

CEOS Data Management - Seabird TSG Data Processing Cookbook

CENTRE FOR EARTH OBSERVATION SCIENCE



Document Control

0.1 Version History

| Version | Author(s) | Туре | Date Modified | Comments |
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| 1.0 | Hunt, J., Campbell, Y. | Working Copy | | |

0.2 Document Location

A hard copy of the document can be found in the Lab 489 document cupboard.

A digital copy of this document can be found here:

0.3 License

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1 Introduction

1.1 Description

This document outlines the steps for data conversion of Seabird Thermosalinograph data using SBE Data Processing software, and subsequent curation to transform them into standardized CSV files. The initial data processing steps are created specifically for processing data from the SBE 21 instrument collecting flow-through data aboard the RV William Kennedy while it is underway. This is supplementary to the SBE Data Processing manual.

You will need to download SBE Data Processing software to begin processing.

2 Initial Data

2.1 .hex files

Files containing raw data of each cast. Files names should include cruise ID (WKxx_dd-mm-yy) and the download date of the leg (WKxx_dd-mm-yy). For example, WK01_01-08-22 indicates the first leg of cruise #1 was completed on August 1, 2022.

2.2 .xmlcon files

.xmlcon are configuration files needed to convert to the .hex data to a usable format (.cnv).

The .xmlcon file is created by Seabird when the instruments are sent for calibration. It stores the calibration coefficients of the sensors. You do not need to edit it unless there is a change to an auxiliary sensor. Keep it with the raw data.

2.3 creating .cnv files

Open SBE Data processing. Select "Run", "1. Data Conversion", "File setup". Select appropriate instrument configuration file (.xmlcon). Select the input directory where your raw .hex and .xmlcon files are stored. Select all casts as the input files. Select your desired output directory... (see "suggested directory setup?" make a table?—>file source and location...)

Open the "Data Setup" tab. Leave the default settings except for "source for start time in output .cnv header". For this select "System UTC" (Figure 1).

| Data Conversion File Options Help | _ | | \times |
|--|--------------|-----|----------|
| File Setup Data Setup Miscellaneous Header View | | | |
| File Setup Data Setup Miscellaneous Header View Image: Process scans to end of file Begin scans to skip over 0 Scans to process 1 0 Output format ASCII output Image: Convert data from Output format ASCII output Image: Convert data from Convert data from Upcast and downcast Image: Convert data (CNV) file only Source of scan range data Scans marked with bottle constrained on the scans marked with bottle constrained on the scans range duration [s] 0 Scan range duration [s] 0 0 Scan range duration [s] 2 0 Merge separate header file Select Output Variables Source for start time in output .cnv header C Instrument's time stamp Image: System C C NMEA time C Upload | onfirm bit v | | |
| Prompt for start time and/or note | | | |
| Start Process | Exit | Can | cel |

Figure 1. Thermosalinograph data conversion settings

Select output variables (table 1.1).

Table 2.1: Variables to select when creating .cnv files from TSG .hex files

| Variable |
|-----------------------------|
| Scan count |
| Latitude |
| Longitude |
| Temperature (ITS-90, deg C) |
| Salinity (psu) |
| Conductivity (mS/cm) |

Then click the "Start Process" button. The .cnv files will be placed into the output file location.

3 Intermediate Data

The intermediate process involves converting the CNV files produced by the SBE Data processing to CSV files. This was done by using a python script.

For more details on the script, see the TSG codebook on the Datahub here, and the scripts can be found here.

3.1 Overview of script

- 1. Create a loop to read all the cnv files. The following steps are performed for each file.
- 2. Begin reading the CNV file line by line
- 3. Extract the metadata into a dictionary. Metadata are preceded by * in the CNV file
- 4. Write the metadata with XML form into an XML file. XML metadata are preceded by # in the CNV file
- 5. Check for the start date/time tag: *start_time* and extract the date
- 6. Check for the time interval (tag containing the word *interval*)
- 7. Extract the variable names
- 8. Get the actual data
- 9. Create a data frame from the variable names (column headers) and the data
- 10. Calculate a range of dates starting with the start date and interval taken from the cnv file
- 11. Add as a column in the data frame
- 12. Save as a csv file

3.2 File names and variables

Intermediate File Name(s)

- leg1.csv
- leg2.csv
- leg2.1.csv

- leg3.csv
- leg4.csv
- leg5.csv

Intermediate Dataset Variables

- scan
- latitude
- longitude
- t090C
- sal00
- date_time

4 Final Data

4.1 Vocabulary standardization

Column headers are standardized in accordance with the NERC Vocabulary, and units added after an underscore(_). See the converted headers under Dataset Variables below. Once the variables were standardized, a template was created for the final output files, and a python script was used to convert all the intermediate files to the format of this template.

