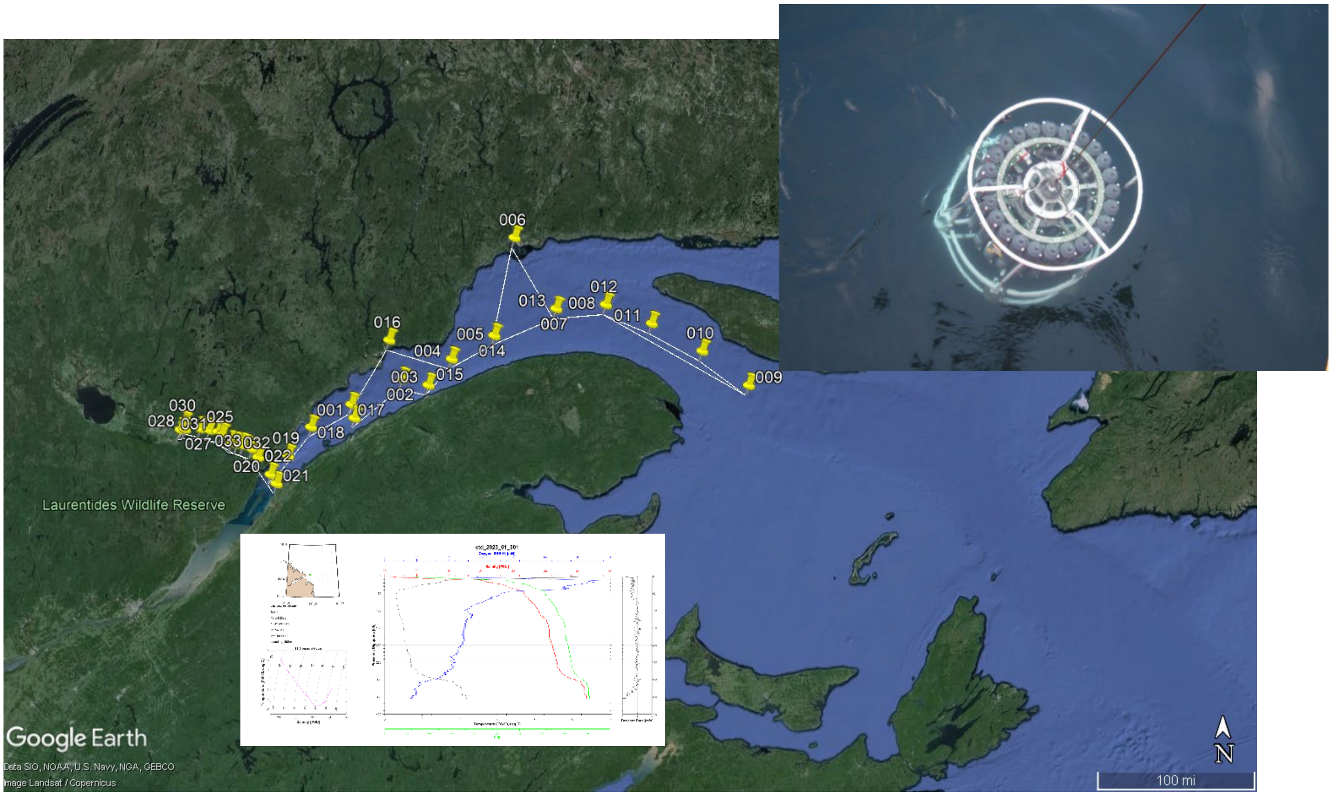
Cruise MAP 2023_13 CTD processing notes



Pascal Guillot
Pascal_Guillot@qo.ulaval.ca

Québec OCÉAN

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Revision History

Date	Description
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Cruise 2023_13 CTD Processing Notes

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1. Foreword.

Québec-Océan and Amundsen Science have developed a procedure to process oceanographic data collected from a Sea-Bird Conductivity Temperature Depth (CTD) sensor (Guillot, 2007). This procedure should ensure that both the quality and the durability of the data are acceptable for scientific use.

The data processing is performed through the “Sea-Bird SBE Data Processing” program offered as free software from Sea-Bird Electronics (Sea-Bird, n.d.). The quality control is mainly based on the GTSPP algorithms (Unesco, 1990) and is performed through the Matlab toolbox developed by the Maurice-Lamontagne Institute, Fisheries and Ocean Canada (OGSL, n.d.).

2. Data preparation.

There are 33 casts recorded with a Sea-Bird SBE 911plus Profiler (24 Hz).

For each cast, several kinds of files are saved:

- hex files: raw data files in hexadecimal format.
- bl files: contain information regarding the bottle firing sequence.
- xmlcon files: the files define the instrument configuration, integrated and auxiliary sensors with the serial number, calibration date and coefficients. This ensures that the right configuration is used for the quality control processing.

2.1. Configuration file checking.

There are 8 sensors (Tables 1 and 2) with an unique instrumental configuration.

Table 1. List of the sensors installed on the SBE 911*plus* CTD during the MAP 2023 cruise.

Sensor	Type and Web link	Unit	Serial number	Calibration date
Temperature	SBE 3plus	ITS-90 deg C	5769 6622	2023-03-14 2022-08-06
Conductivity	SBE 4	mS/cm	4244 6090	2023-03-31 2022-08-05
Pressure	ParoscientificDigiquartz®	db	1168	2023-03-03
Oxygen	SBE 43	ml/l	2766	2023-03-25
pH	SBE 18		1078	2023-04-13
Fluorescence	Seabird ECO	µg/l	FLRT-3363	2023-01-25
Transmissometer	Sea-Bird C-Star (WetLabs)	%	CST-1628PR	2023-04-14
PAR/Irradiance	QCP-2300 Bioshperical	µEinsteins/m^2/sec	70455	2023-01-25

Table 2. Sensor main specifications.

Sensor	Specifications	Values
SBE 3plus	Resolution at 24 Hz Initial accuracy	0.0003 °C at 24 Hz ± 0.001 °C
SBE 4	Resolution at 24 Hz Initial accuracy	0.00004 at 24 Hz 0.0003 S/m
ParoscientificDigiquartz®	Range Initial accuracy Resolution at 24 Hz	0 to 6800 m 0.015% 0.001%
Oxygen SBE43	Range Accuracy	120% of surface saturation 2% of saturation
Fluorescence seabird	Range Sensitivity Fluorescence EX/EM	0.025 µg/l 470/695 nm
Transmissometer WetLabs	Optical pathlength Wavelength Sensitivity Response time	25 cm 650 nm 1.25 mV 0.167 sec

2.2.Metadata checking.

Metadata saving into the logbook, the rosette sheets and the header files are checked and compared. Main problems generally include typing errors, missing errors, difference between pressure and depth. Missing meteorological in the rosette sheet files are updated from the closest data of the validated meteorological data files or the navigation data files. Parameters such as Sea state and Ice could be determined from the Amundsen 3d camera.

2.3.Checking the bottle data summary files (extension btl).

There may be problems concerning the bottle position between the bottle log file (extension bl) and the bottle summary file (extension btl) for some casts.

There is no firing issue concerning this cruise.

3. Data processing.

3.1. Sensor post cruise validation.

First, all the sensors are factory calibrated before the start of the cruise season. To get the highest accuracy data, most of sensor calibration can be performed from field sampling. When field data are not available, the data should be considered with some cares.

Table 3 Field calibration summary.

Parameter	Field calibration	Comment
Salinity	yes	dual sensor system
Temperature	no	dual sensor system
Oxygen	yes	
Fluorescence	yes	
Transmissiometer	no	normalisation to 100%
Irradiance	no	

3.1.1. CTD Oxygen data field validation

Winkler titrations are used to validate SBE43 data. A regression between the two datasets is determined.

The regression shows very good agreement between the 2 datasets (see the following figure). The mean average (see the next table) is very small. The regression was applied to the oxygen data.
The difference between the Winkler titrations and the regression is about 6%.

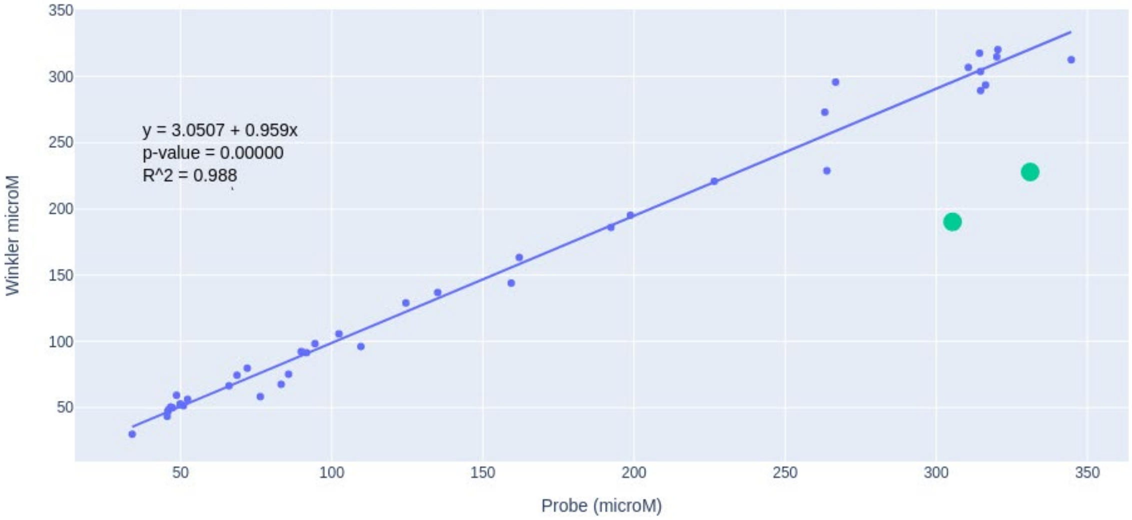


Figure 1 Regression between the probe and the Winkler titration for the cruise MAP 2023 (the green dot are outliers.).

Table 4. Comparison between the Winkler titrations and the SBE 43 data (the fit difference is: (regression-winkler)/winkler * 100)).

