ICES WGOH CTD Intercomparison Project: Methodology Document

Participant Number: [Your Participant Number]

1. Introduction

From the Cruise Report we extracted the following relevant information:

"The main workhorse of CE17007 was the Seabird SBE911*plus* CTD connected to a SBE32 carousel. Power to the CTD and sensors was provided through the sea cable from an SBE11*plus* deck unit located in the dry lab in the ship. The sensor setup employed during CE17007 is located below in the Table. The calibration dates and coefficients are checked (against the SBE calibration sheet, which in this case we did not have). Serial numbers are also noted.

Sensor Code	Parameter	Serial Number	Calibration/Service date
CTD SBE911*plus* PSO513		09P19835-0513	M: 10 Nov 2014 POMs: 25 Jan 2015
SBE32	Bottle firing mechanism	unknown	unknown
SBE3	T1: Primary Temperature Sensor	4023	01 Sep 2016
SBE3	T2: Secondary Temperature Sensor	4927	28 Sep 2016
SBE35	Discrete depth bottle triggered Temperature sensor	0020	17 Oct 2016
SBE4	C1: Primary Conductivity Sensor	3480	20 Sep 2016
SBE4	C2: Primary Conductivity Sensor	2764	06 Oct 2016
SBE43	Oxygen Sensor[1]	3339	16 Feb 2017
SBE43	Oxygen Sensor[1]	1416	18 Mar 2017
VA500	Altimeter	46504	unknown
Wetlabs C-star	Transmissometer	CST-1101DR	08 Dec 2016
Wetlabs ECO-FLNTURTD	Fluorometer and Turbidity	1609	12 Oct 2009

[1]The original oxygen sensor (S/N 3339) was found to be performing poorly at station 3 and was swapped out for a replacement sensor (S/N 1416).

Note that after station 3 a different oxygen sensor was used.

The CTD supplied a standard SBE-format data stream at a rate of 24 Hz. The CTD provided pressure plus dual temperature and conductivity data, with single sensors for oxygen, optical transmission, a combined fluorometry/turbidity sensor and an altimeter. The CTD system was equipped with dual pumps. Primary temperature, conductivity and dissolved oxygen were plumbed into one pump circuit; and the secondary temperature and conductivity was on the other circuit. A Lowered Acoustic Doppler Profiler (LADCP) was also mounted on the rosette frame; it was powered separately and collected data internally. The original altimeter from this unit (Benthos) was swapped with a Valeport VA500 on loan from WHOI as the LADCP interferes with the Benthos device. Prior to every CTD deployment the transmissometer was checked and cleaned and a zero reading in air taken. The primary temperature and conductivity sensors were used for reported CTD temperatures and salinities on all casts; the exception was station 27, were there was an initial problem with the primary signal, as evidenced by anomalously low O2 readings and significant deviations from the values of secondary temperature and conductivity sensors, due to what is suspected was a transient pump blockage.

At station 11 the pump stopped and started intermittently. Bottom connection warning alarm triggered a couple of times. Bottle firing communication error occurred. Water ingress on secondary pump connector, loose connections were tightened, the secondary pump was cleaned and the bottle firing mechanism was also cleaned. […] Routine maintenance was carried out on the Niskin bottles after station 33 (May 13: 0200 UTC) in response to comments returned by the sampling group. The spigots were checked on all bottles (3 had been reported as difficult to open), the outer flange was removed, the valve body was taken out, the 2 inner o-rings were lifted and put back in, pushed inside, and then the reinstalled flange. No change of parts were made. The CTD data and bottle trip files were acquired by SBE Seabird SeaSave V7 version 23.0.2 on the ship's Windows 7 workstation located in the dry lab. Pre-cruise calibration data were applied to CTD Pressure, Temperature and Conductivity sensor data acquired at full 24 Hz resolution. Bottles were close on the upcast through the software and were tripped 30 seconds after stopping at the required bottle depth to allow the rosette wake to dissipate and the bottles to flush. The upcast continued 30 seconds after closing a bottle to ensure that stable CTD and reference temperature data (SBE35) were associated with the bottle trip.

[…] An issue was identified with the SBE 43 sensor (SN 3339) for stations CE17007-01 to 03. The sensor was swapped out for station 4 and replaced with SBE 43 (SN 1416). Thereafter, the dissolved oxygen laboratory and sensor values correlated very well (r2 = 0.97 Figure 4.4.2) with the exception of station 27 where a problem with the CTD pump was noted."

We are using SBE Data Processing Version 7.26.7.

2. Initial Data Processing Workflow

2.1. Data Conversion

The initial step in our data processing workflow involves converting the raw CTD data to engineering units using the SBE Data Processing software. The following procedures were followed:

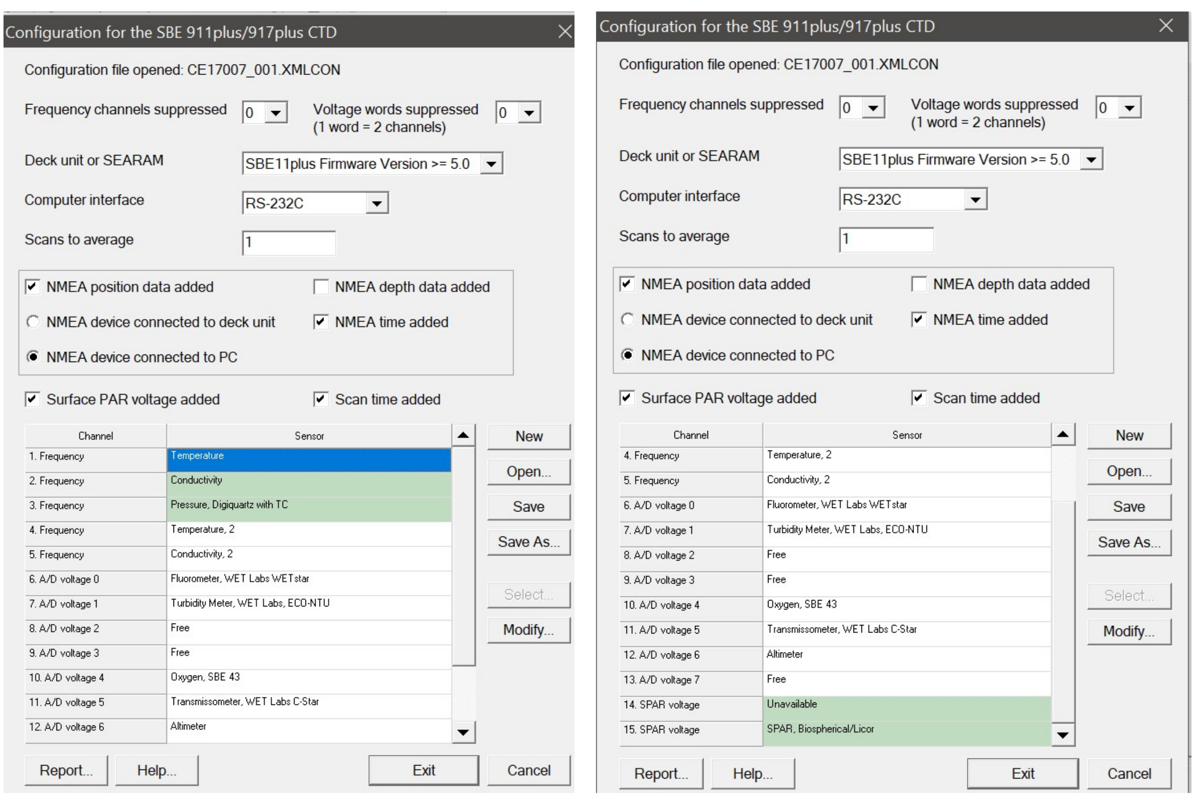

Fig. 1: View of the configuration file, to see which sensors are mounted

The raw data files, typically in .hex format, were loaded into the SBE Data Processing software. The Data Conversion module in the SBE software was used to convert the raw data to engineering units. This conversion process translates the raw sensor outputs into meaningful physical measurements such as temperature (°C), conductivity (S/m), and pressure (dbar)

The option “Match instrument configuration to input file” has been selected.

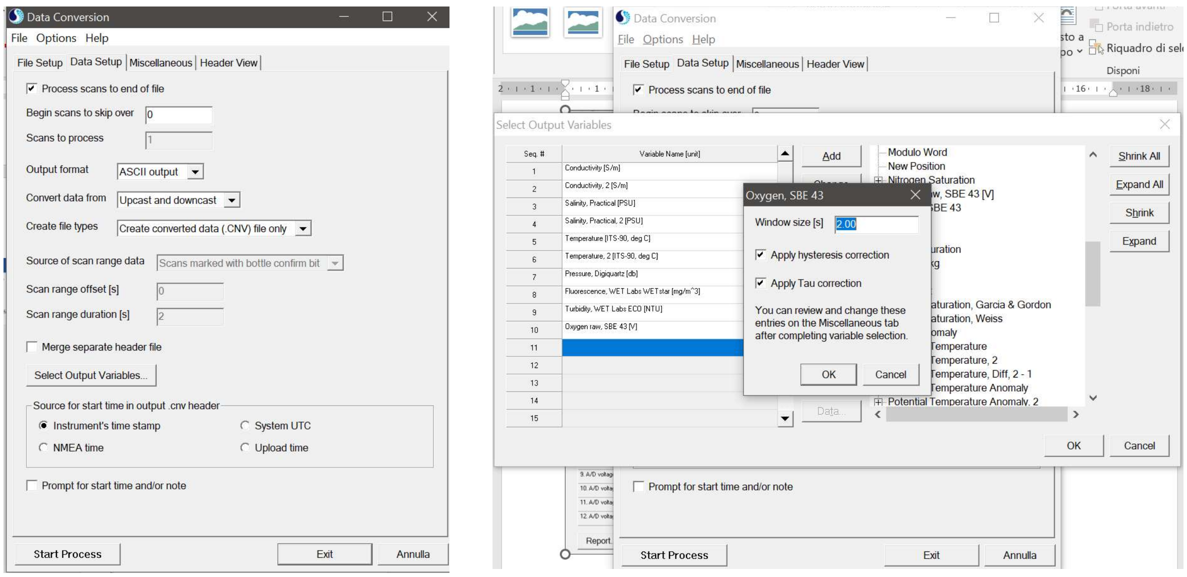

Fig. 2 Other selected options during the DataConv step

The list of variables that we chose to convert is shown in Fig. 3. Given that LADCPs were mounted on the carousel, we decided to also extract latitude and longitude during the cast.

