CTD Data Processing

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This document discusses processing of the rosette CTD dataset from the 2019 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 5-29, 2019

Spatial region: Hudson Bay

Notes:

- Many errors were found in the rosette bottle files produced by the technician handling these data in 2019. Users are encouraged to no longer use those files.
- SPAR was disconnected after the first two casts.
- Station 7 Cast 2 did not have an acclimation period, and the data manager has reason to believe the CTD pump was not working when the first five bottles were fired.
- Notes arising from scanned copies of rosette logs:
    - It was indicated in rosette logs that NMEA data stream was connected to PC after the first two casts, however, the raw data has no records of NMEA coordinates or NMEA time. Coordinates from the logbook were used in the final files here.
    - Station 12 Cast 1: one of the two bottles fired at 60 meters depth was seemingly not registered in the software. Rosette log indicates all 12 bottles were fired, but bottle file only has record of 11 bottles fired.
    - Station 14 Cast 2: rosette log indicates that bottles 10 and 11 were fired out of order, but this was not observed in the bottle file. Bottle file was not edited as it is unknown why the previous technician believed the bottles fired out of order.
    - Station 15 Cast 2: bottle file did not register bottles 5 through 12 firing. Users can pull data from upcast if needed. Additionally, the rosette log indicates that bottles 1 through 4 were collected at 40 m, however, in the bottle file, bottle 4 was fired at 30 m.
    - Station 23 Cast 2: bottle file registered 13 bottles firing. By looking at the rosette log, four bottles were supposed to be fired at 10 m, but the bottle file indicates that five bottles were fired at that depth, so it is likely that one of those records is erroneous. However, cannot know with certainty which of the bottle records is false by looking at the bottle file alone. Needs further investigation.
    - Station 26 Cast 1: bottle file registered 14 bottles firing. Cannot know with certainty which of the bottle records are false by looking at the bottle file alone. Needs further investigation.

The following steps were taken to process the data:

1. Create the following folder structure:
   a. 2019_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. Based on looking at .xmlcon files, there was a change in configuration after station 10, the SPAR sensor was removed. The .xmlcon files were identical for these earlier stations-casts: 3-1, 3-2, 5-1, 6-1, 7-1, 7-2, 8-1, 9-1, 9-2, 10-1. After the configuration change, the remaining .xmlcon files were identical for the later stations-casts. The main .xmlcon file (non-cast specific) aligns with the earlier cast-specific .xmlcon files with SPAR added.

   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 was also compared to the one used in 2018; they were identical.

   In rosette log scans (scans of rosette sheets filled out by hand by the rosette operator during rosette operations), it is noted on station-cast 5-1 that "casts 1 & 2 of stn 3 did not use NMEA to PC in XMLCON. Will be added for all further casts". The addition of NMEA was not reflected in any cast-specific .xmlcon files, and in the next step, when the data conversion module was run, there were scan length errors for cast 5-1 onwards, confirming that the present .xmlcon files are not compatible with the raw data. Upon further investigation, it was found that SPAR was removed from the rosette configuration following station-cast 3-2, not 10-1 as suggested by cast-specific .xmlcon files.

The main .xmlcon file was zipped and saved to the originals folder. A copy of the main .xmlcon file was modified to include NMEA and exclude SPAR. Station-casts 3-1 and 3-2 will be processed separately using a separate .xmlcon file with SPAR.

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 "Edited 2019 configuration file.XMLCON"
      iii. Under Input directory, select all .hex files in "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.
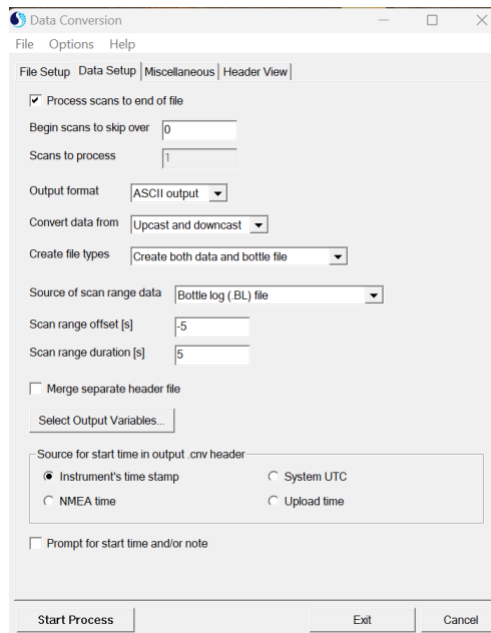
      i. Click Select Output Variables…, and choose the following:

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

a.