Sn	Nb	Original mean and std difference [µM]	Mean and std difference after regression [µM]	Fit difference average [%]
2766	40	8.3±9.0	7.8±8.0	6.4

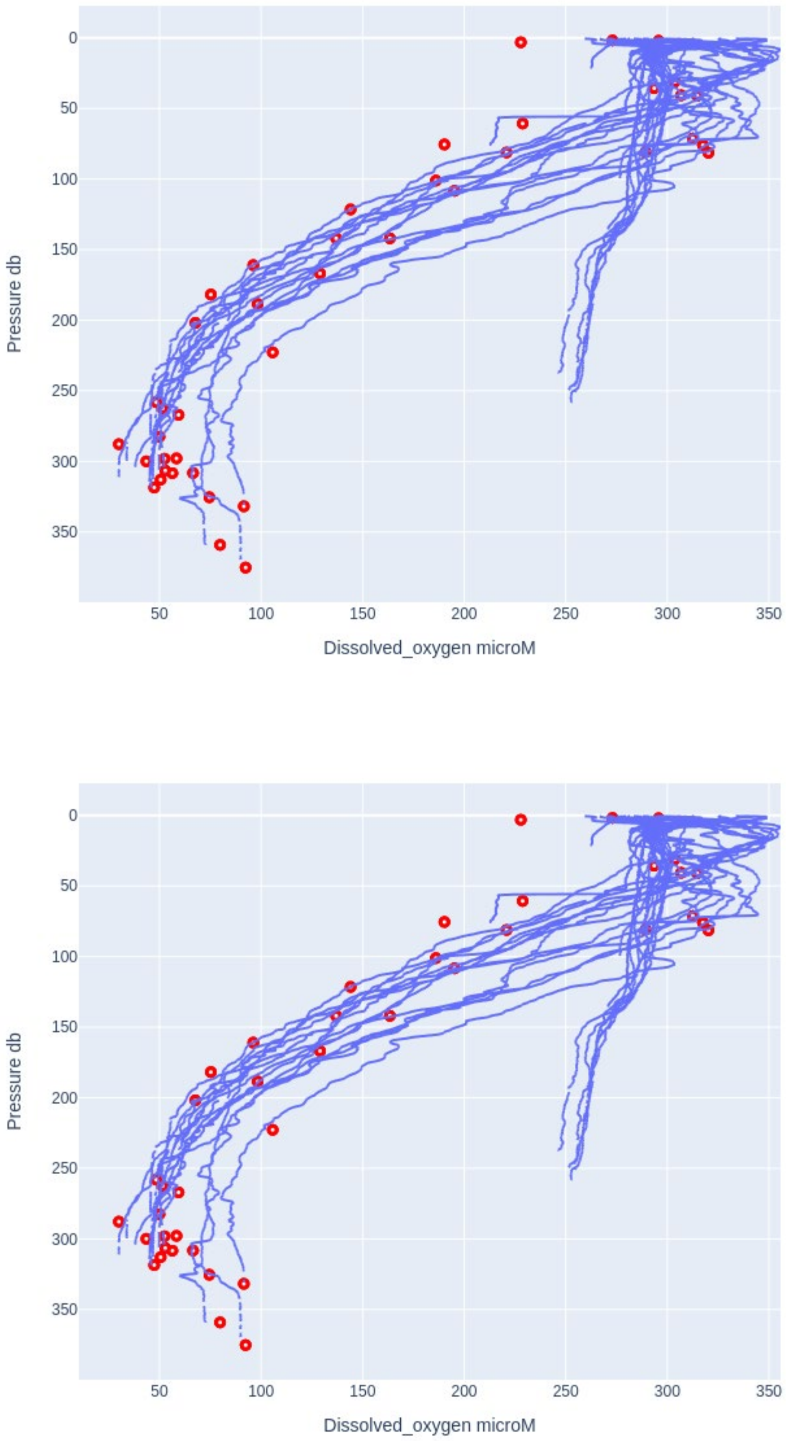


Figure 2 Dissolved oxygen concentrations measured during the 2023_13 cruise. In red bottle titrations, in blue ascending profiles recorded by the SB43 sensor with the original coefficients (top) and optimized coefficients (bottom).

3.1.2. Compute new calibration coefficient for the Wet Labs fluorescence sensor.

It is also possible to post-calibrate the Wet Labs (Seabird) fluorescence sensor from fluorescence concentrations taken from *in situ* samples. The relationship between the output probe voltage and the derived concentration is very simple as following:

$$Output(\mu g/l) = (voltage - Dark\ Ouput) * scale\ factor$$

All fluorometric measurements of chlorophyll *a* (with and without acidification) and Phaeopigments were performed as described by Parsons *et al.* (1984).

It seems that there are 2 modes of profiles: casts 001 to 018 and 019 to 033. The first cast series were recorded in the St-Lawrence estuary and gulf while the second batch was mostly recorded in the Saguenay fjord. The data presents one major issue: the calibration seems inappropriate since the deepest part of the profiles are less than zero. Moreover, the shape of the first profile batch is odd since the minimum value occurred at the base bottom of the subsurface part and so, the concentration at the bottom is higher (see the next figure). This type of odd shape is depicted both on the ascending profiles.

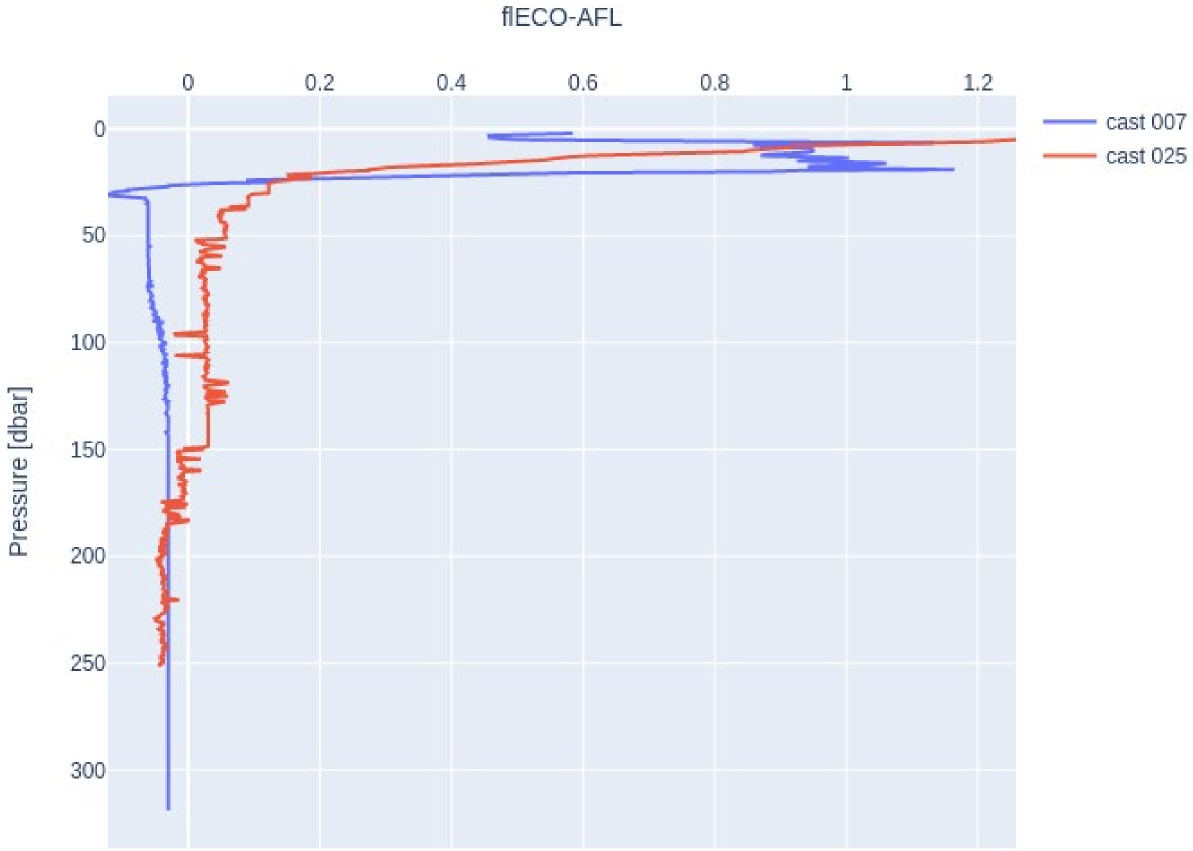


Figure 3 Example of fluorescence profiles depicting the two profile modes: 001 to 018 and 019 to 033.

The regression between the fluorescence titration and the sensor output in voltage shows that there is a good relationship between the 2 datasets for both batches. That suggests the use of the sensor is reliable for this kind of environment and the calibration is suitable even that an offset is requisite to make the concentrations greater to zero.

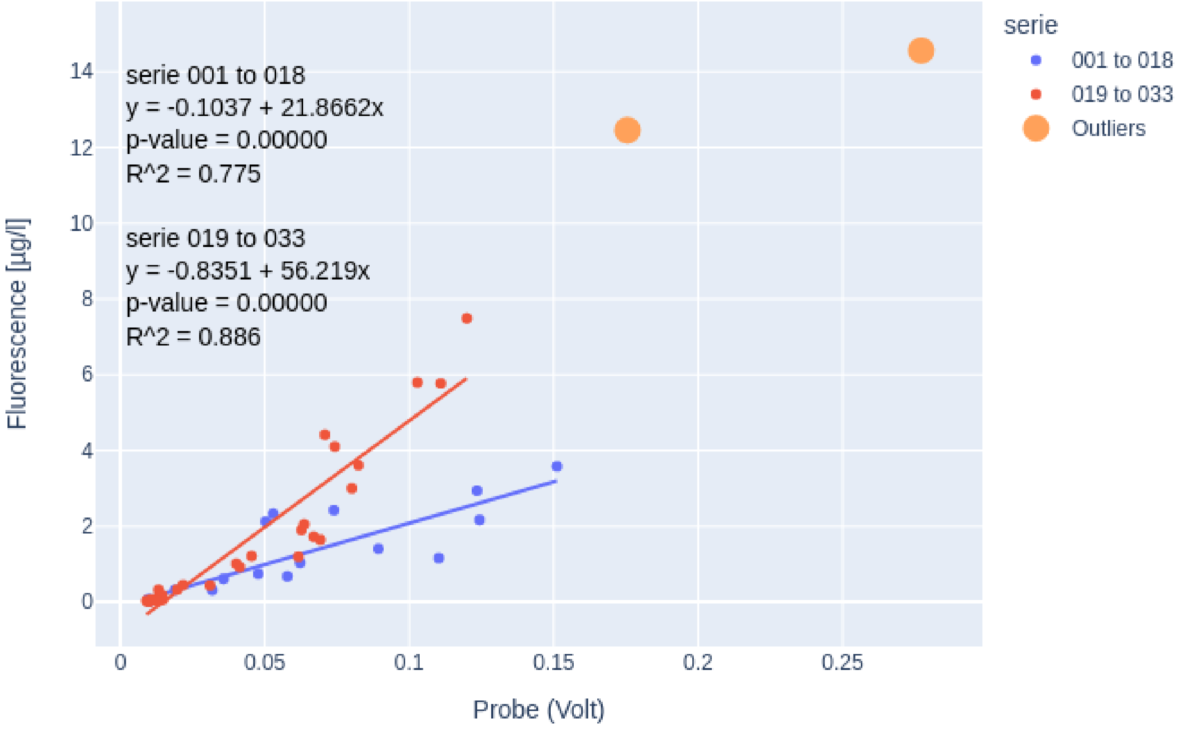


Figure 4 Regression between the probe and the Winkler titration for the cruise MAP 2023.