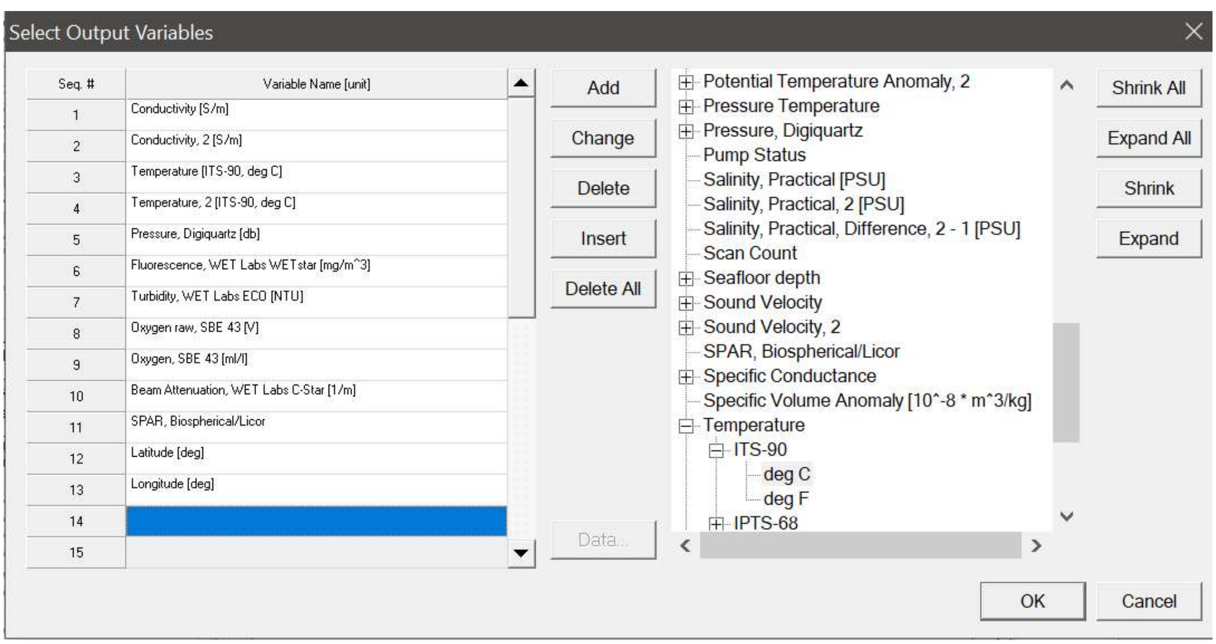

Fig. 3. List of converted variables

The converted data was saved in .cnv format,

2.2. Align CTD

The next step in our data processing workflow involves aligning the CTD data to correct for time lags between different sensors. This ensures that the measurements of temperature, conductivity, and pressure are synchronized. The alignment process corrects for the time delay between the temperature and conductivity measurements, which is caused by the time it takes for water to transit from the thermistor to the conductivity cell. The converted data files (.cnv format) from the previous step were loaded into the Align CTD module in the SBE Data Processing software. From the Header View (Fig. 4), we learn that the deck unit is already taking care of the advancement of both the primary and the secondary sensors (0.073 seconds).

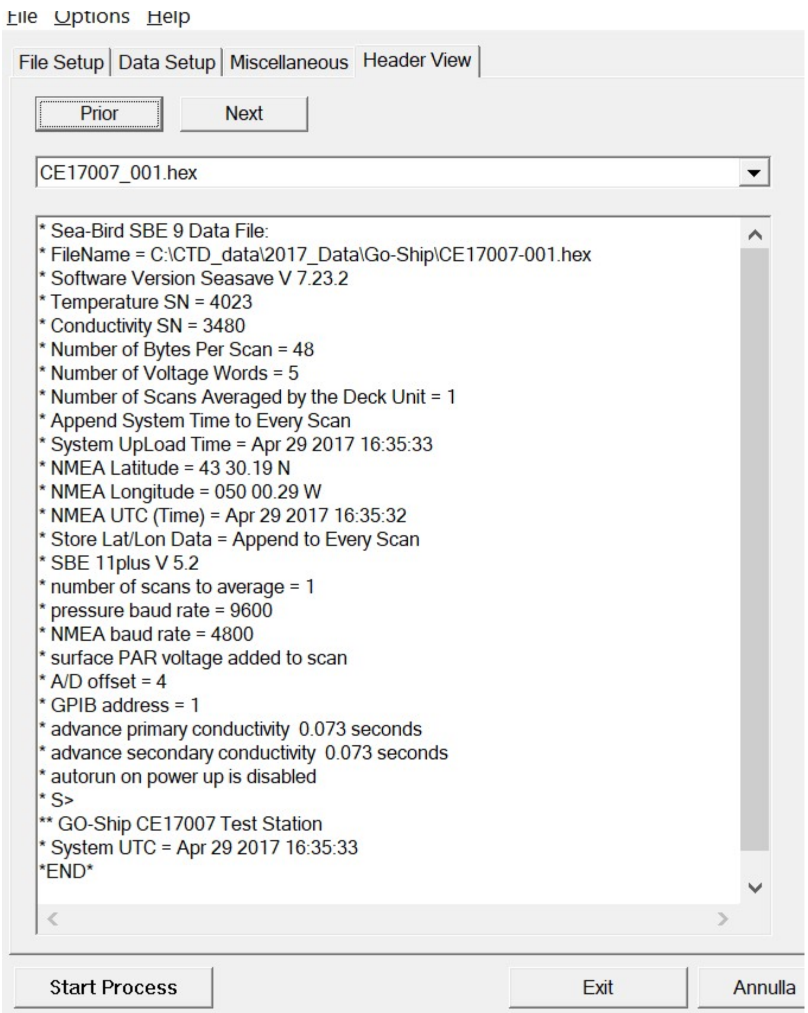

Fig. 4. Header View containing information about the configuration of the data acquisition

For the dissolved oxygen sensor (SBE 43), an additional alignment was performed to account for the transit time of water through the plumbing. The delay for the SBE 43 sensor is estimated to be approximately 3 seconds, with adjustments made based on the temperature-dependent response time. The same delay was applied to the optical sensors installed.

The aligned data was saved in .cnv format, ensuring that the temperature, conductivity, and pressure measurements were synchronized.

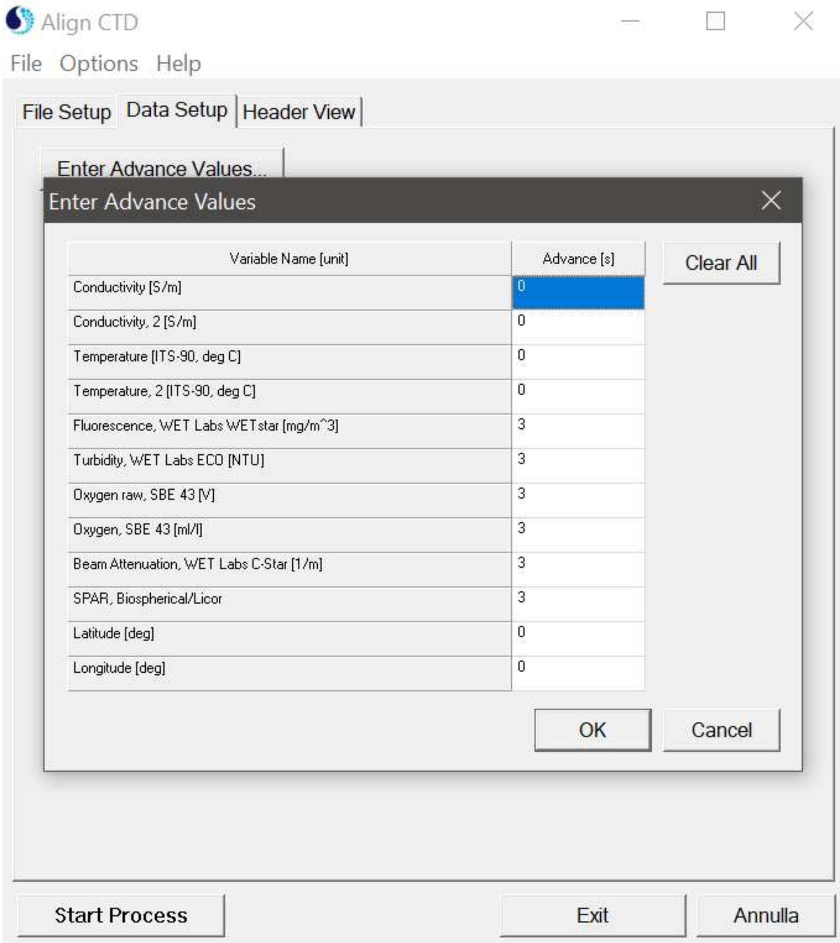

Fig. 5. Advanced values for each sensor to be aligned

2.3. Cell Thermal Mass

The cell thermal mass correction is an essential step in our data processing workflow to account for the thermal inertia of the conductivity cell. This correction helps to improve the accuracy of salinity measurements by compensating for the thermal lag between the temperature and conductivity sensors. The thermal mass of the conductivity cell can cause a lag in the response of the conductivity sensor to changes in water temperature. This lag can introduce errors in the calculated salinity, especially in regions with sharp temperature gradients. The aligned data files (.cnv format) from the previous step were loaded into the Cell Thermal Mass module in the SBE Data Processing software. The software applies a correction algorithm that compensates for the thermal mass effect. This algorithm adjusts the conductivity measurements based on the rate of change of temperature. The default parameters provided by SeaBird were used (0.03 for thermal anomaly amplitude and 7 for thermal anomaly time constant). The primary (secondary) temperature sensor was used to correct the primary (secondary) conductivity sensor.

