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RV *Investigator* CTD Data Processing Report

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|------------------------|--|
| Voyage ID | IN2022_T01 |
| Voyage Title | Transit: Cairns to Darwin 2022 |
| Depart | Cairns, 10 September 2022, 23:26 UTC |
| Return | Darwin, 16 September 2022, 22:49 UTC |
| Chief Scientist | N/A |
| Data Processor | Stephanie Petillo (CSIRO – E&T Data Acquisition & Processing) |

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| 9 March 2023 | 1.0 | Stephanie Petillo | Initial version |
| 24 March 2023 | 1.1 | Stephanie Petillo, Steven Van Graas | Updates from initial review |
| 12 April 2023 | 1.2 | Stephanie Petillo, Steven Van Graas | Final updates |

Contents

| | | |
|-----|--|----|
| 1 | Summary..... | 3 |
| 1.1 | Voyage Track | 4 |
| 2 | Data Processing..... | 4 |
| 2.1 | Background Information..... | 4 |
| 2.2 | Pressure and Temperature Calibration | 5 |
| 2.3 | Conductivity Calibration | 7 |
| 2.4 | Dissolved Oxygen Sensor Calibration | 10 |
| 2.5 | Other Sensors | 12 |
| 2.6 | Bad-Data Detection | 13 |
| 2.7 | Heave Filtering..... | 13 |
| 2.8 | Temperature-Conductivity Lag..... | 13 |
| 2.9 | Averaging | 14 |
| 3 | References | 15 |
| 4 | Appendices | 16 |

1 Summary

The primary objective of this voyage was to transit the RV Investigator from Cairns to Darwin between scientific voyages and to allow time for underway training, repairs, and maintenance. Additionally, some opportunistic science operations were undertaken.

Science operations on board included one CTD deployment and water sampling immediately prior to a BGC-Argo float deployment, as well as geophysical mapping enroute (diverting somewhat for improved coverage), with a focus on the reef's edge for Project 3D-GBR.

This report describes the production of quality controlled, calibrated CTD data from RV *Investigator* voyage IN2022_T01.

Data for 1 CTD deployment were acquired using the Sea-Bird SBE911 CTD unit #22 (S/N 1039), fitted with 36 twelve-litre bottles on the rosette sampler. Sea-Bird-supplied calibration factors were used to compute the pressures and preliminary conductivity values. CSIRO-supplied calibrations were applied to the temperature data. The data were subjected to automated QC to remove spikes and out-of-range values.

During the deployment, the Niskin bottles labelled #18 & #19 were in swapped positions on the rosette. The bottle in *position* #19 was not fired at the planned depth (which was the chlorophyll maximum), but it was fired at the next depth stop. This was accounted for in the hydrology data and did not impact processing or data quality.

The final conductivity calibration from the secondary sensor had a standard deviation (SD) of 0.0024157 PSU, outside our target of 'less than 0.002 PSU'. The standard product of 1-decibar binned averages were produced using data from the secondary sensors.

The dissolved oxygen data calibration fit had a SD of 0.85269 μM . The agreement between the CTD and bottle data was good.

An ECO Triplet was also installed on the auxiliary A/D channels of the CTD, and its data were logged in Seasave with calibration values applied. The only processing applied by CapPro was NaN filtering, and the resulting ECO Triplet data are present in the average file.

To access the full voyage plan and other reports and data associated with this voyage, please see the contact information at the end of this report.