Several tests were performed to try to improve the sensor data based on the field titrations. Eventually, a simple offset (one per batch) was added to the fluorescence concentrations to reduce the gap between the two datasets and with the “zero signal” at the deepest part. Also, a linear regression between the titrations and sensor concentrations were tested to try to minimise the gap between the 2 datasets. Moreover, a new scale factor was calculated from the titration and tested for the same purpose. The following table shows no optimization allows to improve the CTD data for the casts 001 to 018. On the other hand, both the linear regression and an optimized scale factor allow to reduce the gap between the CTD data and the titrations for the second group of profiles. After a visual check, I decided to keep the new scale factor method.

Table 5 Comparison between the fluorescence titrations and the Wet Labs data.

Serie	Original mean and std difference (µg/l)	Mean and std difference after regression (µg/l)	Mean and std difference with a new scale factor (µg/l)
001 to 018	0.35±0.42	0.34±0.39	0.71±0.84
019 to 033	0.71±1.23	0.52±0.44	0.50±0.62

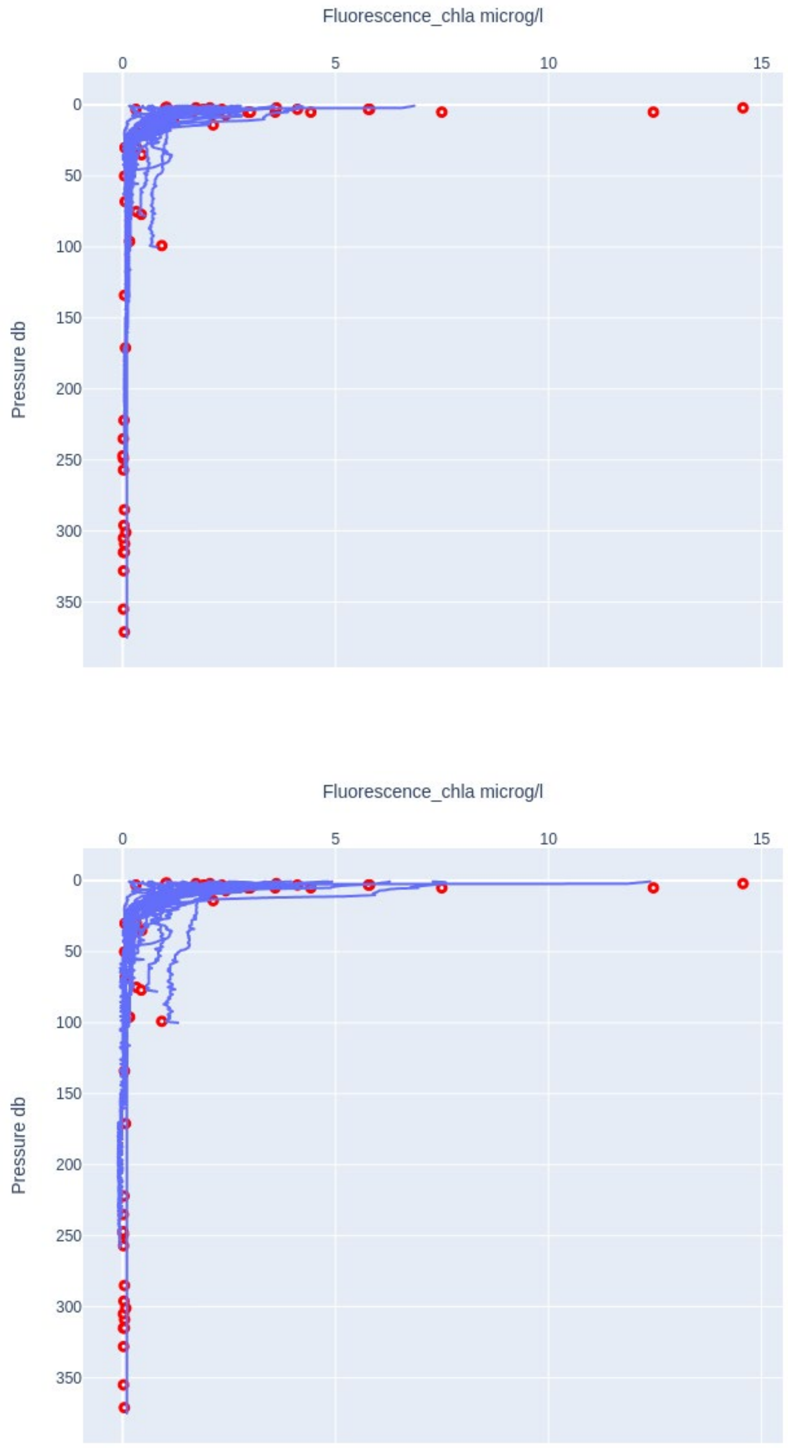


Figure 5 Fluorescence chla concentrations measured during the 2023_13 cruise. In red bottle titrations, in blue ascending profiles recorded by the Seabird sensor with the original coefficients (top) and optimized coefficients (bottom).

3.2.Beam transmission data normalisation.

The C-Star transmissometer measures light attenuation: the maximal signal (100%) is recorded when there is no target through the light beam.

Due to the factory calibration (Seabird 2011), there may be values greater than 100% or more rarely less than 0%. In such case, it is possible to normalize the transmission values using the following equation:

$$ValueN = (ValueO - MinT) * (maxO - minO)/((maxT - minT) + minO)$$

Where:

- ValueN: normalized values according to the target interval minT and maxT,
- ValueO: original values recorded according to the initial interval.

Concerning this cruise, the maximal value is about 102.5 % and so, a small normalization was performed.

3.3.CTD data processing.

This stage concerns mainly the Sea-Bird probe. The typical sequence suggested by Sea-Bird to process 9*plus* CTD data is used.

Table 6 Data processing sequence for the SBE *9plus* instrument.

Module	**Function**	**Parameter**
Data conversion	Convert raw data to engineering unit	Temperature, conductivity, pressure, oxygen voltage, nitrate, transmission, SPAR…
Wild edit	Mark data value with badflag to eliminate wild points	Temperature, conductivity, pressure, oxygen voltage, nitrate, transmission, SPAR…
Filter	Increase pressure resolution	Pressure time constant 0.15 sec.
Align CTD	Advance oxygen in time relative to pressure	Oxygen voltage correction 4.5 sec
Cell Thermal Mass	Conductivity cell thermal mass correction	Alpha 0.03 1/beta 7
Loop Edit	Mark scans with minimum and backward velocity	Minimum CTD velocity 0.1 m/s
Median filter*	Data smoothing	Suna nitrate
Derive	Compute derived parameter	Salinity, density, dissolved oxygen
Bin Average	Average data	Pressure 1 db

*The median filter was used to remove a configuration issue inducing non reliable data.

3.4.Data Extraction.

This stage is applied just after the Sea-Bird “Data Conversion” module. It is particularly useful to eliminate useless data such as those corresponding to the soaking period and to reduce the size of the files. This step is performed through the Matlab software.

In addition, this step allows to detect rare pressure spikes (see next figure for an example). The original values are replaced by the Sea-Bird "bad flag" value (-9.990e-29) into the corresponding Sea-Bird converted files. Pressure spikes are usually associated by unreliable value of other parameters such as conductivity and temperature. Major temperature spikes have an impact upon conductivity data (module Cell Thermal Mass) and upon derived variables using temperature such as salinity and oxygen from SBE43 (see the following figures as example).

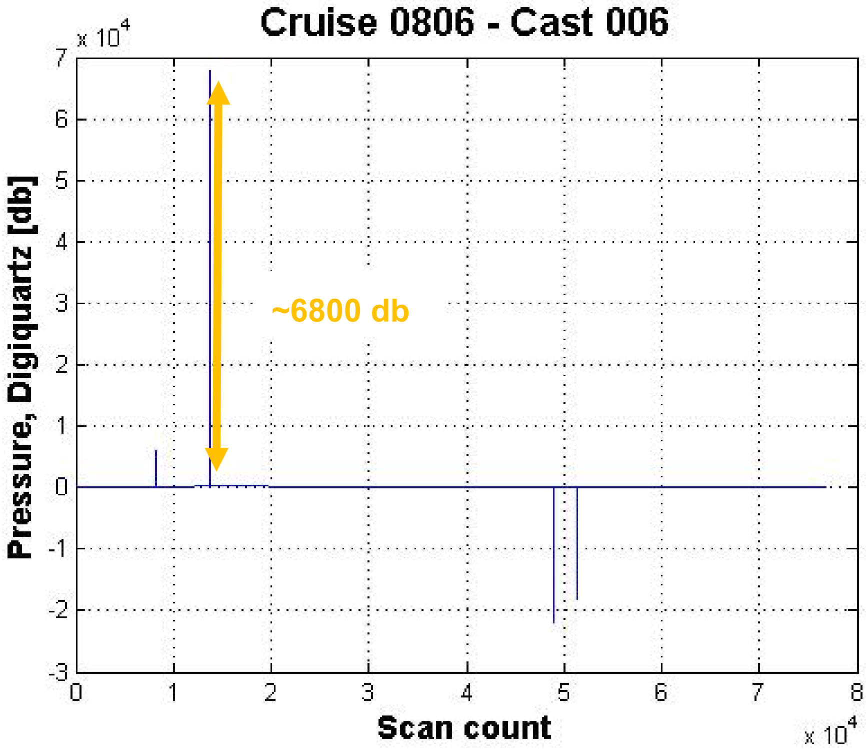


Figure 6. Example of the evolution of spiked pressures.