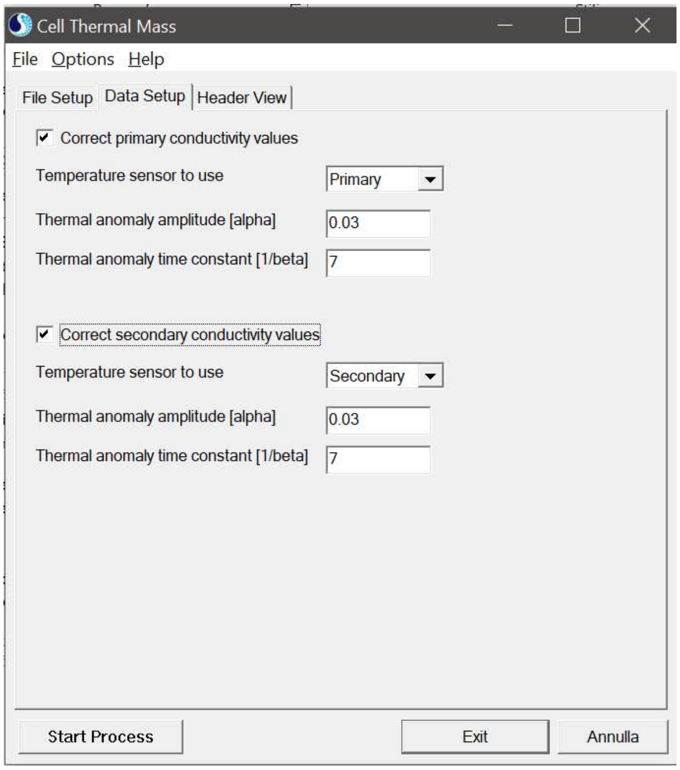

Fig. 6. Data Setup for Cell thermal Mass coeffficients

2.4. Derive

The "Derive" module in the SBE Data Processing Software is used to calculate additional parameters from the primary CTD measurements. This step is crucial for obtaining accurate and meaningful oceanographic data. Derived parameters include:

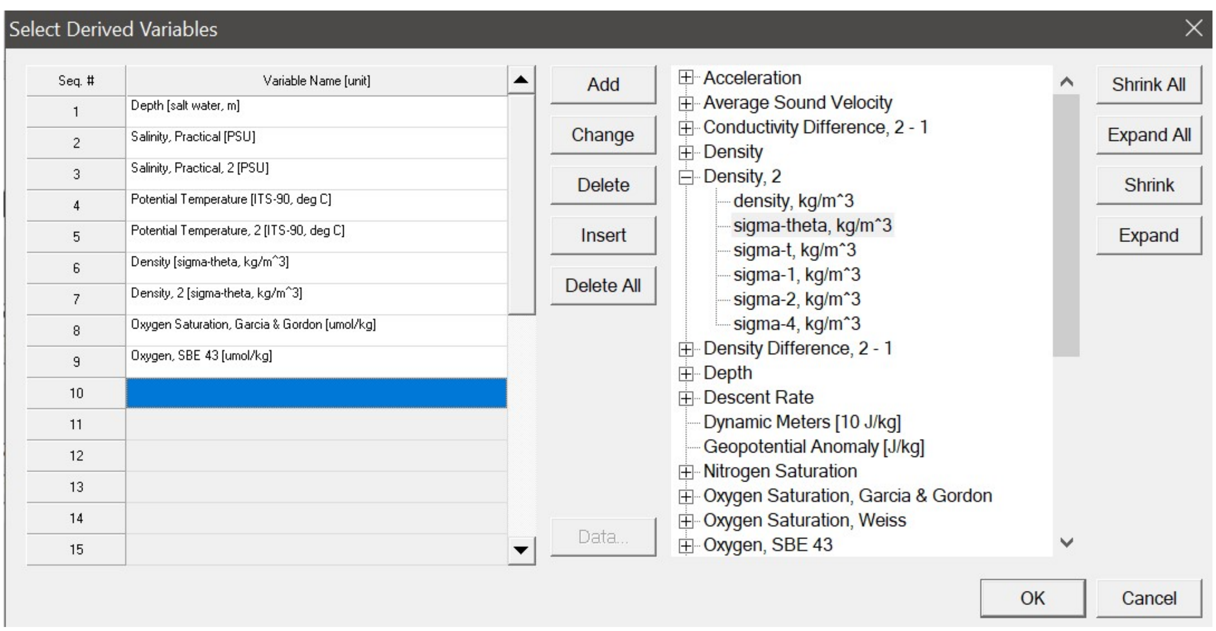

Fig. 6. Derived parameters selected

The oxygen concentration is corrected for hysteresis[1]., which is recommended for profiles exceeding a depth of 1000 m. This step ensures that the derived oxygen concentration is accurate over varying pressures.

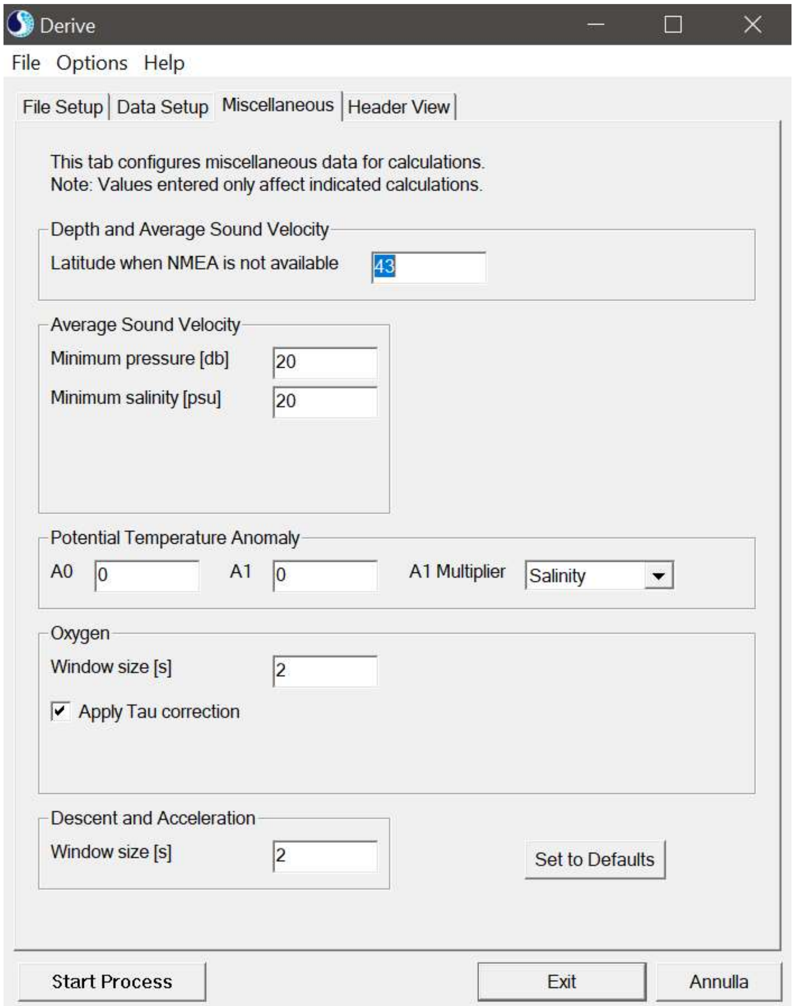

Fig. 7. Miscellaneous parameter settings used

2.5. Bin Average

The "Bin Average" step was performed using the SBE Data Processing Software to average the data into specified depth bins, as part of the intercomparison exercise on CTD data post-processing. The bin size was set to 1 decibar, in accordance with the participants' instructions. To prevent overwriting the .cnv files so far created, the output files were saved in a different folder, and the output files were named with the suffix *_1db.cnv to indicate the bin size used.

[1] https://www.seabird.com/asset-get.download.jsa?code=251035

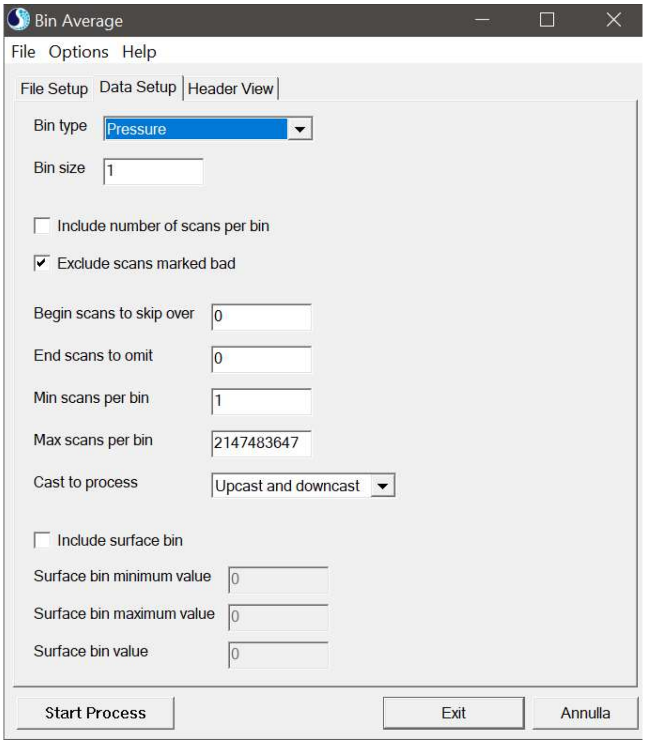

Fig. 8. Data setup used to bin average

2.6. Split

The "Split" step in the SBE Data Processing Software was used to separate the upcast and downcast portions of the CTD profile. This separation is essential for analyzing the data collected during the descent (downcast) and ascent (upcast) of the CTD instrument independently. The binned data file from the previous "Bin Average" step was selected for processing. The split process was executed, resulting in the division of the data file into two segments: one for the downcast (prefix “d”) and one for the upcast (prefix “u”). The resulting segments were saved as separate files in a designated folder (/split).