1.1 Voyage Track

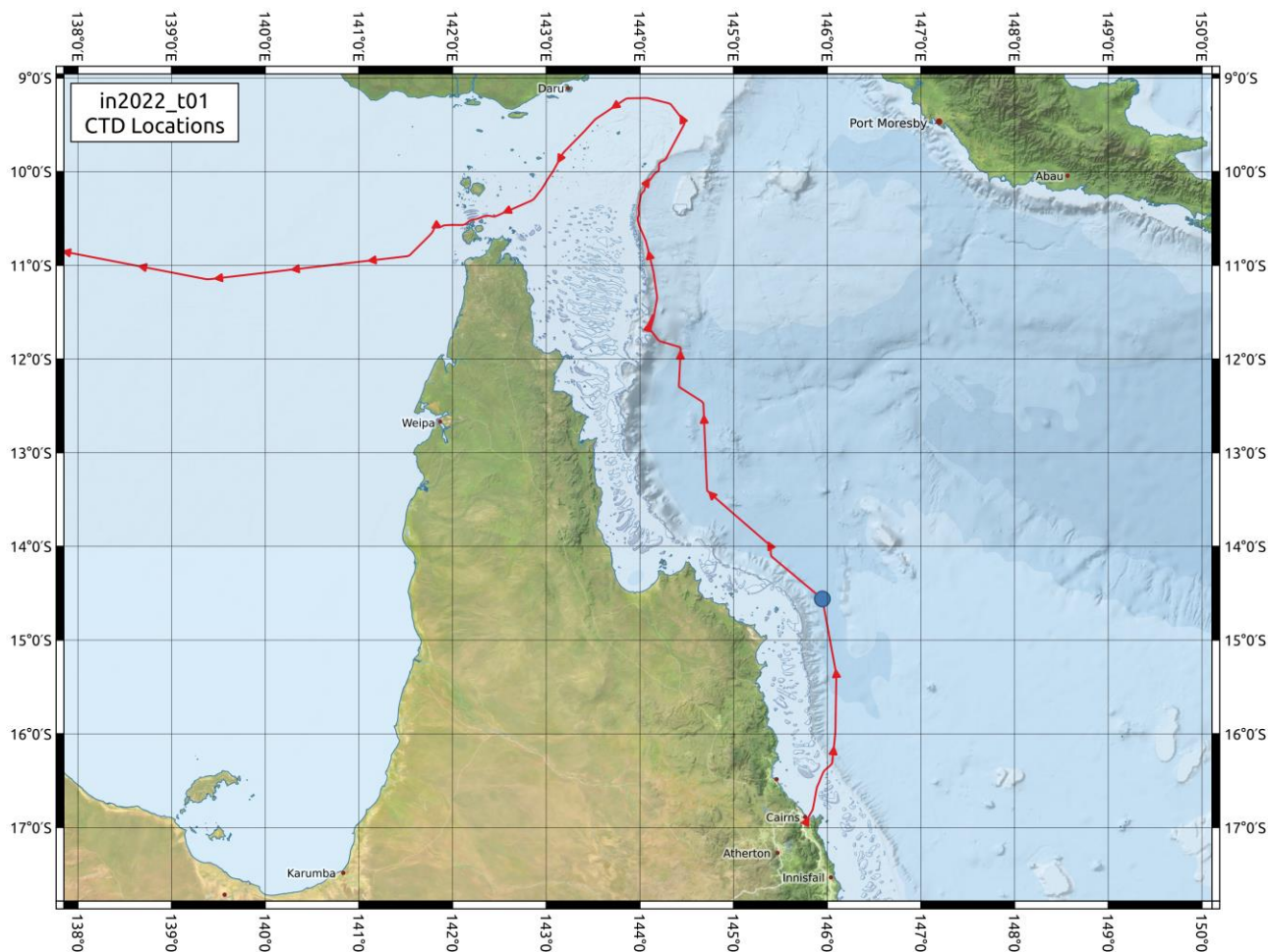


Figure 1: Voyage track with CTD cast locations

2 Data Processing

2.1 Background Information

1 CTD deployment was conducted on this voyage prior to the BGC-Argo float deployment. The data were acquired with the CSIRO CTD unit #22 (S/N 1039), a Sea-Bird SBE911 with dual conductivity and temperature sensors.