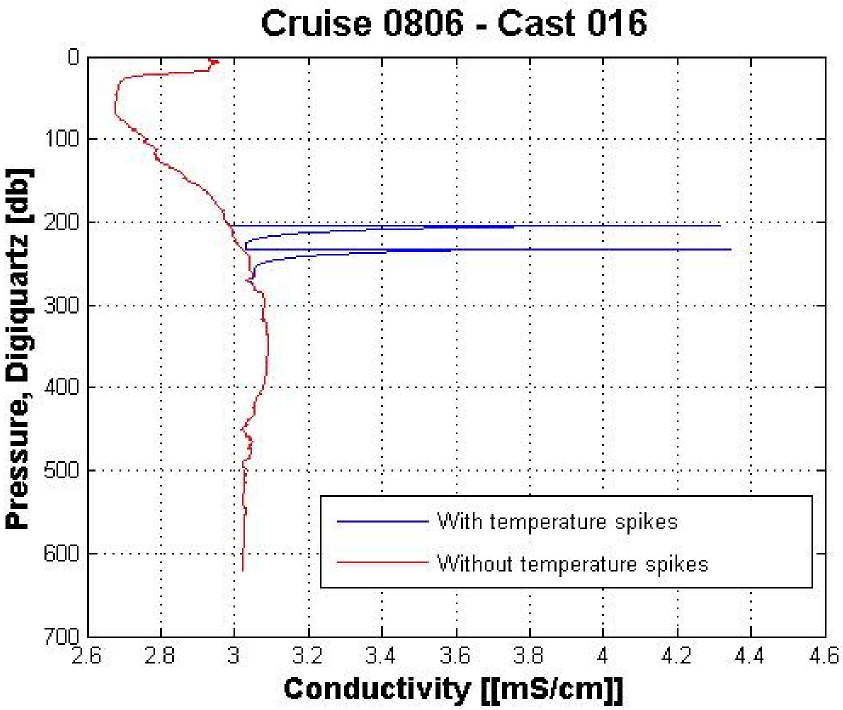


Figure 7 Example of the impact of temperature spikes upon the conductivity variable through the "Cell Thermal" module.

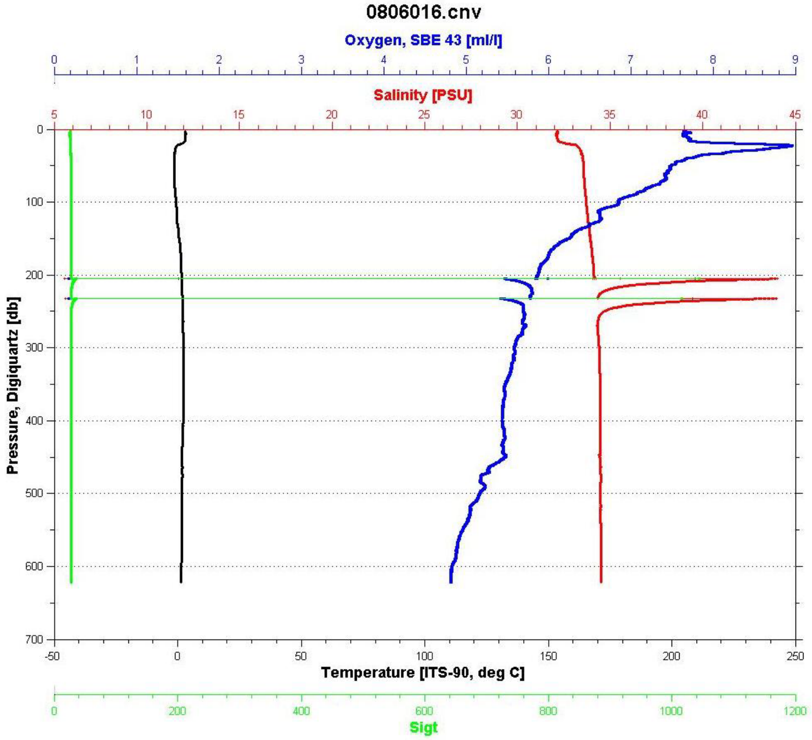


Figure 8 Example of the impact of temperature spikes upon the derived variables such as oxygen, salinity, and density.

4. The data quality control.

Most of the tests are based on the GTSPP ’s tests which are divided in several series. Both metadata (such as time and position) and data values (such as depth, temperature, salinity, and density) are tested.

Additional tests concerning to Sea-Bird CTD (such as pump status and low velocity) have been included.

Other parameters such as oxygen and fluorescence could have been tested to remove doubtful data.

4.1.Causes of irregular and doubtful data.

- The first portion of the data set collected, corresponding to the subsurface (about the first 5 - 10 db), may be characterized by large and sporadic variations or even by large density inversions. It is well known that salinity data is influenced greatly by temperature at low velocities. As such, the best quality data is collected from a 1 m/s CTD descent rate. For some casts in the subsurface, it is difficult to detect if salinity and temperature variations are physically valid or if a low CTD velocity (acceleration from 0 to 1 m /s) causes the data profile.

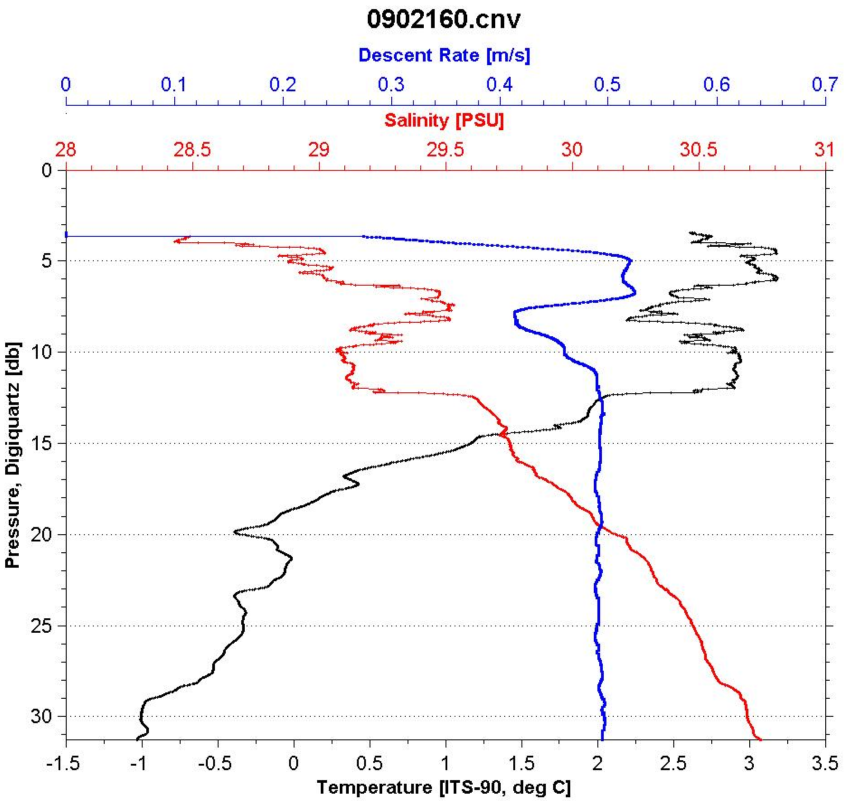


Figure 9 An example of irregular temperature and salinity variations at the surface.

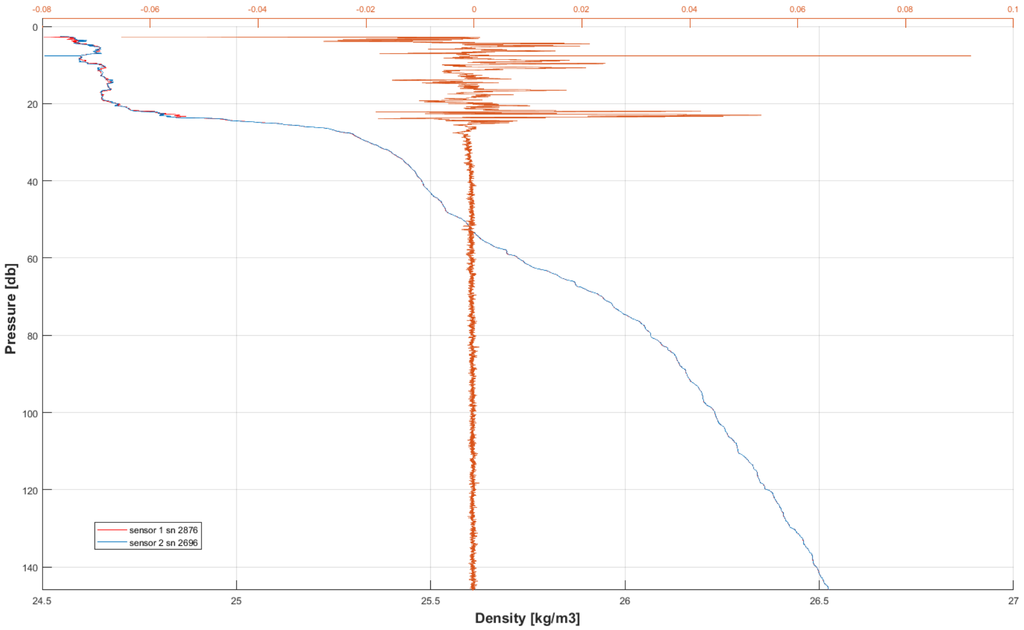


Figure 10 Density difference recorded by a dual conductivity/temperature system.

- At the bottom of the descent, it is common to record noisy data and chaotic variations. These artefacts may often be linked with the CTD deceleration.