3. Correction of T, S and Oxygen

In order to follow on with the correction, and reprocessing data with new configuration files containing the corrected factors, for Temperature, Salinity and Oxygen, we need to create “bottle files”. We followed the procedure described below.

3.1. Bottle file creation

The first step is to create .ros bottle files, which contain CTD data for a user-selected range of scans before and after each bottle firing. This means re-run the Data Conversion step again, and on the Data Setup tab, set the following: Create file types = create bottle file only (source of scan range data = scans marked with bottle confirm bit; scan range offset = 0; scan range duration = 2). The selected output variables were:

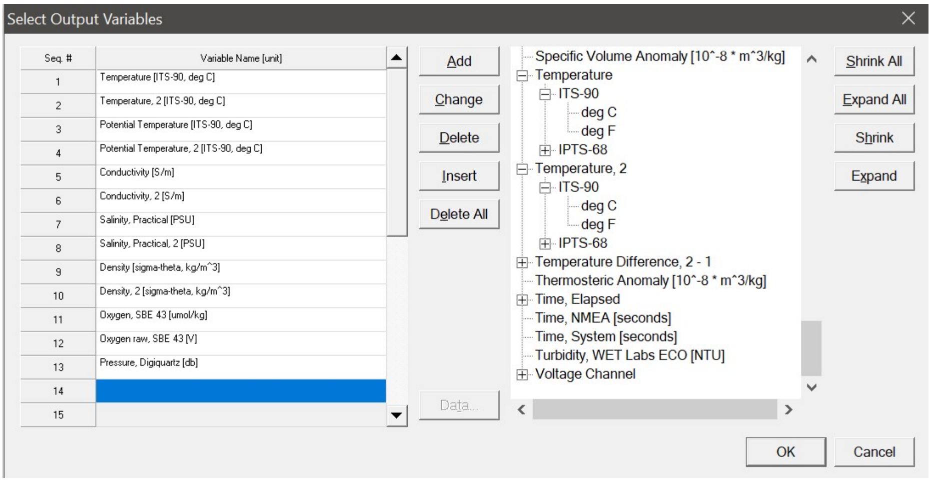

Fig. 9. Output variables for the bottle files

Then it is needed to create .btl bottle summary files, by running the "Bottle Summary" step was performed using the SBE Data Processing Software to generate a summary of the CTD data associated with each bottle firing. This step is crucial for obtaining averaged values and other statistical parameters for the data collected at each bottle closure depth. The following actions were taken: the "Bottle Summary" module in the SBE Data Processing Software was accessed; the configuration (.xmlcon) file from the campaign and the .ROS files created in the previous step were selected for processing; the input directory containing the .ROS files was specified; averaged variables were selected to be included in the summary; the bottle summary process was executed, resulting in the creation of btl files, containing averaged values and standard deviation for each parameter at the bottle closure depths.

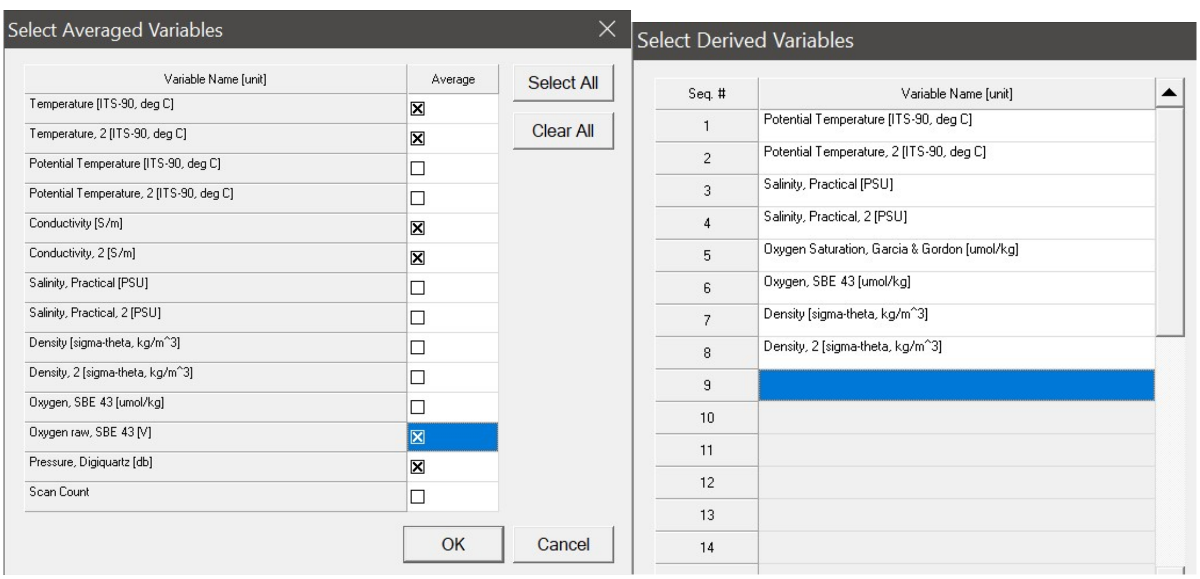

Fig. 10. Selected Averaged Variables and Selected Derived Variables

In this way SBE Data Processing creates .btl files with summary CTD data for the scans associated with each bottle firing.

3.2. Field Calibrations, Temperature

To ensure the accuracy of the CTD temperature measurements, we conducted a thorough calibration check using the SBE35 Deep Ocean Standards Thermometer. This process involved comparing the temperature readings from the primary and secondary CTD temperature sensors with the SBE35 measurements taken at bottle closure depths. The SBE 35 is an internally recording temperature sensor that operates independently of the CTD. The SBE 35 is triggered by the SBE 32 carousel in response to each bottle closure.

We first plotted the differences between the primary and secondary CTD temperature sensors. The average difference observed was 0.0025°C. However, there were two data points with differences exceeding 0.05°C. For these points, no SBE35 data were available, indicating potential anomalies or sensor issues at those specific depths (at stations 6 and 8).

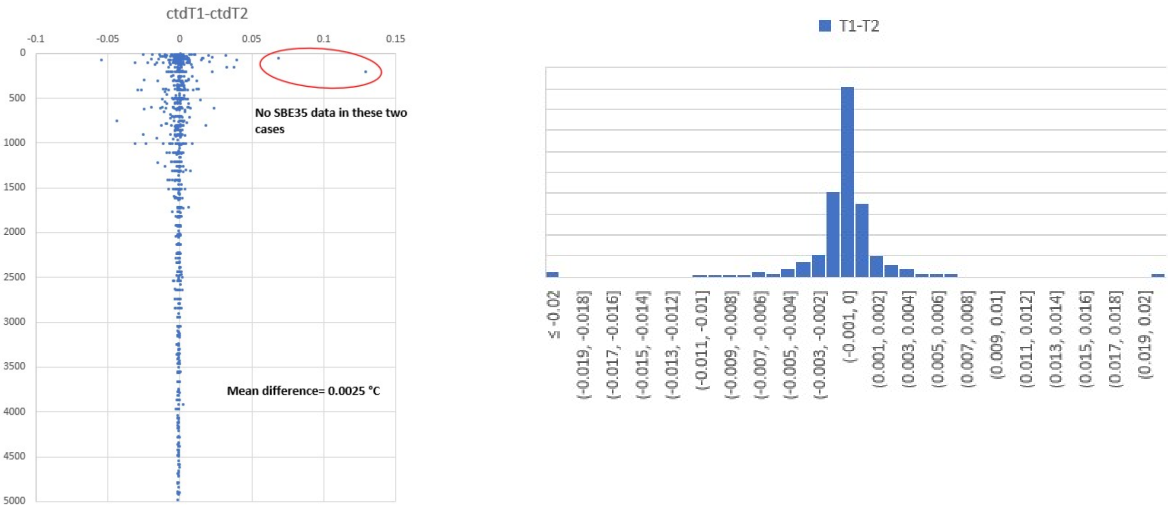

Fig. 11. (left) differences between the primary and the secondary temperature sensors; (right) frequency distribution of the differences T1-T2.

Next, we compared the temperature readings from each CTD sensor with the corresponding values measured by the SBE35. These differences were plotted against pressure to identify any depth-related trends. The mean difference for the primary CTD temperature sensor was 0.0028°C, while the secondary sensor showed a mean difference of 0.0025°C. Notably, the discrepancies were more pronounced at depths above 1000-1500 meters, suggesting potential calibration drift or environmental factors affecting sensor performance at greater depths.

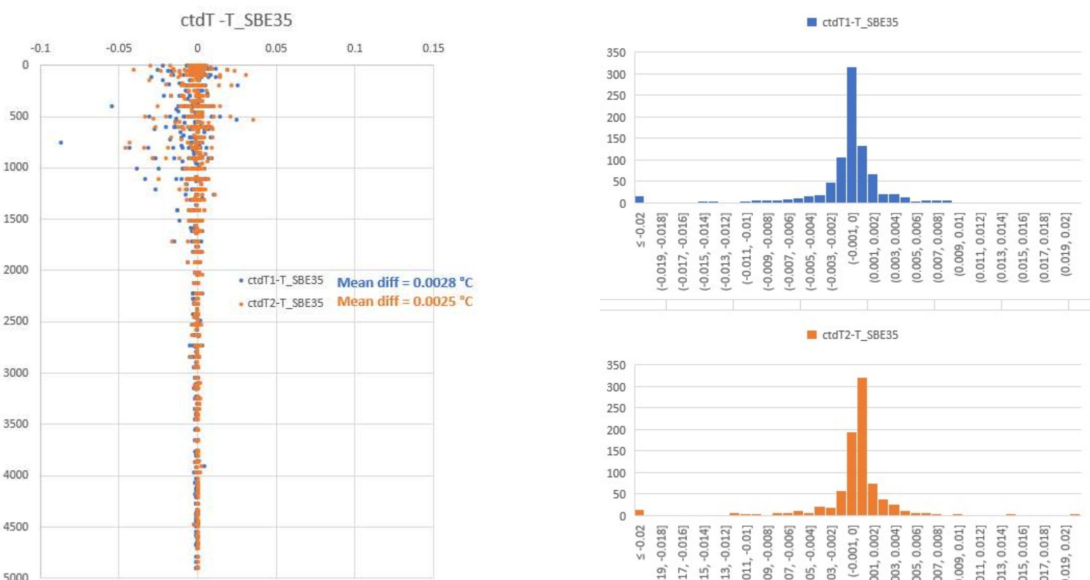

Fig. 12. (left) differences between the CTD temperatures and the SBE35 data; (right) frequency distributions of these differences for the primary and for the secondary sensors.