The CTD was additionally fitted with SBE43 dissolved oxygen sensors, an LADCP, a PAR sensor, a transmissometer, and CDOM, Chlorophyll-a and scattering sensors. These sensors are described in Table 1.

| Sensor Description | Model | Serial No. | A/D Channel | Calibration Date | Calibration Source |
|-----------------------|---------------------|------------|-------------|------------------|--------------------|
| Pressure | Digiquartz 410K-134 | 1039 | P | 21-Apr-2022 | Sea-Bird |
| Primary Temperature | Sea-Bird SBE3plus | 4722 | T0 | 11-Jun-2022 | Sea-Bird |
| Secondary Temperature | Sea-Bird SBE3plus | 6022 | T1 | 9-Oct-2021 | Sea-Bird |
| Primary Conductivity | Sea-Bird SBE4C | 4662 | C0 | 6-Apr-2022 | Sea-Bird |

| | | | | | |
|----------------------------|------------------------|--------|----|-------------|------------------|
| Secondary Conductivity | Sea-Bird SBE4C | 4685 | C1 | 3-Jun-2022 | Sea-Bird |
| Primary Dissolved Oxygen | SBE43 | 1794 | A0 | 16-Nov-2021 | Sea-Bird |
| Secondary Dissolved Oxygen | SBE43 | 3155 | A1 | 21-Dec-2021 | Sea-Bird |
| Altimeter | Tritech PA500 | 316739 | A2 | 7-May-2019 | Tritech |
| PAR | Biospherical QCP2300HP | 70562 | A3 | 14-Sep-2021 | Biospherical |
| Transmissometer | Wetlabs C-Star | 1735DR | A4 | 16-Jun-2021 | Wetlabs/Sea-Bird |
| CDOM | Wetlabs ECO FLCDRTD | 7138 | A5 | 8-Dec-2021 | Wetlabs |
| Chlorophyll-a | Wetlabs ECO FLBBRTD | 6890 | A6 | 27-Jul-2021 | Wetlabs/Sea-Bird |
| Scattering | Wetlabs ECO FLBBRTD | 6890 | A7 | 27-Jul-2021 | Wetlabs/Sea-Bird |

| | | | | | |
|----------------------|------------------|-------|----------|--|--|
| Additional Payloads: | | | | | |
| LADCP Slave (Up) | Teledyne 300 kHz | 24502 | Internal | | |
| LADCP Master (Down) | Teledyne 150 kHz | 16710 | Internal | | |

Table 1: CTD Sensor configuration on IN2022_T01

Water samples were collected using a Sea-Bird SBE32, 36-bottle rosette sampler. Sampling was from 26 out of the 36 twelve-litre bottles which were fitted to the frame.

The raw CTD data were collected in SBE SeaSave version 7.26.4.0, converted to scientific units using SBE Data Processing version 7.26.4.0 and written to NetCDF files with CNV_to_Scan (cnv_to_scan_ui2.py, from the CSIRO MNF Data Acquisition and Processing “marinotech” git repository) for processing using the MATLAB-based CapPro software.

The CapPro software version 2.12 was used to apply automated QC and preliminary processing to the data. This included spike removal, identification of water entry and exit times, conductivity sensor lag corrections, conductivity cell thermal inertia corrections, and the determination of the pressure offsets. It also loaded the hydrology data and computed the matching CTD sample burst data (i.e., averaged sensor data) for water-sample-to-sensor data comparisons. The automatically determined pressure offsets and in-water points were inspected and verified during data processing.

The bottle sample data were used to compute final conductivity and dissolved oxygen calibrations. These were applied to the data, after which files of binned 1-decibar averaged data were produced.

2.2 Pressure and Temperature Calibration

The pressure offsets for each deployment are plotted in Figure 2. The blue circles refer to initial out-of-water values (beginning of downcast) and the red circles the final out-of-water values (end of upcast).