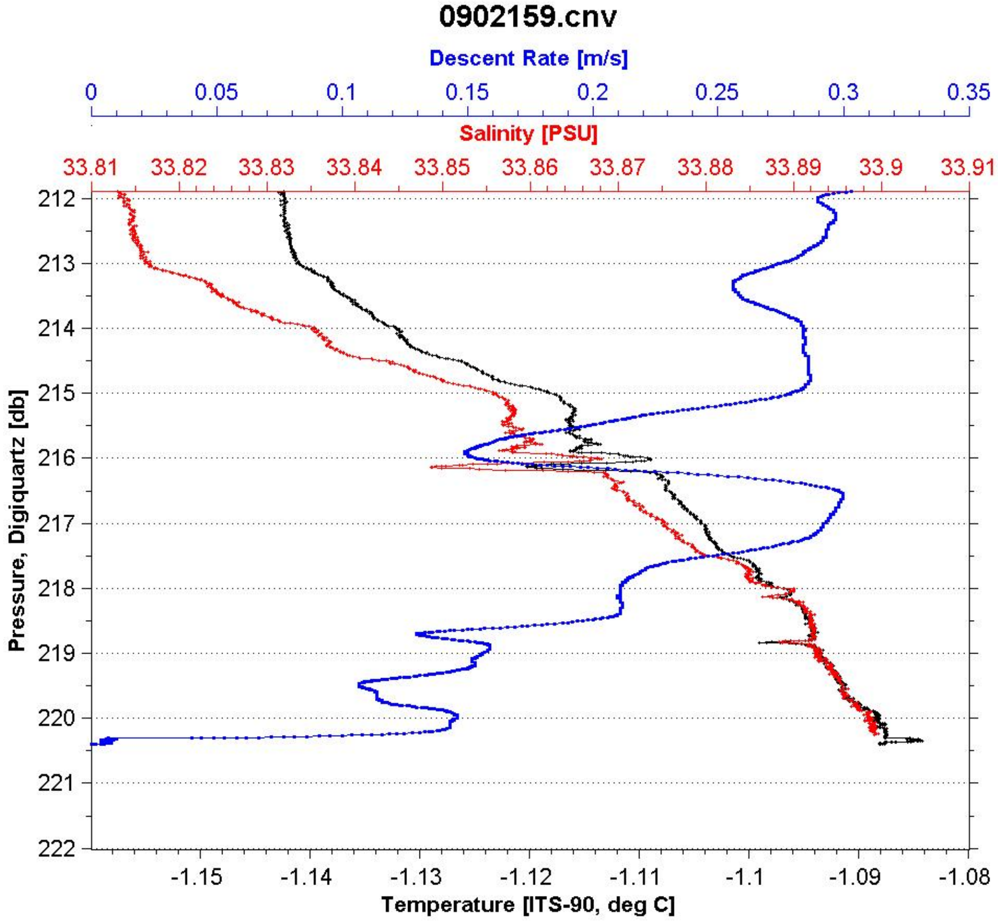
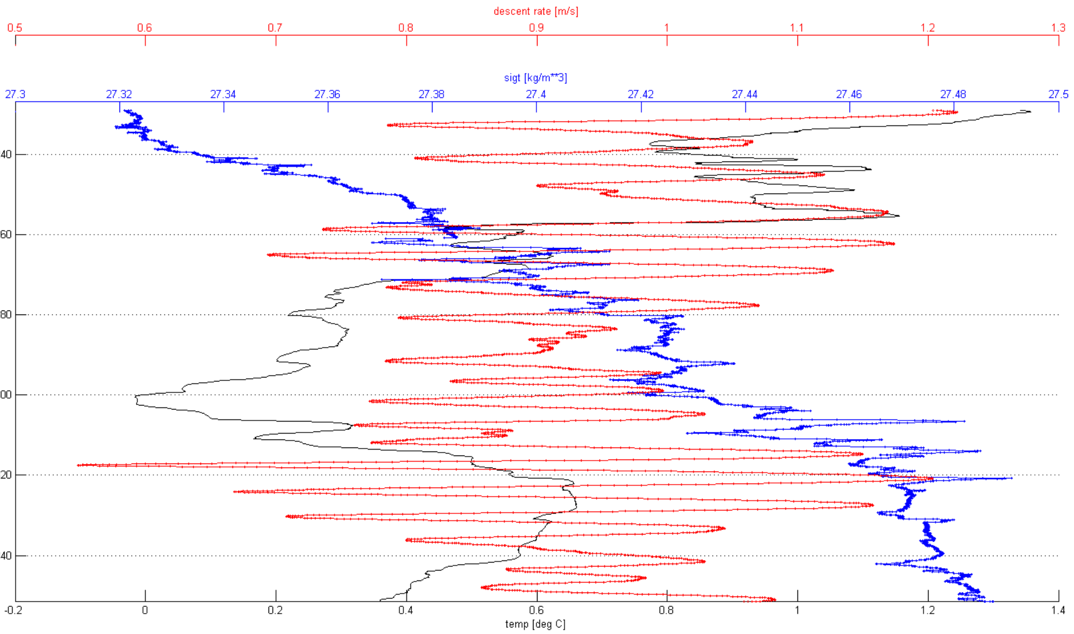


Figure 11 An example of doubtful data occurring during the rosette deceleration at the bottom.

- For some casts, the salinity and density profiles are very noisy, exhibiting large spikes in values. These features may be caused by sensor misalignment and/or irregular CTD/Rosette descent and a succession of thermoclines.



Mois,

Figure 12 An example of salinity spikes coinciding with temperature gradients and irregular descent rates.

- The sea state (specifically the pitch and roll) can have a major impact on the CTD data quality, as the descent is uncompensated from the ship's movement (Figure 15).

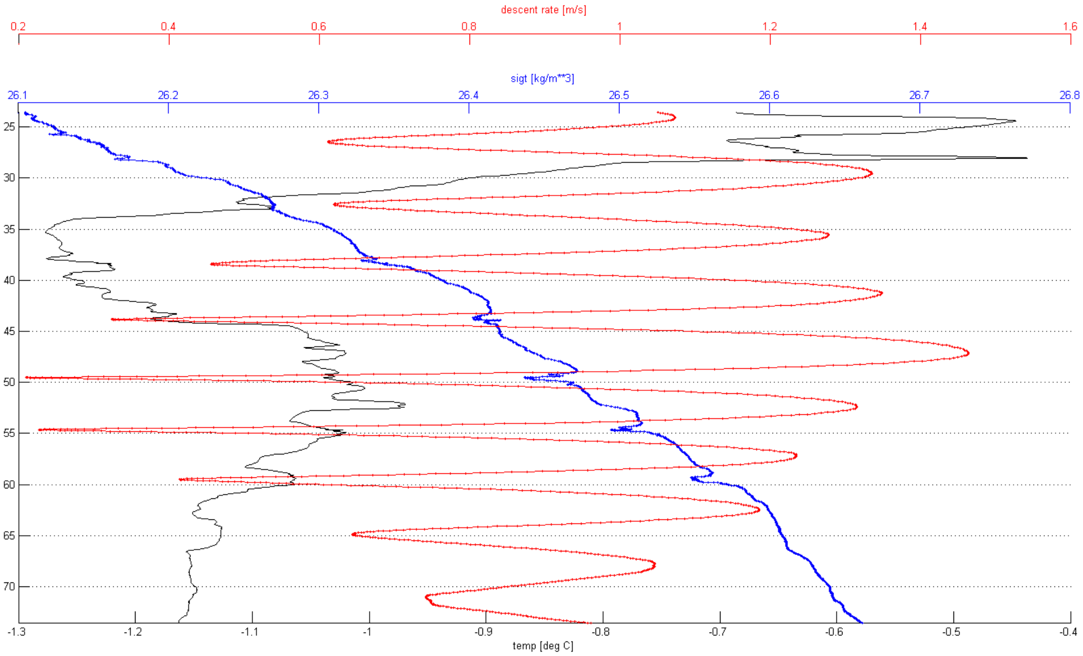


Figure 13 An example of typical impact of heave on the CTD data.

- Spikes in dissolved oxygen levels can coincide with abrupt temperature gradients. Although these data artefacts seem to be doubtful and may be produced by an inappropriate Sea-Bird algorithm, no data is flagged (Appendix A).
- For some casts, there may be a subsurface fluorescence maximum mismatch between the ascending and descending profile. The gap can vary up to 5 m. During the cruise, we tried to overcome this issue by reducing the rosette speed (down to 0.7 m/s) for the first 80 meters.

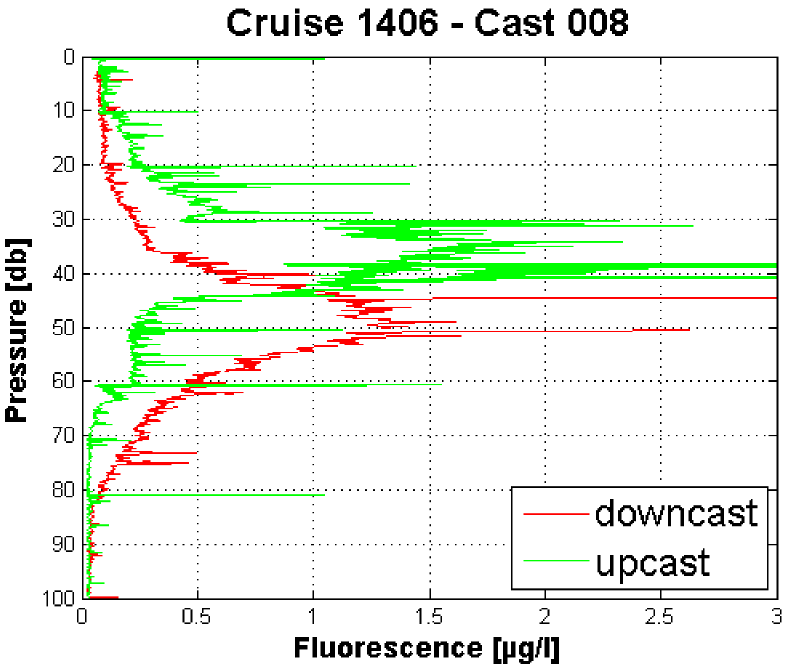


Figure 14 An example of descending and ascending fluorescence profile mismatch.

4.2.Checking the CTD pump status

This step allows to detect that the CTD pump is on that ensures that a best data quality for the sensors plumbed with the pump as conductivity and oxygen (Sea-Bird 2012).

