19plus or 19plus V2 with a standard 2000-rpm pump, do not advance conductivity." Second statement is: "If temperature is advanced relative to pressure and you do not want to change the relative timing of temperature and conductivity, you must add the same advance to conductivity."
            2. Pascal applies a +0.5 second advance to both temperature and conductivity, Pascal's method will be followed.

        iv. Oxygen raw, SBE43 (V): no advance
            1. The data processing manual suggests +3 to 7 seconds for an SBE19Plus
            2. Janine noted that this only works if the Oxygen raw, SBE43 (V) variable is being aligned. Janine tried several delays and the 0s delay seemed best for 2021 data.
            3. Pascal noted that at the beginning, he tried to estimate the right correction. You need to remove the gap between the downcast and upcast because of the long sensor response time. When you are going to apply a correction, you shift all oxygen values X seconds below their original place. Therefore, if you are moving at a speed of 1m/s, a +5 second shift would shift all values 5 m below where they were recorded. For oceanic waters with little variation, this could be okay. But for Arctic

waters with chlorophyll maxima and oxygen peaks, this could create a big shift between these two events (SCM and O_2 peak). In Pascal's opinion, it is scientifically incorrect to create a gap between SCM and O_2 peak. Pascal either does not apply an oxygen correction, or he applies a 0.5s correction (same as for temperature and conductivity).

c. Click Start Process

15. Cell Thermal Mass

    a. As per the data processing manual, "Perform conductivity cell thermal mass correction if salinity accuracy of better than 0.01 PSU is desired in regions with steep gradients. Note: do not use Cell Thermal Mass for freshwater data."
    b. SBE Data processing → Run → Cell Thermal Mass (#4) → File Setup
        i. Program setup file: 06_CTMass_SN7798_ROSCTD.psa
        ii. Input directory: 04_align folder (all casts)
        iii. Output directory: 05_ctmass folder
    c. → Data setup → Correct primary conductivity values
        i. Thermal anomaly amplitude (alpha): 0.04
        ii. Thermal anomaly time constant (1/beta) = 8.0
    d. Click Start Process

16. Loop Edit (flags scans with very low and backward velocity)
    a. SBE Data processing → Run → Loop Edit (#5) → File Setup
        i. Program setup file: 07_LoopEdit_SN7798_ROSCTD.psa
        ii. Input directory: 05_ctmass folder (all casts)
        iii. Output directory: 06_loopedit folder
    b. → Data Setup
        i. Minimum velocity type: Fixed minimum velocity
        ii. Minimum CTD velocity (m/s): 0.05. Note that Pascal recommended using velocity < 0.1 m/s (as opposed to the SBE recommended 0.25 m/s).
        iii. Uncheck "Remove surface soak"
        iv. Check "Exclude scans marked bad"
    c. Click Start Process

17. Derive (computes thermodynamic properties based on EOS-80 (practical salinity))
    a. SBE Data processing → Run → Derive (#6) → File Setup
        i. Program setup file: 08_Derive_SN7798_ROSCTD.psa
        ii. Instrument configuration file: 19-7798 - with SPAR.xmlcon
        iii. Input directory: 06_loopedit folder (all casts)
        iv. Output directory: 07_derive folder
    b. → Data Setup → Select Derived Variables