Considering only depths higher than 1500 m, the differences were reduced to 0.00093 °C (T1-T2), 0.00095 °C (T1-SBE35) and 0.00067 °C (T2-SBE35), values that are fully acceptable (McTaggart et al., 2010[2]).

No temporal drifts were seen in the sensor-to-sensor differences. To further analyze them, we plotted histograms of the temperature discrepancies. The histograms revealed a Gaussian distribution centered around 0, indicating that the differences between the CTD sensors and the SBE35 measurements follow a normal distribution pattern. This Gaussian behavior supports the reliability of the calibration, as most differences are minor and symmetrically distributed around the mean.

We did therefore not apply any correction to the CTD data.

3.3. Field Calibrations, Salinity

To ensure the accuracy of the salinity measurements, we conducted a calibration check using the salinity values obtained from water samples analyzed by a salinometer. Figure xx shows an example of the salinity values from the CTD derived bottle files (blue/green lines), and the corresponding salinity values measured in the samples (red crosses). The existing difference is appreciable by eye, showing that a correction is needed.

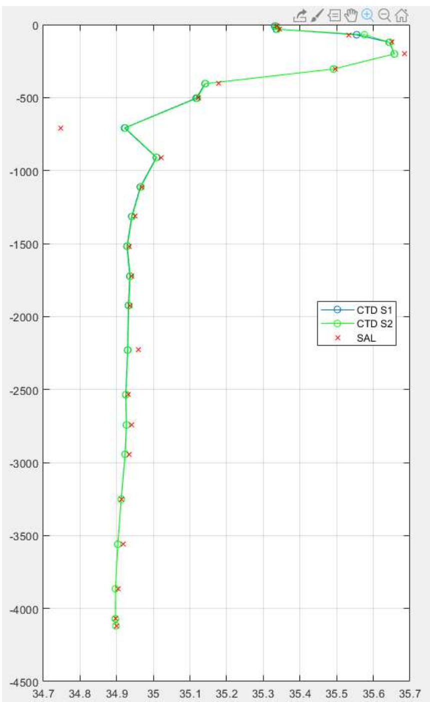

Fig. 13. Example station with Bottle file Salinity data and Salinometer values

The slope factor, needed to correct the CTD salinity data, is calculated as follows:

$$slope = \frac{\sum_{i=1}^{n} \alpha_i \beta_i}{\sum_{i=1}^{n} \alpha_i \alpha_i}$$

Where n is the number of samples, α is the CTD conductivity and β is the true (bottle sample) conductivity.

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[2] https://doi.org/10.25607/OBP-1348

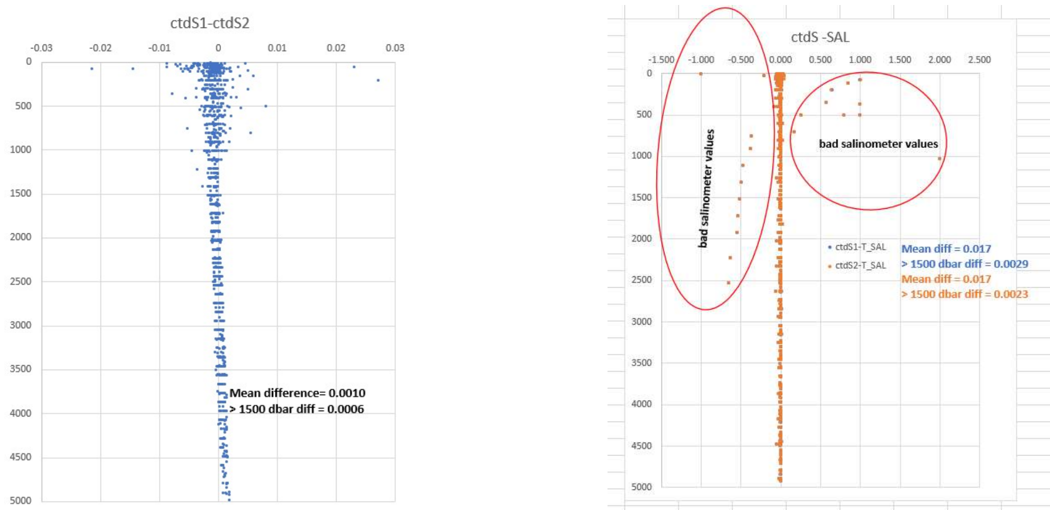


Fig. 14. (left) vertical distribution of the difference between Sal1 and Sal2; (right) differences between each sensor and the salinometer data

Figure 15 shows the pre-corrected Salinity comparison between the primary sensor and the Salinometer measurements. Figure 16 shows the same for the secondary sensor

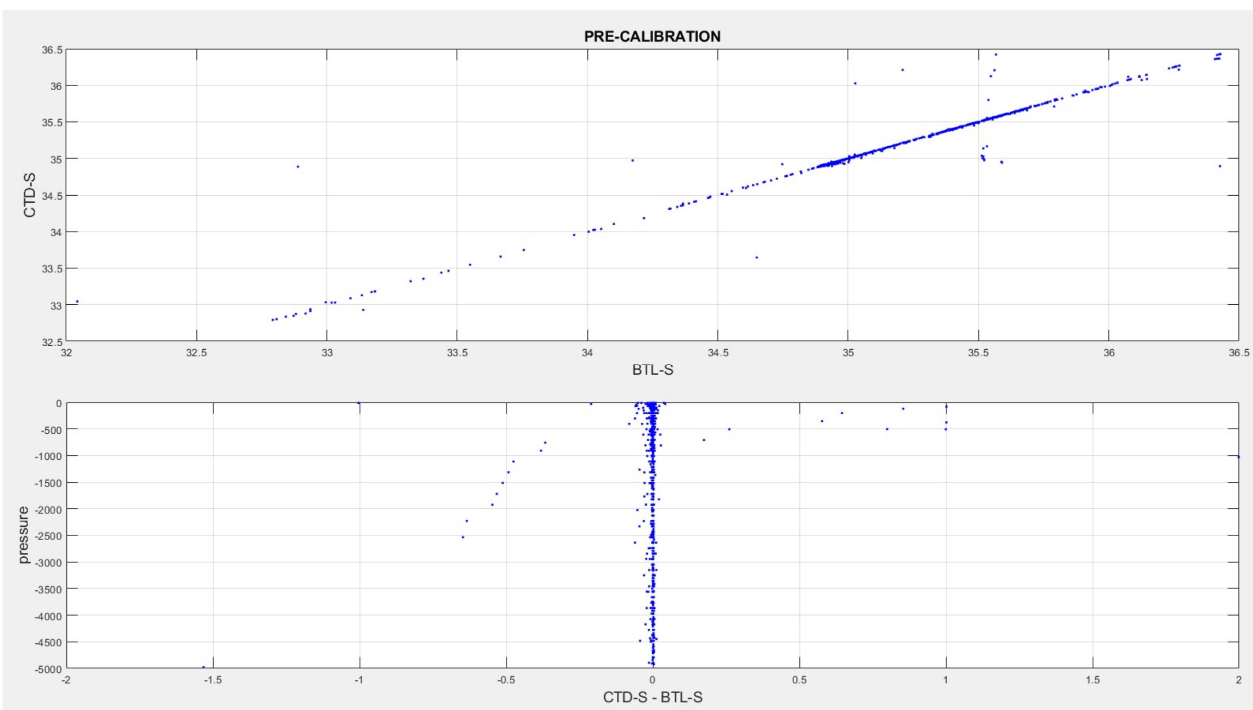


Figure 15: . Scatter plot showing the relation between CTD-salinity (primary sensor) and bottle-salinity and the vertical distribution of the differences between CTD-salinity (primary sensor) and bottle-salinity before applying the slope correction

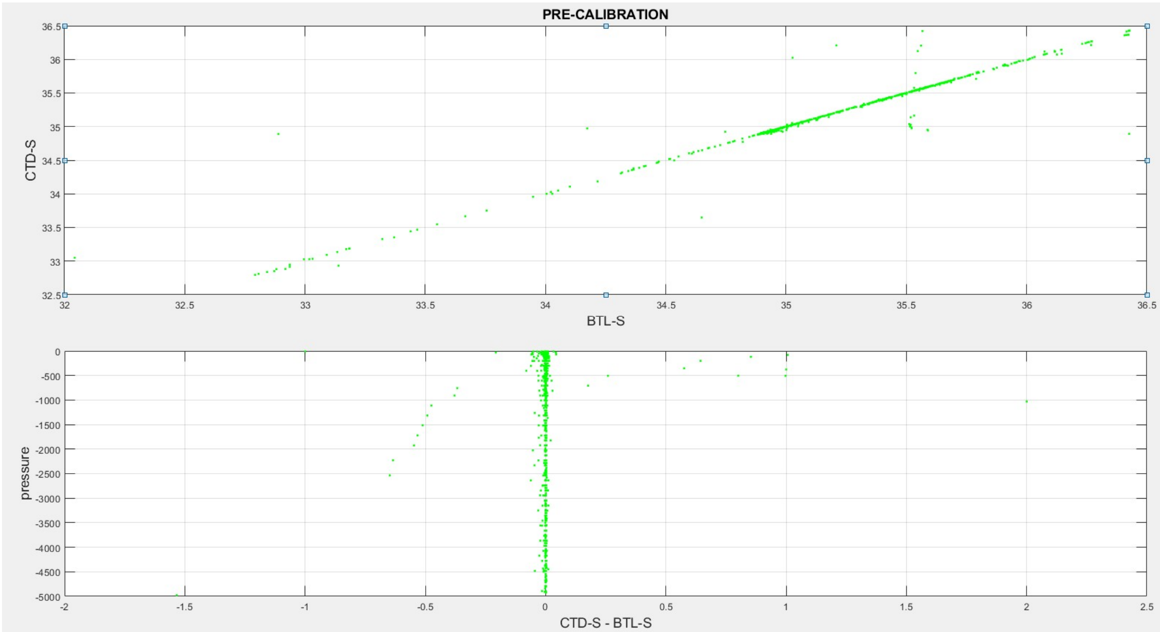


Figure 16: . Scatter plot showing the relation between CTD-salinity (secondary sensor) and bottle-salinity and the vertical distribution of the differences between CTD-salinity (secondary sensor) and bottle-salinity before applying the slope correction

For the primary sensor we calculated a slope of 0.99998288, while for the secondary sensor we calculated a slope of 1.00004677. These values are applied to the raw CTD data (modifying the con files), to correct for this bias. For the calculation of the slopes we excluded data from the first 500 m, as well as flagged salinometer values (those where the difference between the primary/secondary salinity values and the bottle salinity exceeded 0.1).