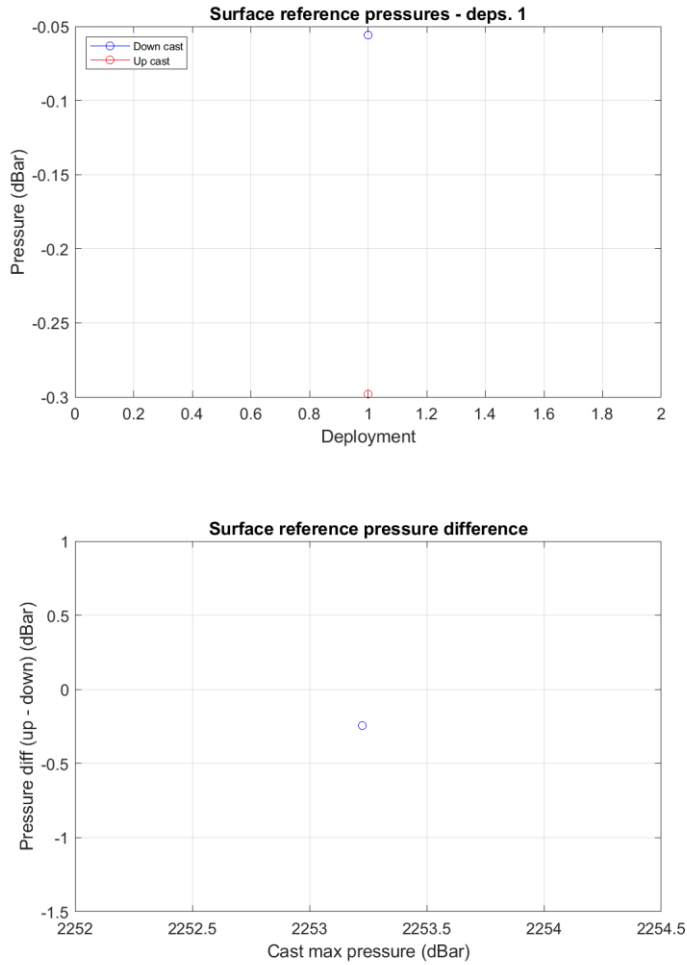


Figure 2: CTD pressure offsets

The difference between the primary and secondary temperature sensors at the bottle sampling depths is plotted in Figure 3. Most deployments plot within ± 0.001 °C of zero – outliers result from sampling in regions of high vertical temperature gradient. Since there was only one CTD deployment on this voyage, no trends can be deduced from the mean difference (red + markers) between the primary and secondary temperature.

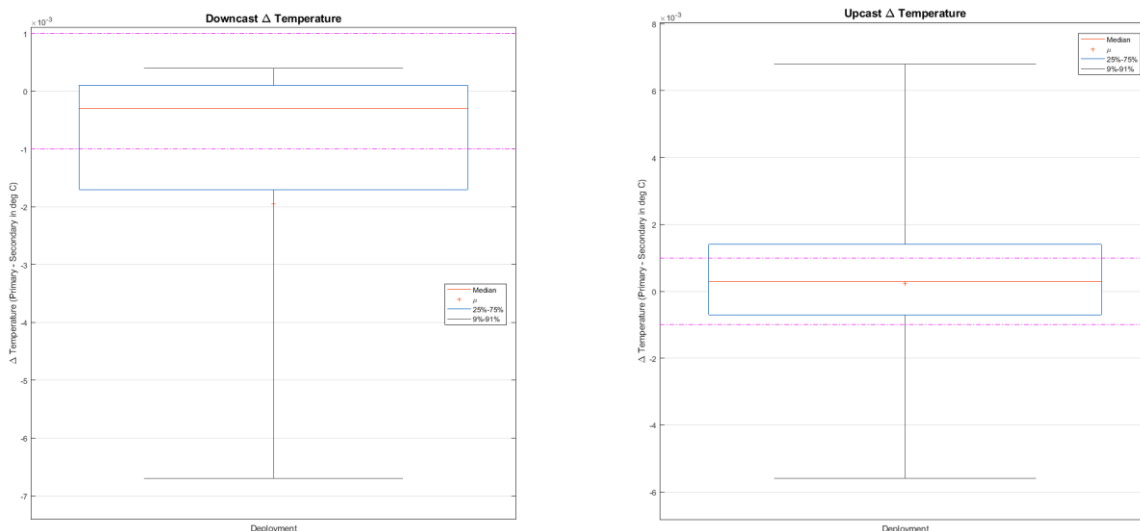


Figure 3: Difference (primary - secondary) between temperature sensor values on downcast (left) and upcast (right)

2.3 Conductivity Calibration

If any discrepancies or sampling problems occurred during bottle salinity sampling or between primary and secondary CTD conductivity measurements, these would show in the conductivity calibration plots in Figure 4. We observed discrepancies based on these calibration results. These discrepancies were due to a large percentage of points being located within the halocline region. The profile plots showing the thermocline and halocline ranges are in Figure 5.