Note that this does not ensure that the pump is working properly: the main problem is due to the pipe blocking by an outside element. This issue is detected by the sensor comparison and with a profile visual inspection.

A simple function has permitted to check that there were no pump problems for this cruise.

4.3. Salinity cross-check.

4.3.1. Double salinity and salinity sensor comparison

Dual conductivity & temperature system allows detecting issues such as drift, pump problem (blockage). The sensor slope and offset in the configuration file permit to make corrections (Sea-Bird Electronics, Inc., 2016) if necessary.

Concerning the current mission, the temperature difference is still close to zero along for all the cruises. The evolution of both difference exhibits no drift.

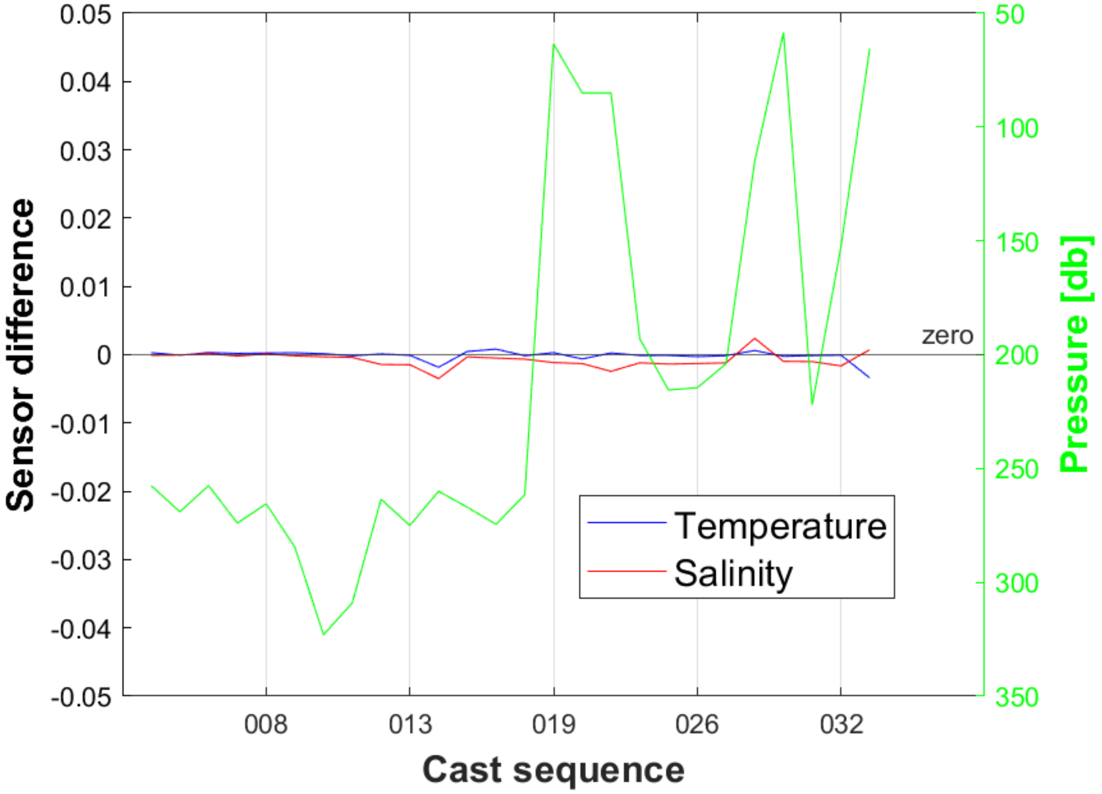


Figure 15 Difference comparison evolution (calculated from the mean pressure data) between the dual Sea-Bird C (red) & T (blue) sensors during the cruise. The salinity and temperature data are extracted from the deepest pressures (last ¼ of the pressure range) displayed in green.

4.3.2. Autosal cross-chek.

The salinity values recorded by the SBE 4 conductivity sensor are cross-checked against bottle samples. The field dataset was analysed with an Guildline salinometer model 8410A.

The comparison between the conductivity sensor and the field measurements is shown in the next table and figures. The comparisons are very good for both sensors and better for deep samples. No correction is needed as far as the conductivity sensors concerned.

Table 7 Comparison between the salinity measurements and the salinity sensors (upcast). The serial number 4244 sensor is the main salinity sensor, the serial sensor 6090 sensor is the redundant probe.

Sn	Dn/Up	Occurrence	Depth	Mean	Std
4244	Up	18	100db-	0.218	0.368
4244	Up	13	100db+	0.010	0.004
6090	Up	18	100db-	0.217	0.365
6090	Up	13	100db+	0.010	0.004

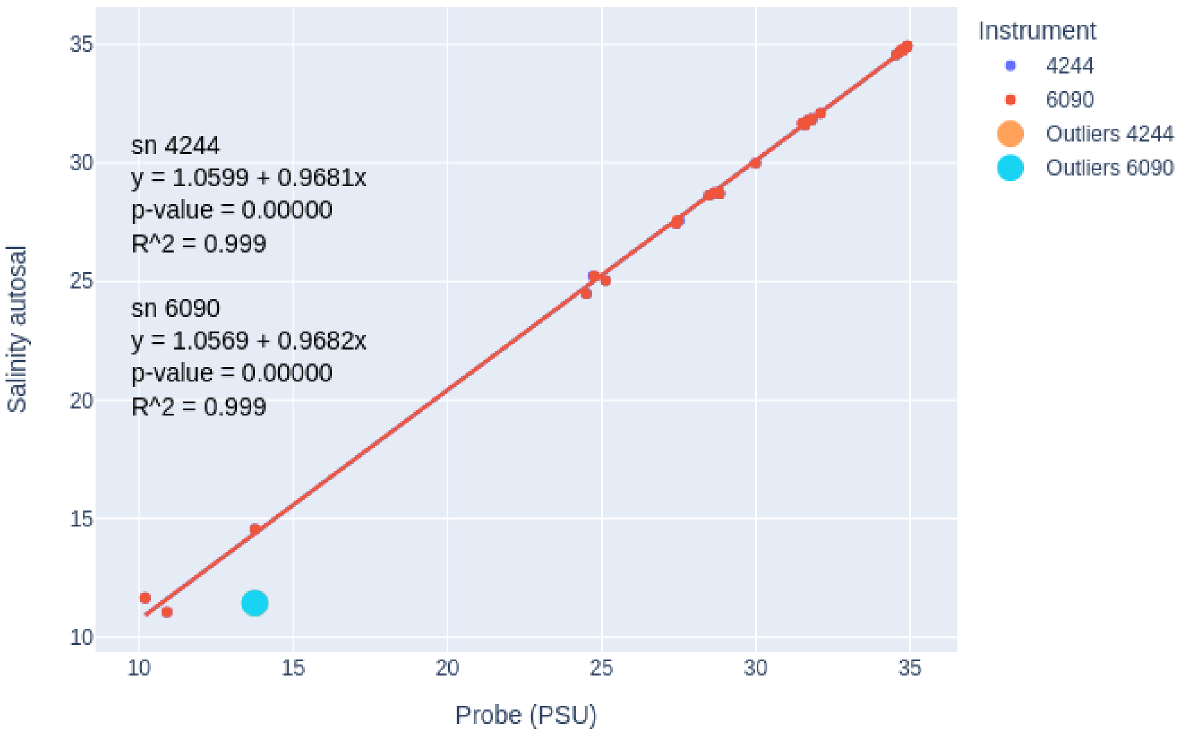


Figure 16 Regression between the bottle and the salinity sensors.

4.4.List of the carried-out tests.

Most of the data/profile tests are performed on the downcast unless a major problem is detected (the profile visual inspection includes a comparison between the upcast and the downcast).

In addition, salinity data recorded with the redundant sensor n°2 (serial number 4981 for this cruise) is considered for the quality control unless a problem is detected (the profile visual inspection includes a comparison between the dual T/C sensors).

Test 1.1: GTSPP Platform Identification
Test 1.2: GTSPP Impossible Date/Time
Test 1.3: GTSPP Impossible Location
Test 1.4: GTSPP Position on Land
Test 1.5: GTSPP Impossible Speed
Test 1.6: GTSPP Impossible Sounding
Test 5.1: GTSPP Cruise Track Visual Inspection
Test 2.0: IML Minimum Descent Rate (2) (0.10m/s)
Test 2.1: GTSPP Global Impossible Parameter Values (4)
Test 2.3: GTSPP Increasing Depth (16)
Test 2.4: GTSPP Profile Envelope (Temperature and Salinity) (32)
Test 2.6: GTSPP Freezing Point (128)
Test 2.7: GTSPP Spike in Temperature and Salinity (one point) (256)
Test 2.8: GTSPP Top and Bottom Spike in Temperature and Salinity (512)
Test 2.9: GTSPP Gradient in Temperature and Salinity (1024)
Test 2.11: IML Spike in Pressure, Temperature and Salinity (one point or more) (4096)
Test 3.5: IML Petrie Monthly Climatology (Temperature, Salinity and Sigma-T)
Test 4.2: IML Annual Deep Water Profile Consistency
Test 5.2: GTSPP Profile Visual Inspection

4.5.Cruise Track Visual Inspection.

Figure 17. The 2023_13 CTD cruise track.

4.6.Profile Visual Inspection.

For most of the casts recorded in the Saguenay fjord, the surface descending and ascending pH profiles are heavily different (see the next figure as an example). This is induced by a combination of a very high stratified surface water plus a technical pH sensor specification which request water temperature. This type of problem could also occur for the oxygen data.