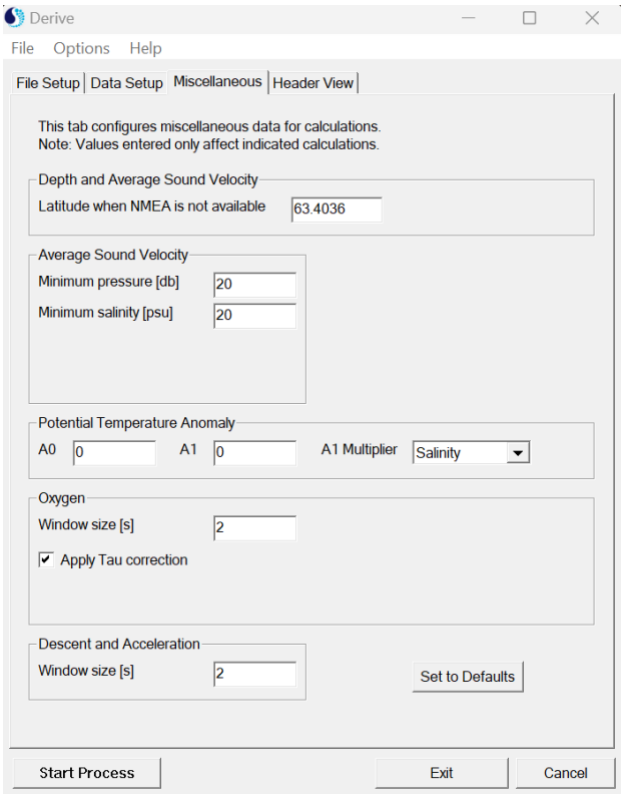
i.

Select Derived Variables

Seq. #	Variable Name [unit]
1	Density [density, kg/m^3]
2	Density [sigma-theta, kg/m^3]
3	Depth [salt water, m]
4	Oxygen, SBE 43 [ml/l]
5	Oxygen, SBE 43 [umol/kg]
6	Oxygen, SBE 43 [% saturation]
7	Potential Temperature [ITS-90, deg C]
8	Salinity, Practical [PSU]
9	Specific Volume Anomaly [10^-8 * m^3/kg]

c. → Miscellaneous

i. Latitude when NMEA is not available: average starting latitude of all casts present in the merge_key.xlsx (63.4036)



d. Click Start Process

e. Optional step that was not done: Use Derive TEOS-10 (absolute salinity) module to derive variables based on TEOS-10.

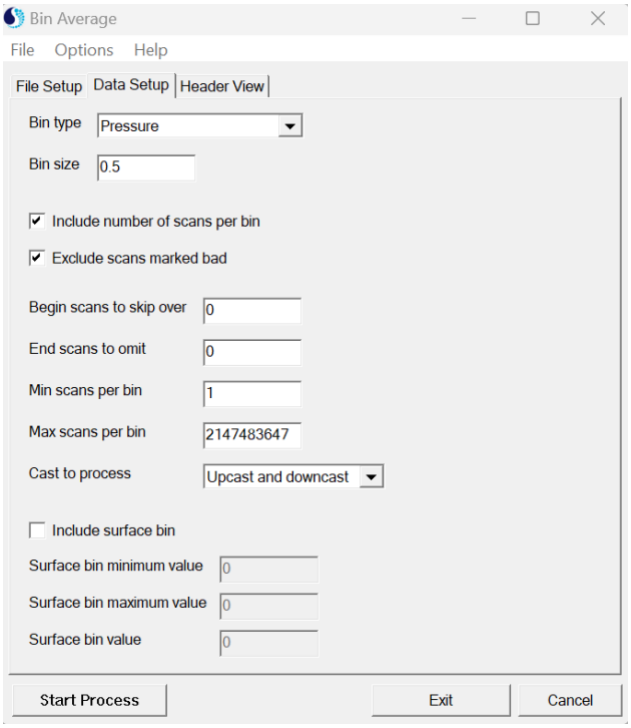
18. Bin Average

a. SBE Data processing → Run → Bin Average (#8) → File Setup

i. Program setup file: 09_BinAvg_SN7798_ROSCTD.psa

ii. Input directory: 07_derive folder (all casts)