The calibrations were based upon the percent of ‘good’ sample data (16 good samples from the primary unit and 16 good samples from the secondary unit), out of a total of 26 samples taken during deployments. To perform the calibration with the preferred (default) CapPro calibration settings, a minimum of 70% of the samples need to be in the ‘good’ range. If there is an insufficient number of good samples for a unit, the conductivity difference ‘cutoff’ value must be increased to continue with the calibration process in CapPro. For this set of conductivity calibrations, the cutoff values used were 0.006 (primary) and 0.006 (secondary).

Figure 4 plots CTD - bottle salinity differences for both upcast (Hydro bottle) and downcast (CTD SBE43) data. The ‘bad’ outliers (magenta dots, red dots and red + markers) are excluded from the calibration, the ‘suspect’ outliers (blue dots) are used in the calibration but are weighted based on their distance from the mean. All green dots are considered ‘good’ data points and are not weighted based on distance from the mean.

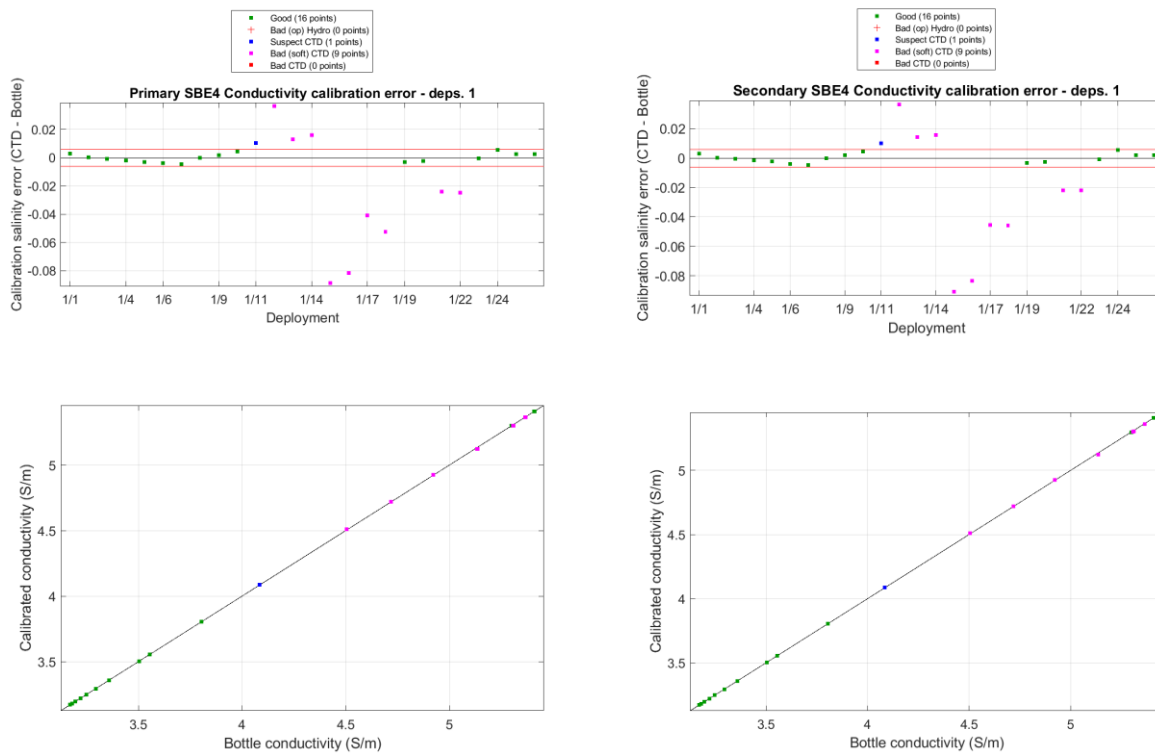


Figure 4: CTD - bottle conductivity difference and salinity calibration error (left: primary, right: secondary)