4.2 File names and variables

Final File Name(s)

- leg1_processed.csv
- leg2_processed.csv
- leg2.1_processed.csv
- leg3_processed.csv
- leg4_processed.csv
- leg5_processed.csv

Final File Location

Processed files can be found on CanWIN's Datahub here.

Final Dataset Variables

| Header | Description | Data Type | Units |
|----------------|--------------------|-----------|-----------------|
| scan | Scan count | numeric | None |
| latitude_north | Latitude | numeric | Decimal degrees |
| longitude_east | Longitude | numeric | Decimal degrees |
| WC_temp90_degC | Temperature | numeric | Degrees Celsius |
| P_sal_psu | Practical Salinity | numeric | PSU |
| Cond_S_m | Conductivity | numeric | S/m |
| Date_time | Date and Time | Timestamp | UTC |

Table 4.1: Variables in the final data files

A Reference Tables

A.1 Data Levels

Level 0 – Raw data: unprocessed data and data products that have not undergone quality control. Depending on the data type and data transmission system, raw data may be available within seconds or minutes after real-time. Examples include real-time precipitation, streamflow, and water quality measurements

Level 0.1 – First pass QC: A first quality control pass has been performed to remove out of range and obviously erroneous values. These values are deleted from the record. E.g: Online Environment Canada stream-flow data, laboratory data

Level 1 – Quality Controlled Data: Data that have passed quality assurance procedures such as Level 0.1 and have been further quality controlled by data provider before being submitted to CanWIN (e.g. Idronaut data with only downwelling (upwelling data removed) data included.

Level 1.5 – Advanced Quality Controlled Data: Data have undergone complete data provenance (i.e. standardized) in CanWIN. Metadata includes links to protocols and methods, sample collection details, incorporates CanWIN's or another standardized vocabulary, and has analytical units standardized. Note: Process still under development in CanWIN (as of May 13, 2020).

Level 2 – Derived Products: Derived products require scientific and technical interpretation and can include multiple data types. E.g.: watershed average stream runoff derived from stream-flow gauges using an interpolation procedure.

Level 3 – Interpreted Products: These products require researcher (PI) driven analysis and interpretation and/or model-based interpretation using other data and/or strong prior assumptions. E.g.: watershed average stream runoff and flow using streamflow gauges and radarsat imagery

Level 4 – Knowledge Products: These products require researcher (PI) driven scientific interpretation and multidisciplinary data integration and include model-based interpretation using other data and/or strong prior assumptions. E.g.: watershed average nutrient runoff concentrations derived from the combination of stream-flow gauges and nutrient values.

Content retrieved from https://lwbin.cc.umanitoba.ca on July 06, 2020.

A.2 Result Value Qualifiers

| ADL | Above Detection Limit | |
|---------------|--|--|
| BDL | Below Detection Limit | |
| FD | Field Duplicate | |
| LD | Lab Duplicate | |
| \$ | Incorrect sample container | |
| EFAI | Equipment failure, sample lost | |
| FEF | Field equipment failed | |
| FEQ | Field Equipment Questionable | |
| FFB | Failed. Field blank not acceptable | |
| FFD | Failed. Field Duplicate | |
| FFS | Failed. Field spike not acceptable | |
| Н | Holding time exceeded | |
| ISP | Improper sample preservation | |
| ITNA | Incubation time not attained | |
| ITNM | Incubation temperature not maintained | |
| JCW | Sample container damaged, sample lost | |
| NaN | Value is missing and reason is not known | |
| NC | Not collected | |
| ND | Not detected | |
| NR | Sample taken/measured on site but information in this field not recorded | |
| NS | Sample collected but not submitted | |
| OC | Master Coordinate List Used | |
| Р | Analysis requested and result pending | |
| prob_good | probably good value. Data value that is probably consistent with real phenom- | |
| | ena but this is unconfirmed or data value forming part of a malfunction that is | |
| | considered too small to affect the overall quality of the data object of which it is | |
| | a part | |
| prob_bad | probably bad value. Data value recognised as unusual during quality control | |
| lutown clotod | that forms part of a feature that is probably inconsistent with real phenomena | |
| Interpolated | This value has been derived by interpolation from other values in the data ob- | |
| 0 | ject Below limit of quantification (LOO). The value was below the LOO of the one | |
| Q | Below limit of quantification (LOQ). The value was below the LOQ of the ana- | |
| | lytical method. The value in the result field is the limit of quantification (limit of detection) for the method | |
| | | |

B Glossary of Options and Packages

B.1 R Packages

Visit https://cran.r-project.org/web/packages/available_packages_by_name.html to learn more about R packages

- Package 1 Description
- Package 2 Description

B.2 Python

B.2.1 Python Script-Specific Options

- Option 1 Description
- Option 2 Description

B.2.2 Python Packages

Visit https://docs.python.org/3/library/ to learn more about python packages

- Package 1 Description
- Package 2 Description

Example: Section 2.1 from Victory's semi-hemi codebook