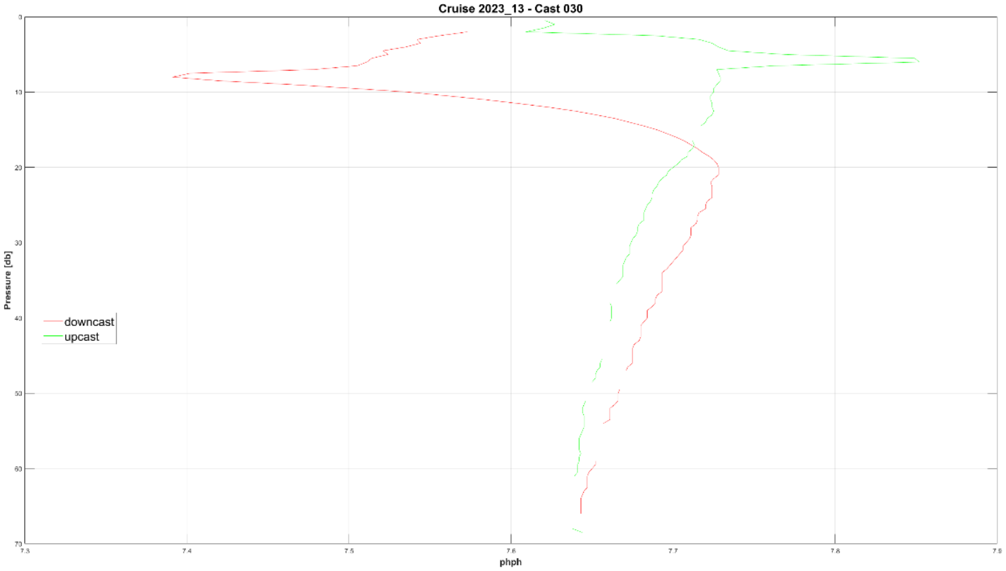


Figure 18 An instance of spurious surface pH profiles.

The casts 004 and 015 are recorded at the same station 5a.

004 ➔ The surface beam transmission signal is quite different with the cast 015. This variation is recorded by other variables.

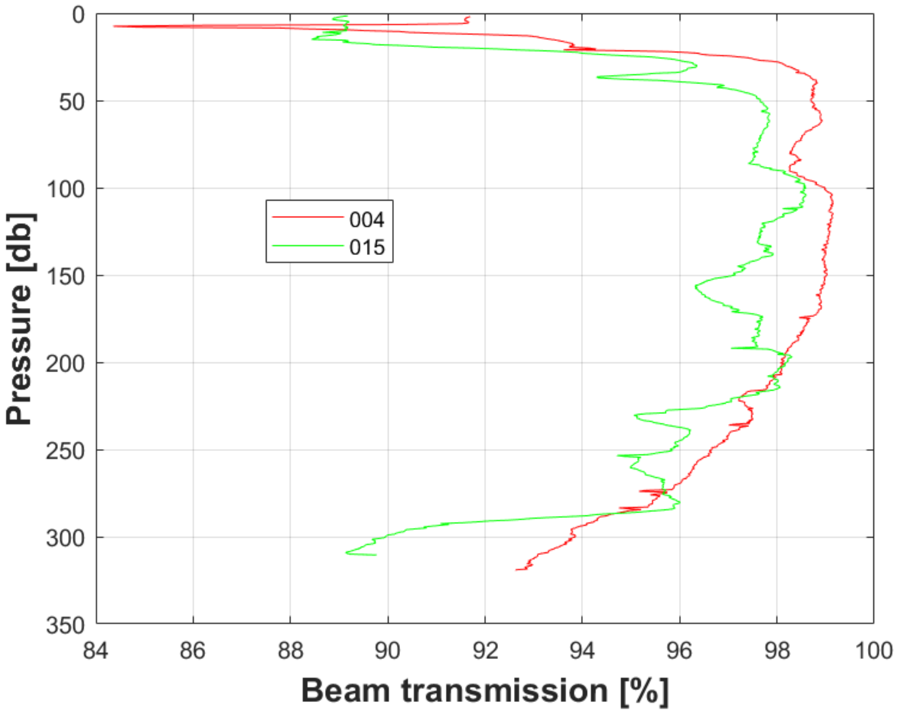


Figure 19 The descending beam transmission profiles recorded at the station 5a.

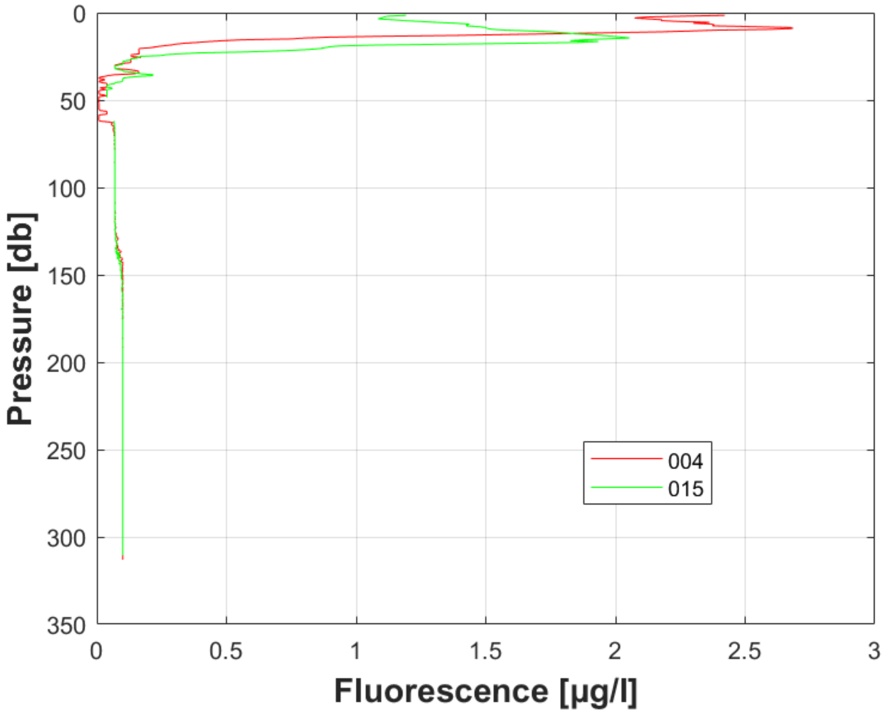


Figure 20 The descending fluorescence profiles recorded at the station 5a.

The casts 005 and 014 are recorded at the same station 6a.

The casts 007 and 013 are recorded at the same station 8a.

007 ➔ The surface beam transmission signal is different with the cast 013.

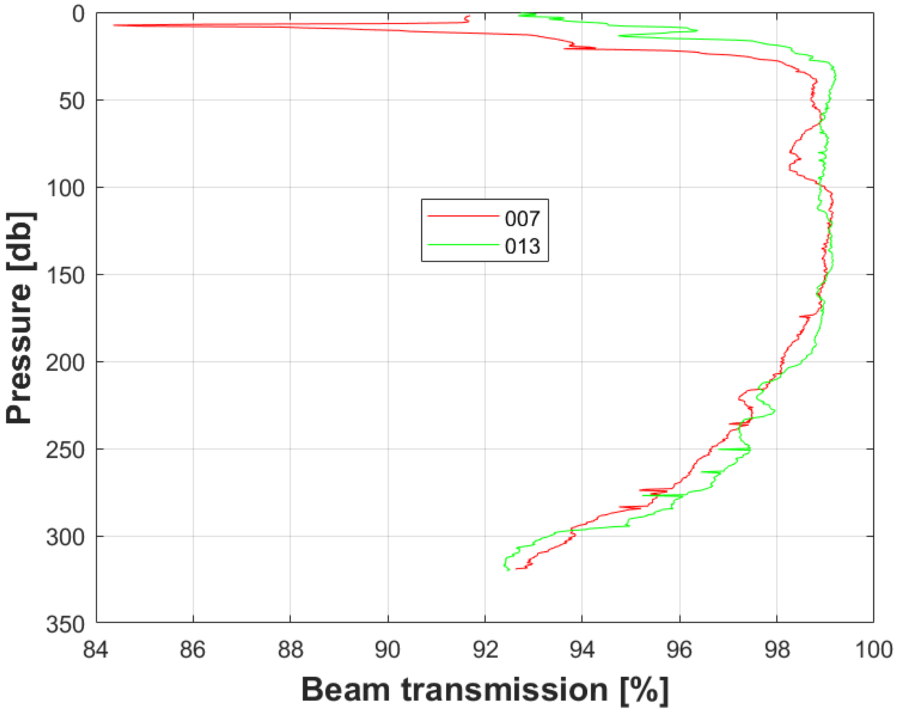


Figure 21 The beam transmission profiles recorded at the station 8a

The casts 008 and 012 are recorded at the same station 10a.

023 ➔ The surface beam transmission profiles mismatch.

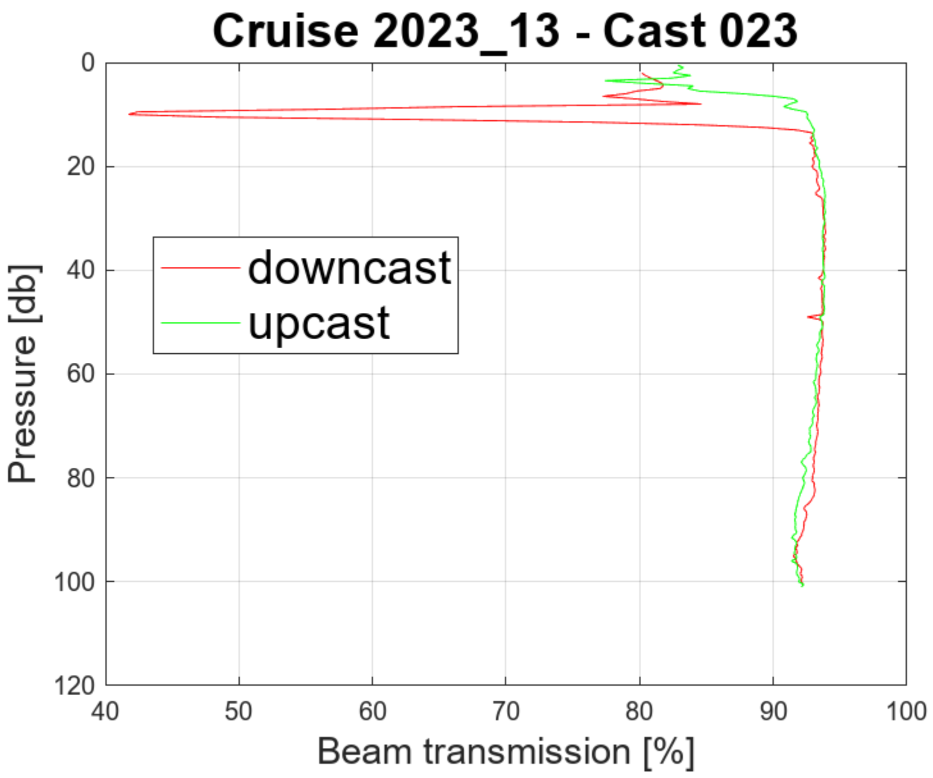


Figure 22 The beam transmission profiles for the cast 023.