The following figures show the post-calibration situation for each sensor.

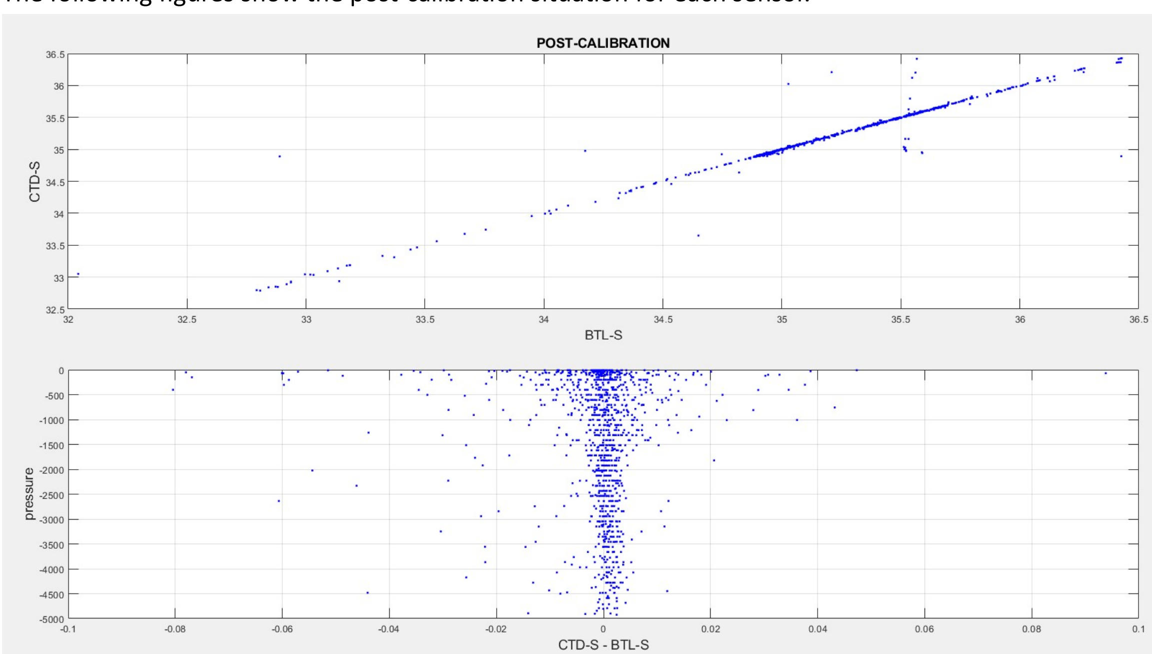


Figure 17: . Scatter plot showing the relation between CTD-salinity (primary sensor) and bottle-salinity and the vertical distribution of the differences between CTD-salinity (primary sensor) and bottle-salinity after applying the slope correction

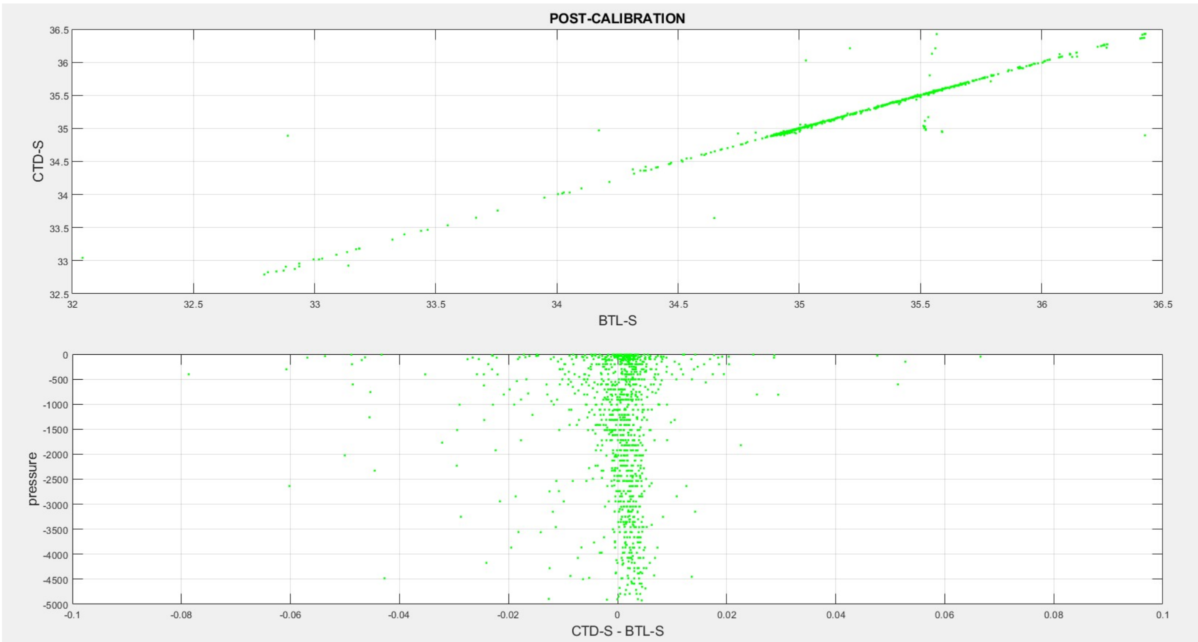


Figure 18: . Scatter plot showing the relation between CTD-salinity (secondary sensor) and bottle-salinity and the vertical distribution of the differences between CTD-salinity (secondary sensor) and bottle-salinity after applying the slope correction

3.4. Field Calibrations, Oxygen

Due to the drift effect observed in the SBE 43 oxygen sensor, it is strongly recommended to correct the sensor response by adjusting the calibration coefficients using Winkler titration measurements, which serve as reference values for oxygen concentrations (Uchida et al., 2010; Coppola et al. (2018).

Step 1: Data status assessment

This step is involves aligning the upcast CTD profiles with the corresponding upcast water sample data based on pressure. This process includes importing all relevant .BTL files and merging them with the Winkler .XLS data. it is essential to ensure that all datasets are in a consistent format and that units are standardized, specially, oxygen concentrations should be expressed in µmol/kg. Then, we investigate the sensor's performance by plotting the residuals calculated as (Winkler - SBE43)

The analysis of these residuals reveals a trend of increasing values from the surface down to 2000 dbar. Below 2000 dbar, the residuals appear to stabilize and minimal variation.

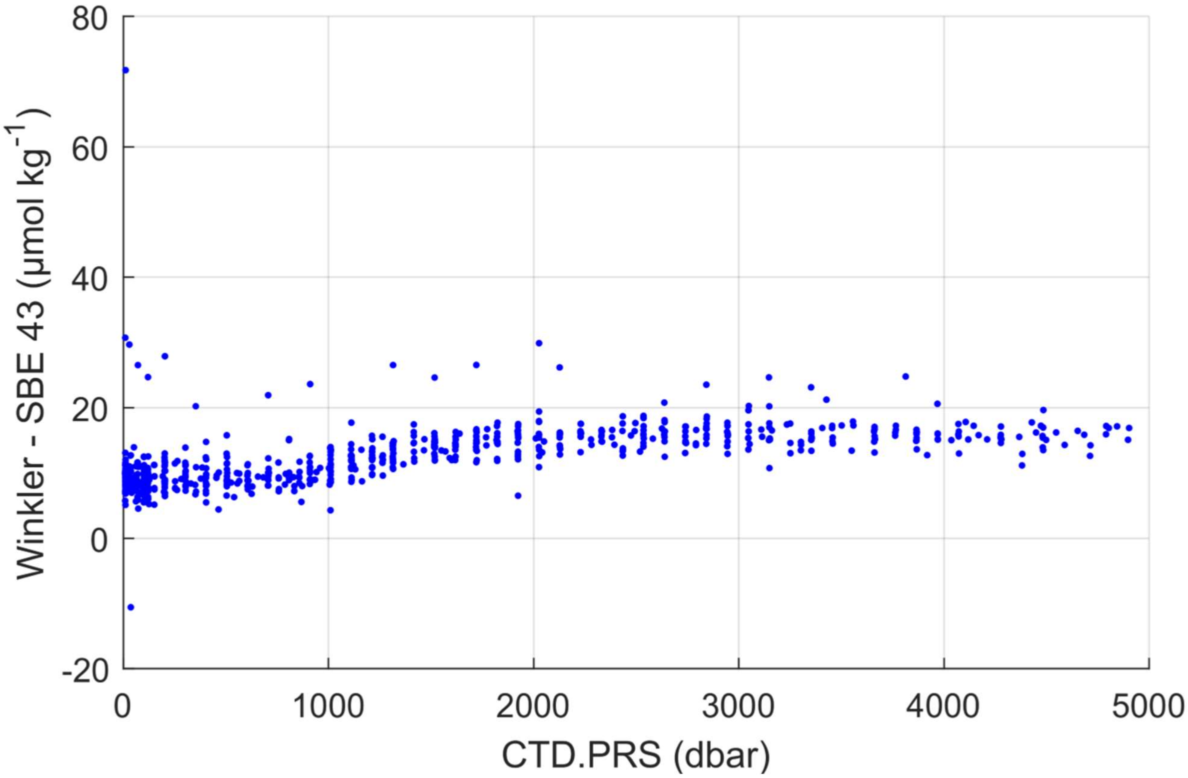
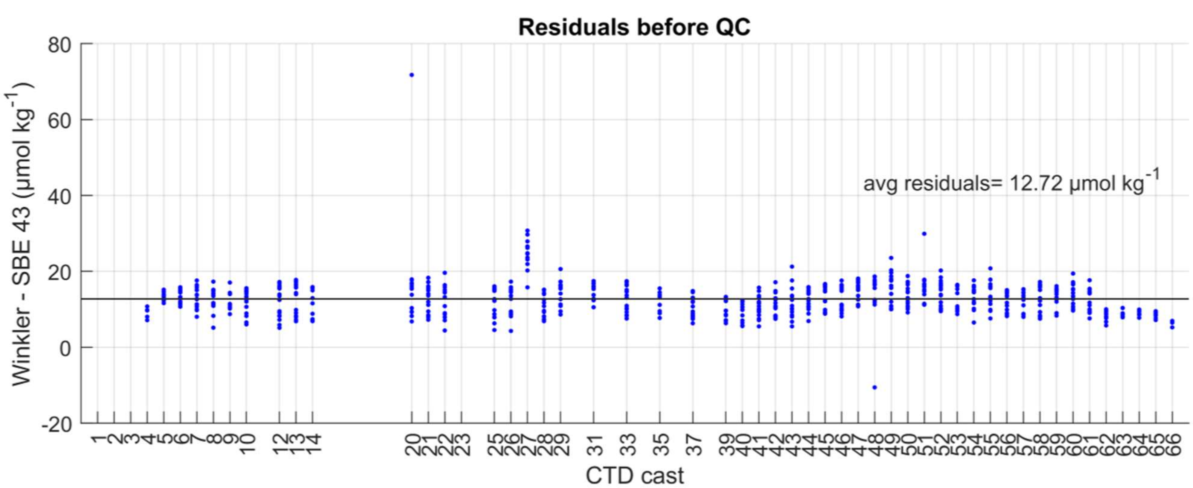