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	Bottle Position in Carousel
23	Bottles Fired
24	Latitude [deg]
25	Longitude [deg]
26	
27	
28	
29	
30	

b.

   c. Click Start Process
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. Will not be proceeding with processing the following casts:
> > > > 1. 7-2 (no acclimation period, rosette was lowered to ~2m, held there for a bit, bottles were fired, then rosette was brought back on deck). The .ros file for this cast will be processed further, but the .cnv file will not be.
> > > > 2. 18-2, cancelled cast.
> > > ii. Station-cast 14-1 was "cancelled" due to the rosette line getting caught on ice, but the downcast is still usable, so the cast will be processed further.
> 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. Only station-cast 7-2 did not have an acclimation period (and was not sectioned), all other casts had a good acclimation period.

a. A test pump check (test_pump_check.R) was run with minimum conductivity frequency of 3257, pump delay of 60 seconds, and sample rate of 0.25 (4 samples/second), all casts passed (downcast began after the pump started working), except 7-2.

b. Station-cast 7-2 did not have an acclimation period, and based on the test pump check, the pump did not start working until scan #587. This means that the pump was only working when bottle 6 was fired. For bottles 1-5, the pump was likely not yet working.

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

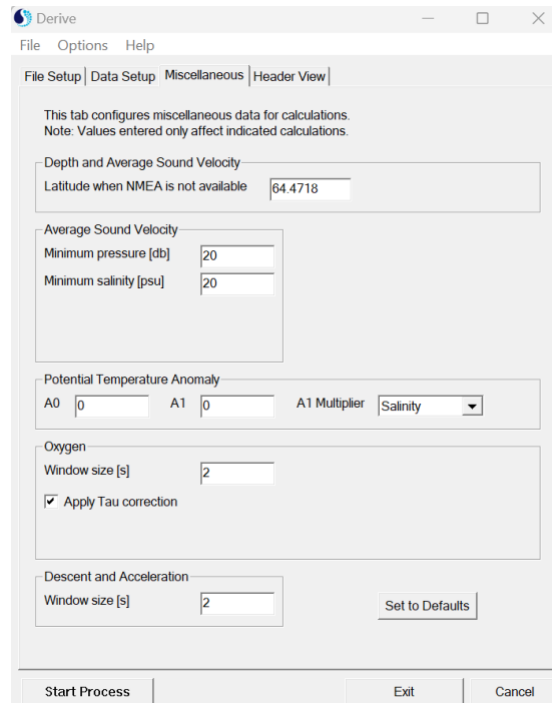17. Derive (computes thermodynamic properties based on EOS-80 (practical salinity))
    a.   SBE Data processing → Run → Derive (#6) → File Setup
        i.   Program setup file: 08_Derive_SN7798_ROSCTD.psa

ii. Instrument configuration file: Edited 2019 configuration file.XMLCON
iii. Input directory: 06_loopedit folder (all casts)
iv. Output directory: 07_derive folder
b. → Data Setup → Select Derived Variables

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]

i.
c. → Miscellaneous

i. Latitude when NMEA is not available: average starting latitude of all casts present in the merge_key.xlsx (64.4718)
   a. When processing Station 3 casts separately, latitude of 63.5214 was used (average starting latitude of both Station 3 casts as seen in the merge_key.xlsx).

Derive

File   Options   Help

File Setup | Data Setup | Miscellaneous | Header View

This tab configures miscellaneous data for calculations.
Note: Values entered only affect indicated calculations.