025 ➔ The surface beam transmission profiles mismatch.

026 ➔ The surface beam transmission profiles mismatch.

031 ➔ The surface beam transmission profiles mismatch.

4.7.TS diagram from controlled data.

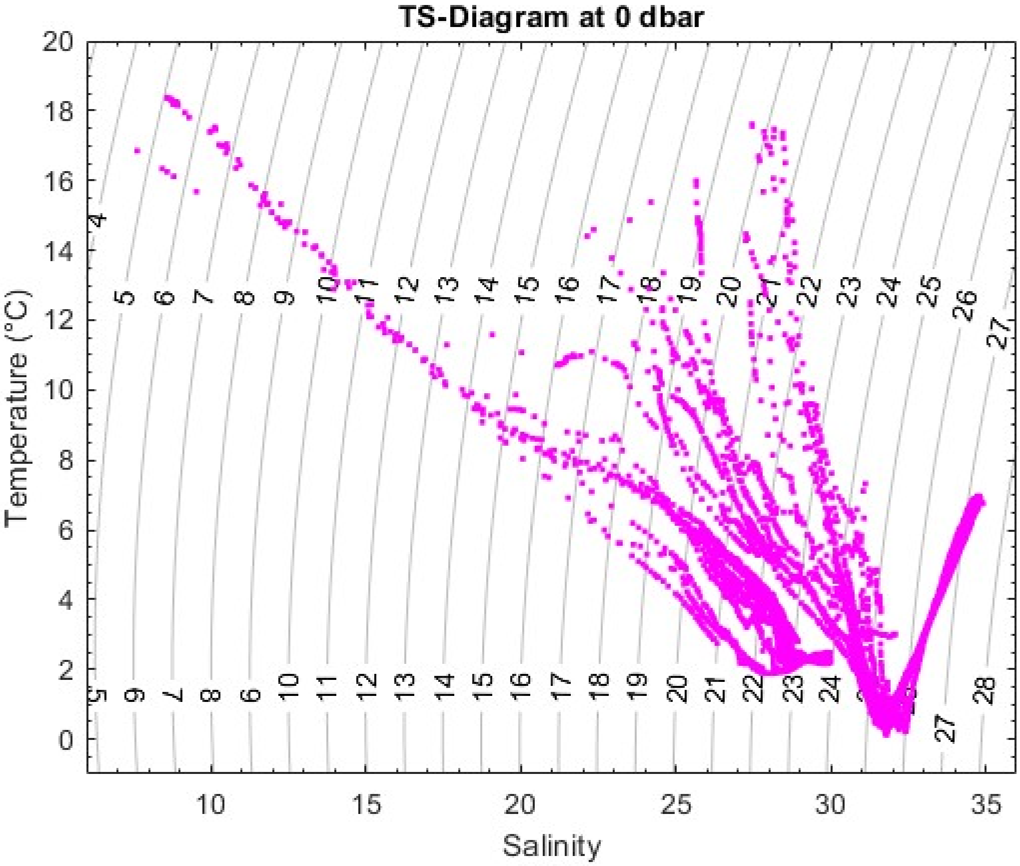


Figure 23.TS-diagram for the cruise 2023_13.

5. Compute derived parameters.

Oceanographic parameters could be computed from control and averaged data. Typically, the following variables are included into the data files:

- Density,
- Specific volume anomaly,
- Brunt Vaissala Frequency,
- Potential temperature,
- Freezing temperature,

In 2009, a new Thermodynamic Properties of Seawater (TEOS-10) has been adopted to replace the EOS-80. TEOS-10 introduces Absolute Salinity instead of the Practical

Salinity which is based on the conductivity.

The Joint Committee has provided some new routines to calculate for evaluating the thermodynamic properties of seawater. Therefore, four new parameters have been included into the files. The correspondence with old parameters is described in the following table.

Table 8. Correspondence between EOS-80 and TEOS-10 parameters.

EOS-80	TEOS-10
Practical Salinity [PSU]	Absolute Salinity [g/kg]
TE90 Temperature [°C]	Conservative Temperature [°C]
Density Dens [kg/m3]	In situ density D_CT [kg/m3]
Sigma-T SIGT [kg/m3]	In situ density D0CT [kg/m3]

Appendix.A. Note about problem of the SBE 43 oxygen data.

Dissolved oxygen profiles recorded by the Sea-Bird SBE 43 sensor may show some doubtful sections. This doubtful data could have some origins. Two are presented in this paper.

1. The oxygen data processing mainly consists in two steps.

    1) Improve sensor coefficient calibration with Winkler titrations. This step allows to calculate much accurate calibration values by fitting SBE 43 oxygen profiles with Winkler derived oxygen concentration coinciding in space and time. This step has no impact on doubtful data.

    2) Align data in time, relative to pressure.
    Dissolved oxygen data collected by the Sea-Bird 911*plus* CTD probe are characterized by a systematic delay with respect to pressure. The main causes are: 1) a time transit of the water through the pipe;according to Sea-Bird a typical plumbing delay for the SBE 43 DO sensor is about 5 seconds. 2) a long time constant of the oxygen sensor which is temperature inversely dependant; according to Sea-Bird this constant varies from approximately 2 seconds at 25 °C to up to 10 seconds at 0 °C. So the total delay should vary from 7 to 12 seconds. This delay must be corrected to ensure that the temperature and the salinity used to calculate the dissolved oxygen concentration from the SBE 43 voltage come from the same parcel of water, the higher the time correction, the greater the vertical shift of the oxygen data relative to the pressure. Sea-Bird suggests testing the “ALIGN CTD” module of the “SBE Data Processing-Win 32” software with different values in order to reduce the misalignment of the dissolved oxygen data between the upcast and the downcast profiles.

So, choosing a correction value is a compromise between the different casts of a leg and between the different sections of a profile. As a unique time correction is used for every cast and for all oxygen data of a cast, some misalignment issues may occur that could lead to hysteresis (hysteresis is a delay in the evolution of a physical or chemical parameter), and so to doubtful dissolved oxygen data.

2. For some oceanographic condition –cold water and sharp temperature gradient, the oxygen profile recorded by the SBE 43 sensor may be characterized by a spike coinciding with the thermocline (see the figure B1 for an example). This artefact should be taken with great care and may not reflect an actual oceanographic phenomenon. Actually, this spike may be an artefact of the equation used to compute dissolved oxygen (see the equation 1). A term of this equation is saturation of oxygen (*Oxsat*) which is function of temperature and salinity. *Oxsat* is changing as fast as these 2 parameters are changing due to very short sensor time constant while the oxygen voltage (*V*) is changing much slower due to a high constant time which is exacerbate by cold temperature.

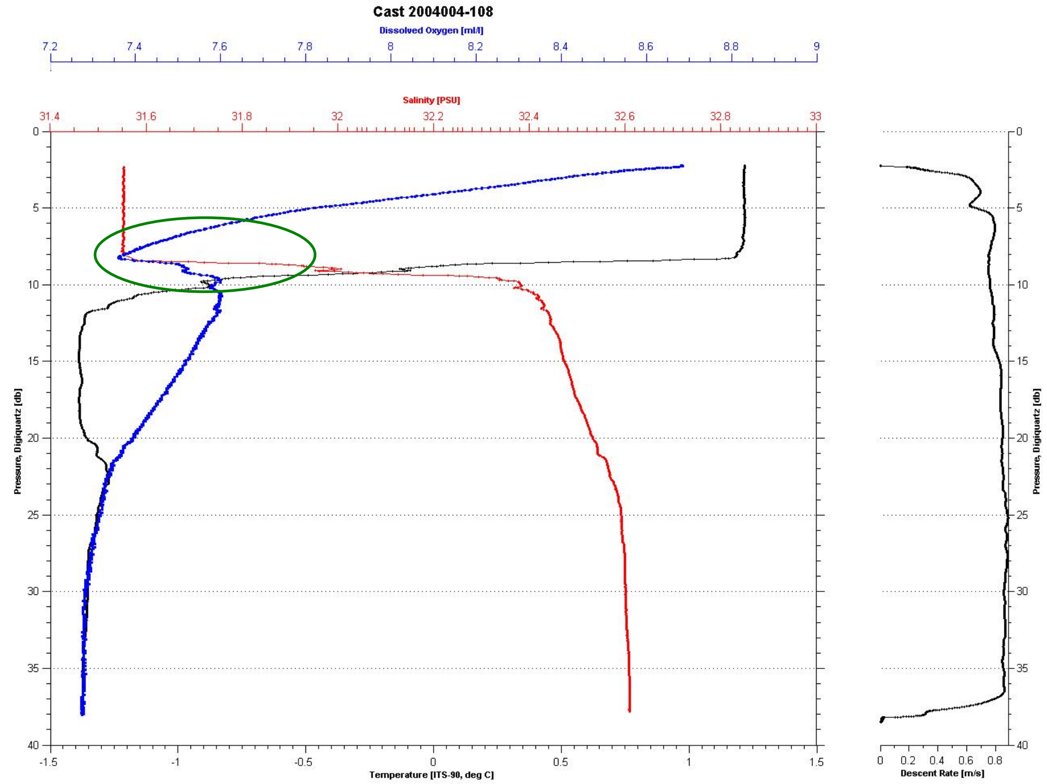


Figure A-1 An example of oxygen artefact coinciding with a thermocline (the alignment correction is 10 seconds).

$$oxygen(ml/l) = Soc * (V + Voffset) * \phi \qquad \text{Equation (1)}$$

Where:

$$\phi = e^{(tcor*T)} * Oxsat(T,S) * e^{(pcor*P)}$$

T = Ctd temperature (°C)

S = Ctd salinity (psu)

P = Ctd pressure (dbars)

V = SBE 43 output voltage signal (volts)

$Oxsat(T,S)$ = oxygen saturation (ml/l)

Soc , $Voffset$, $tcor$, $pcor$ are calibration coefficients

Appendix.B. References

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