Figure 1. difference between Winkler and SBE43

Step 2: outlier identification

Based on the residual plot presented above, specific stations exhibiting anomalies have been identified. The following Winkler measurement issues were detected:

Station 51 one sample (bottle 12) was flagged as Winkler outlier.
Station 48: one sample (bottle 23) at the surface showed a lower value than that indicated by the sensor.



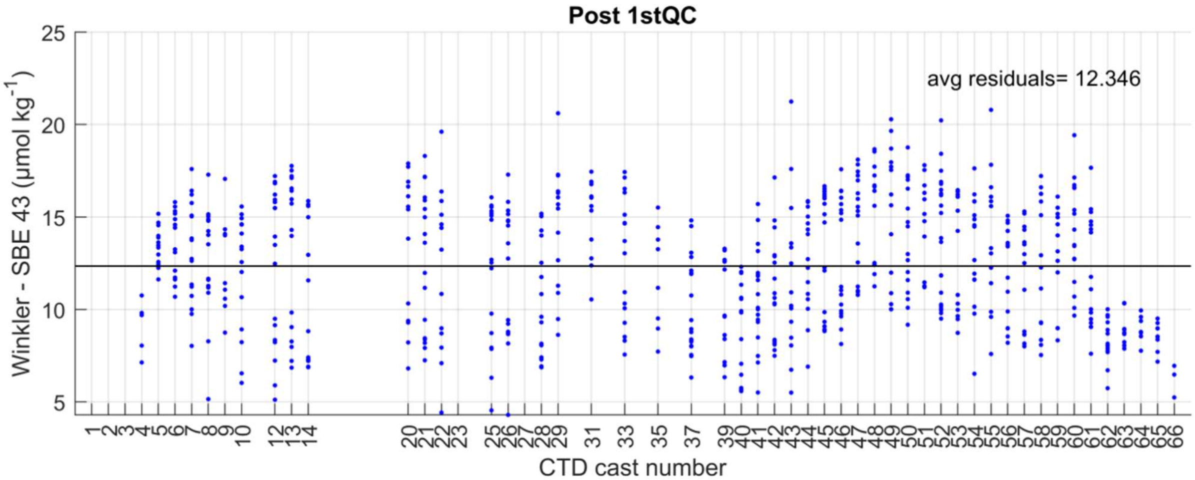


Figure 2. Differences Winkler, SBE43 sensor versus CTD stations.

After removing the outliers (Fig3), Winkler measurements were 12.34 µmol kg^{-1} higher than the sensor.

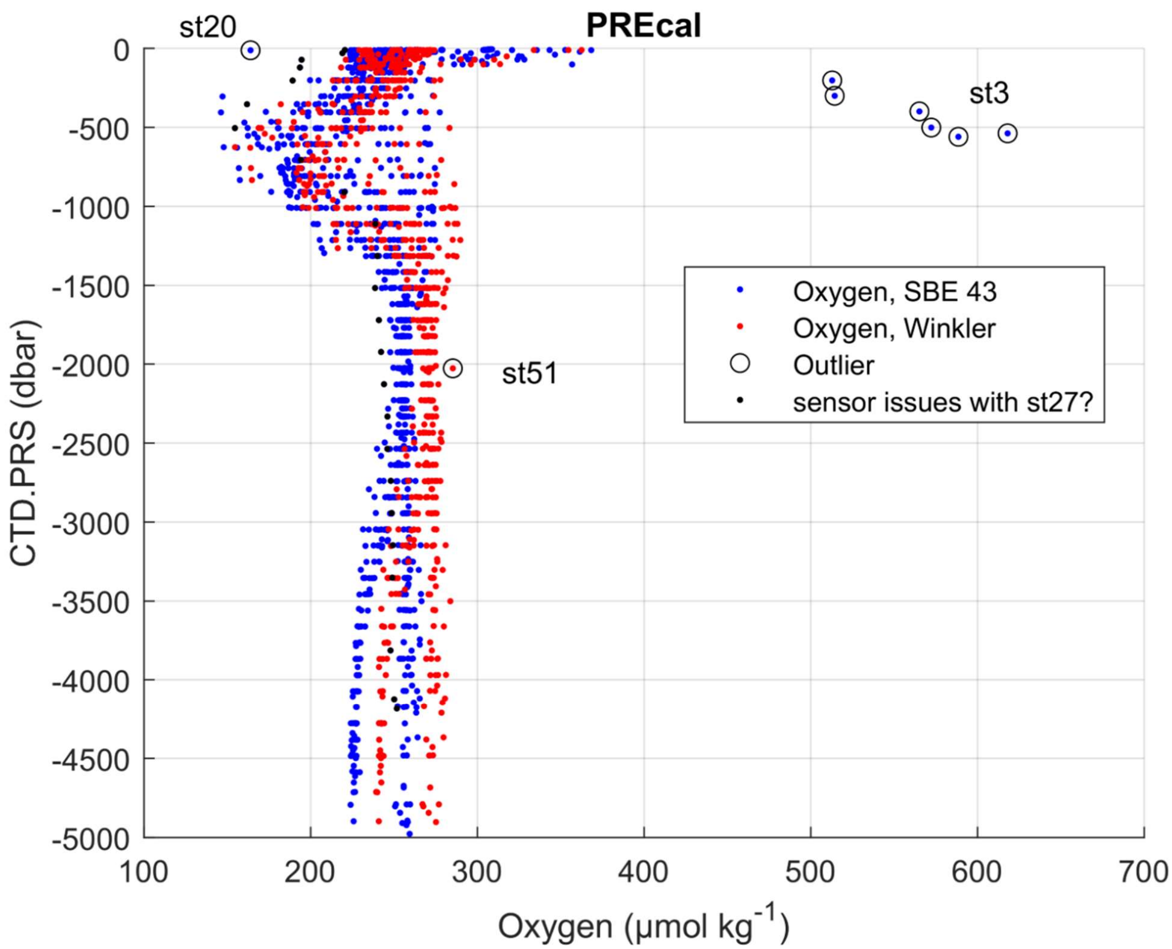


Figure 3. Oxygen data from SBE43 sensor and Winkler values versus pressure.

Step 4: Minimization of Residuals

This step focuses on minimizing the residuals of the squared differences between the calibrated oxygen sensor and the Winkler measurements by adjusting the calibration coefficient: SOC for the slope, VOffset for the offset and E for the pressure correction.

We plot the ratio= Winkler/ SBE43 (Fig.4) to identify any remaining abnormal measurements, which will then be removed. Data reveals a consistent ratio around 1.0511. No measurements are removed.