Depth and Average Sound Velocity
Latitude when NMEA is not available   64.4718

Average Sound Velocity
Minimum pressure [db]   20
Minimum salinity [psu]   20

Potential Temperature Anomaly
A0 0   A1 0   A1 Multiplier Salinity

Oxygen
Window size [s]   2
☑ Apply Tau correction

Descent and Acceleration
Window size [s]   2   Set to Defaults

Start Process   Exit   Cancel

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
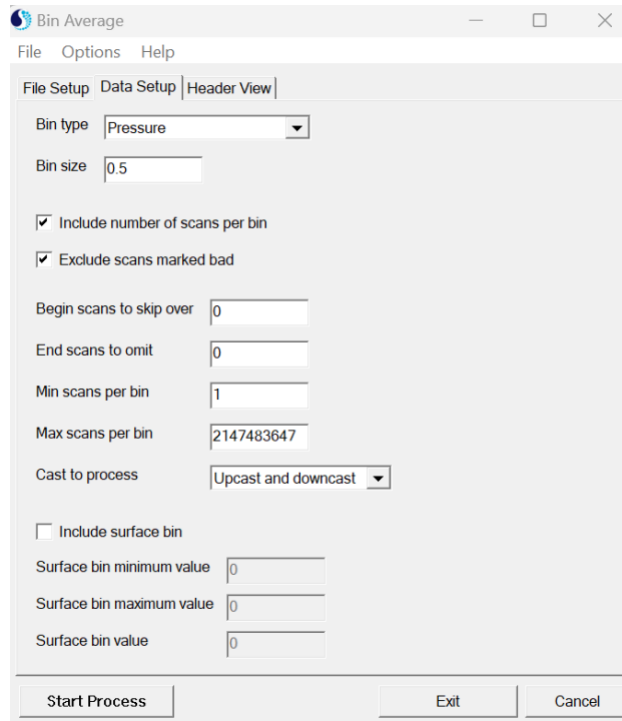
 iii.
c. Click Start Process
19. Split (splitting the downcast from upcast)
 a. SBE Data processing → Run → Split (#17) → File Setup
  i. Program setup file: 10_Split_SN7798_ROSCTD.psa
  ii. Input directory: 08_binavg folder (all casts)
  iii. Output directory: 09_split folder
 b. → Data Setup
  i. Output 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. Follow the same steps to process Station 3 casts in the "12_stn3" folder.
 a. 3-1 scan range for sectioning: 1795-4505
 b. 3-2 scan range for sectioning: 1548-5484
21. 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

ii. It was found that none of the casts actually had NMEA data recorded. NMEA latitude and longitude was 0 for all casts; something must have been wrong with how things were configured on the ship. Logbook coordinates will be used.

22. 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: Edited 2019 configuration file.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
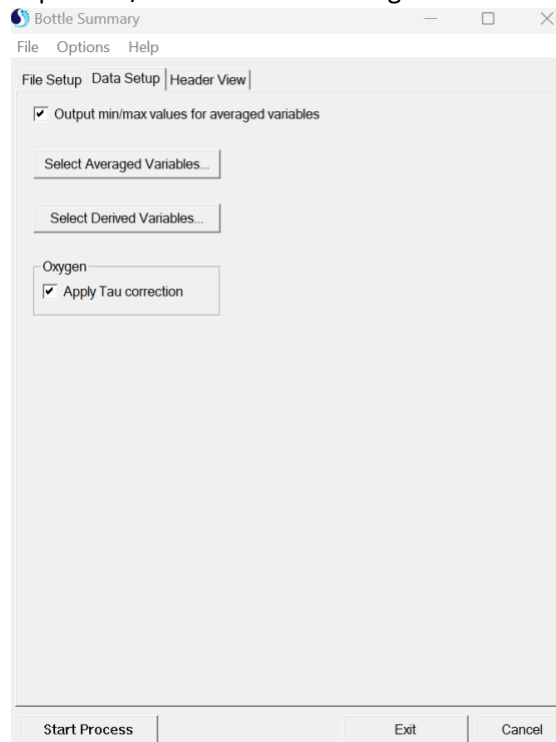
            1.
        ii. Under Select Averaged Variables, Select All, then uncheck Latitude and Longitude given that NMEA data was not actually recorded (see above).
        iii. Under Select Derived Variables, select the following:

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		

         1.

      iv.   Start Process

      v.   Repeat for Station 3 using its configuration file

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