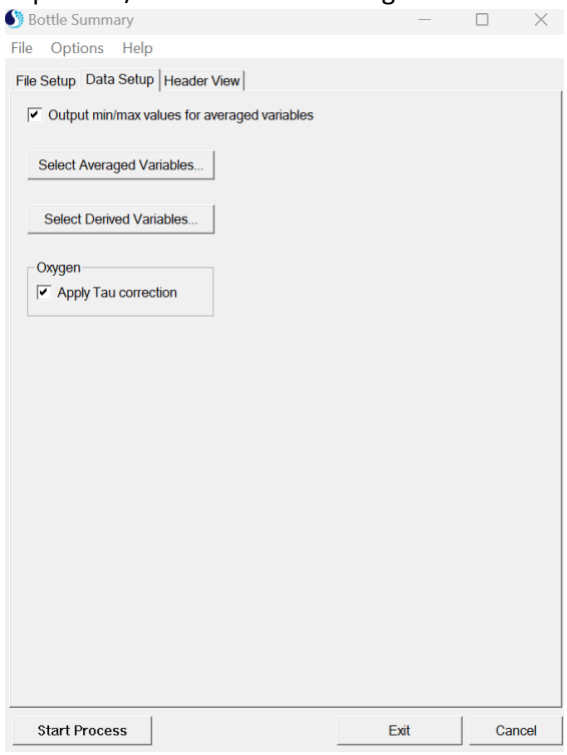
iii. Output directory: 08_binavg folder

b. → Data Setup
    i. Bin type: Pressure
    ii. Bin size = 0.5
    iii. 

c. Click Start Process

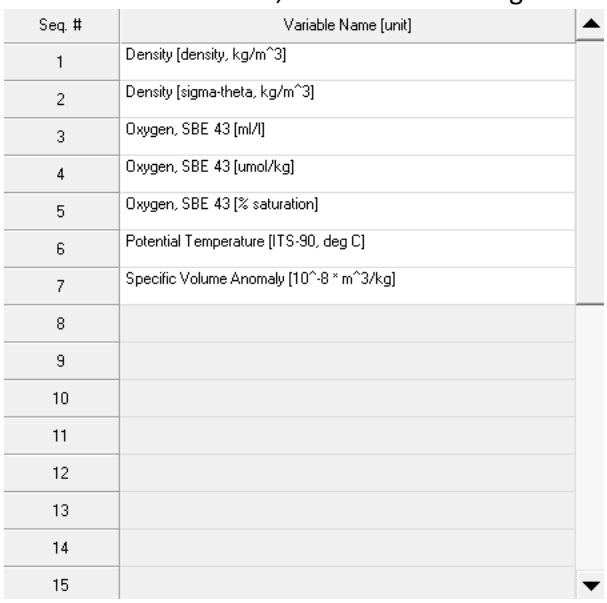
19. Split (splitting the downcast from upcast)
    a. SBE Data processing → Run → Split (#17) → File Setup
        i. Program setup file: 10_Split_SN7798_ROSCTD.psa
        ii. Input directory: 08_binavg folder (all casts)
        iii. Output directory: 09_split folder
    b. → Data Setup
        i. Output files: upcast and downcast (it will rename each file for downcast with a "d" and upcast with a "u" in front of the file name)
        ii. Check "Exclude scans marked bad"
    c. Click Start Process
20. Merging with logbook (using R)
    a. Run the 03_final_file.R script to merge CTD data with the logbook and output Excel and ODV files.
        i. A file named "merge_key.xlsx" was created and saved in the logbooks folder. This file lists which cast filenames correspond to which entries in the logbook
21. Create bottle files
    a. SBE Data Processing → Run → Bottle Summary (#9) → File Setup
        i. Program setup file: 11_BottleSum_SN7798_ROSCTD.psa
        ii. Instrument configuration file: 19-7798 - with SPAR.xmlcon
        iii. Input directory: select all .ros files in 01_datacnv folder
        iv. Output directory: 10_bottlesum folder
    b. → Data Setup

i. Check Output min/max values for averaged variables

1. 

ii. Under Select Averaged Variables, Select All

iii. Under Select Derived Variables, select the following:

1. 

Seq. #	Variable Name [unit]
1	Density [density, kg/m^3]
2	Density [sigma-theta, kg/m^3]
3	Oxygen, SBE 43 [ml/l]
4	Oxygen, SBE 43 [umol/kg]
5	Oxygen, SBE 43 [% saturation]
6	Potential Temperature [ITS-90, deg C]
7	Specific Volume Anomaly [10^-8 * m^3/kg]
8	
9	
10	
11	
12	
13	
14	
15	

iv. Start Process

22. Create final bottle data file
    a. Run the 04_read_bottle_files.R script to output a user-friendly rosette bottle data file.