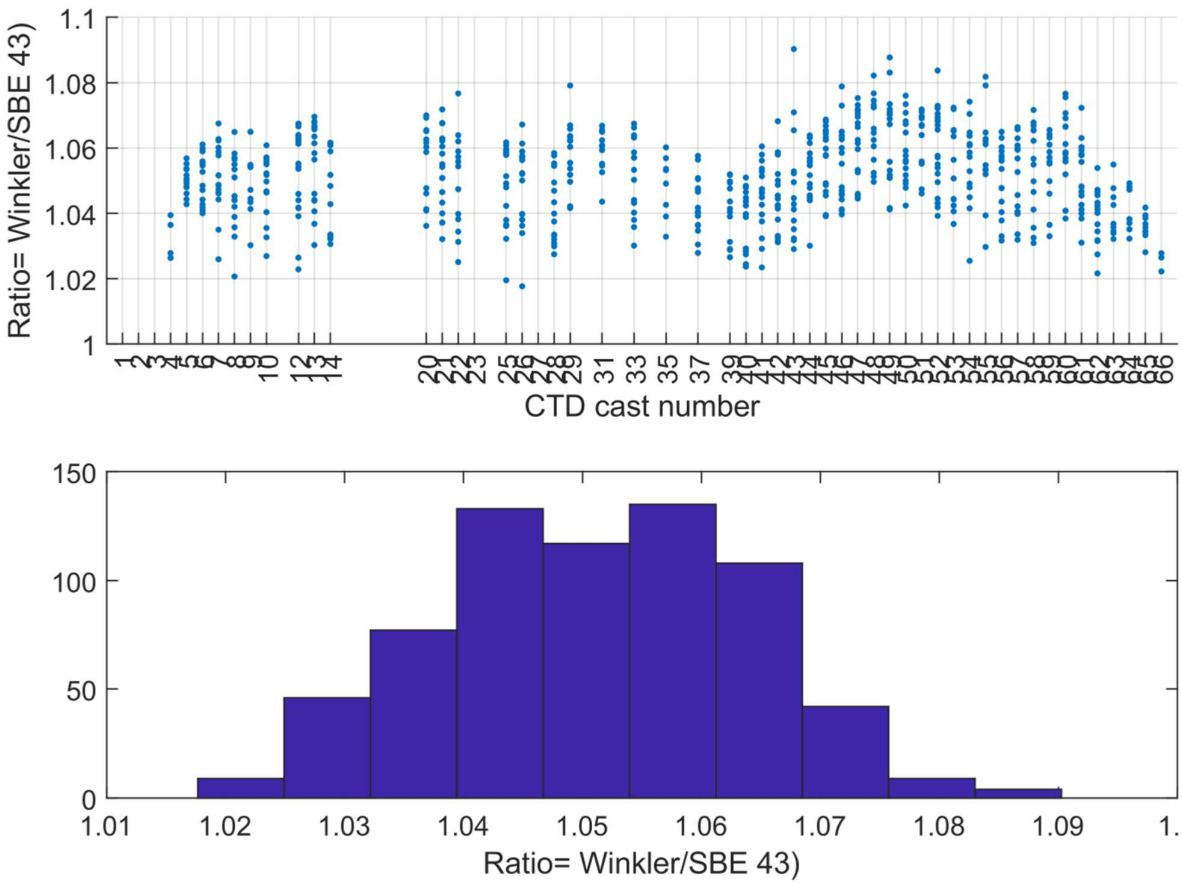


Figure 4. Ratio of Winkler/SBE43 versus CTD stations.

Next, we employ the solver function in excel, starting with the original calibration coefficients presented in table 1, to minimize the residuals of the squared differences between the calibrated oxygen sensor and the Winkler.

Following adjustments to the calibration coefficients in accordance with Seabird's recommendations (APPLICATION NOTE, AN64-2(https://www.seabird.com/oxygen-sensors/sbe-43-dissolved-oxygen-sensor/family-downloads?productCategoryId=54627869932) , we apply the formula outlined below:

$$Oxygen\ (ml/l) = \left\{ Soc * \left(V + Voffset + tau(T,P) * \frac{\partial V}{\partial t} \right) \right\} * Oxsol(T,S) * \left(1.0 + A*T + B*T^2 + C*T^3\right) * e^{\left(\frac{E*P}{K}\right)} \qquad eqn\ 1$$

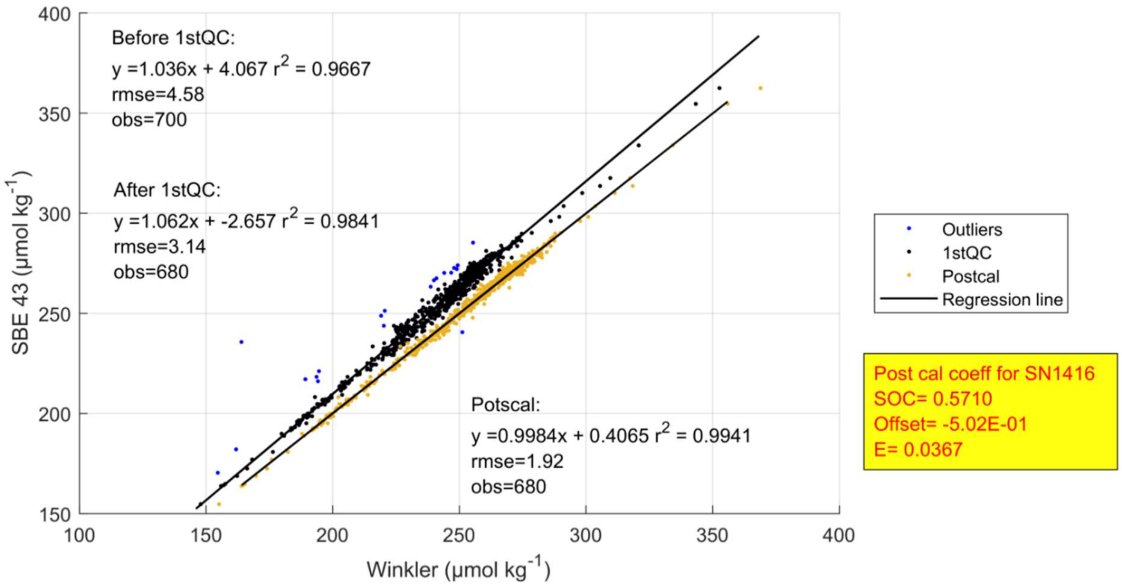
where:

- V = SBE 43 output voltage signal (volts)
- $\partial V/\partial t$ = time derivative of SBE 43 output signal (volts/second), computed over a default window of 2 seconds
- T = CTD temperature (°C)
- S = CTD salinity (psu)
- P = CTD pressure (dbars)
- K = CTD temperature (°K = °C + 273.15)
- *tau(T,P)* = sensor time constant at temperature and pressure
- *Oxsol(T,S)* = oxygen solubility function (ml/L), which converts oxygen partial pressure (sensor measurement) to oxygen concentration (*Garcia and Gordon, 1992*). See Appendix A in *Application Note 64: Background Information, Deployment Recommendations, and Cleaning and Storage* for values at various temperatures and salinities.
- *Soc, Voffset, A, B, C, E*, and *tau20, D1, D2* [terms in calculation of *tau (T,P)*] are calibration coefficients

Table 1. Calibration coefficients for SBE43 SN1416.

Coefficient	**New**	**Original**
Soc	**0.5710**	**0.5518**
Offset	**-5.02E-01**	**-5.09E-01**
A	-0.002519	-0.002519
B	0.000127	0.000127
C	-0.000002	-0.000002
E	0.0367	0.036
Tau20	1.340	1.340
D0	2.5826	2.5826
D1	0.000193	0.000193
D2	-0.046480	-0.046480
H1	-0.033000	-0.033000
H2	5000.00	5000.00
H3	1.45E+03	1.45E+03

Figure 5 illustrated the relationship between SBE43 and Winkler measurements before 1st quality check, after quality control procedures, and following the application of post calibration coefficients



4. Reprocessing raw files

After the coefficients for conductivity and dissolved oxygen were calculated by comparing bottle data with salinometer and Winkler data, the -hex files have been reprocessed with the SBE Data Processing Software, following the same procedure already described, and with new configuration files that contained the new coefficients (one single modified con file was used from station 4 onward, while for 1-3 the configuration files were modified individually, and only for conductivitiies).

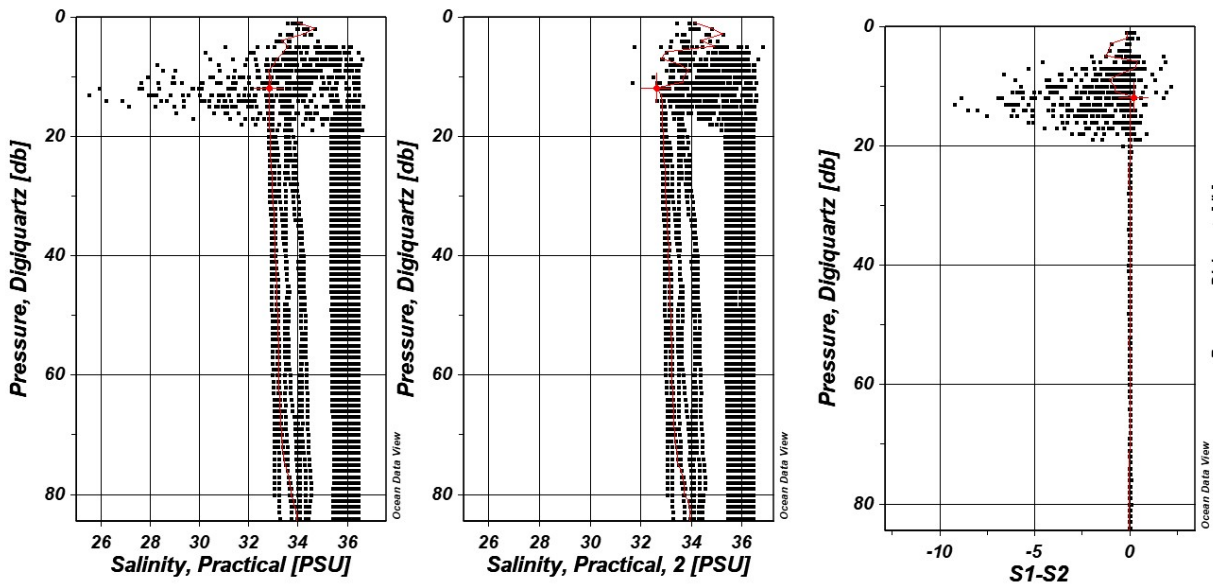
5. Manual and automated Quality Assurance (QA) Process

The reprocessed data (downcast, bin averaged over 1dbar) are collected in a single txt file (ODV format for rapid visualization). ODV was used to detect and flag anomalies and outliers. The flags used were:

0= good data quality

8= bad data quality

The very high and low, and even negative, salinities (Sal1, Sal2) in the surface layer were flagged. There is a zone between 5 and 20 dbar where in many stations the primary salinity is 5-10 units lower than the secondary salinity. Here the primary salinity data have been flagged as well.



Station 3 oxygen data were completely flagged from surface to bottom. All negative Oxygen values were also flagged as "bad".