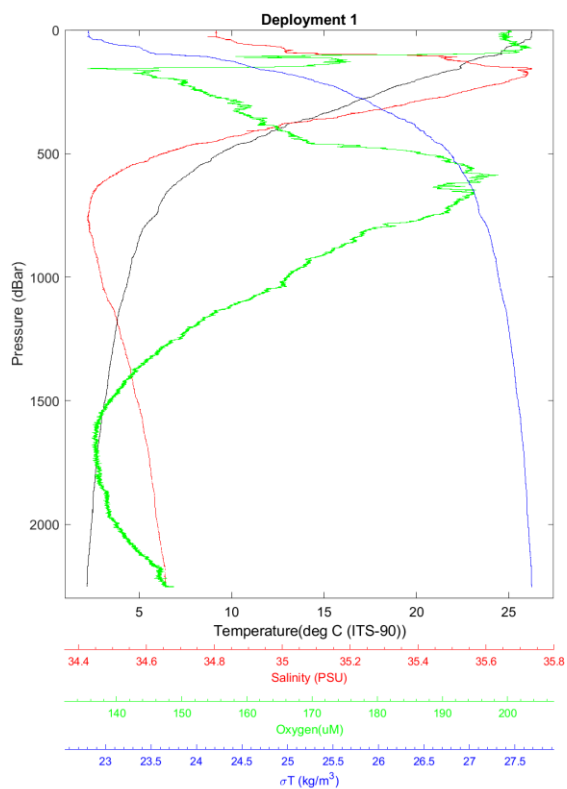


Figure 5: Temperature, salinity, dissolved oxygen and σ_T profiles

The box plot (Figure 6) of calibrated downcast conductivities (primary - secondary) at the bottle sampling depths for all deployments shows that the calibrated primary and secondary conductivity cell responses corresponded reasonably well to each other.

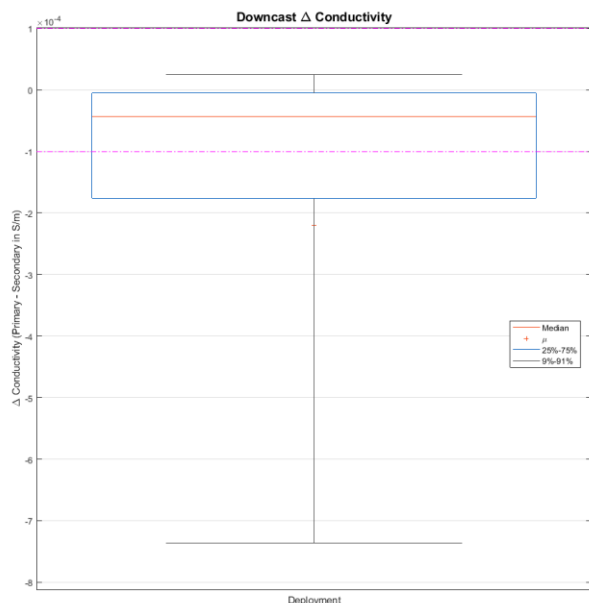


Figure 6: Difference (primary - secondary) between conductivity sensor values on downcast

The final results for the primary and secondary conductivity sensors with respect to their original calibrations are shown in Table 2 and Table 3.

| Sensor Group | Deployments | Scale Factor | | Offset | | Salinity (PSU) | |
|--------------|-------------|--------------|-----------|-------------|----------|----------------|-----------|
| | | a1 | ± | a0 | ± | Residual SD | M.A.D. |
| Primary | 1 | 1.0002 | 0.0038809 | -1.0809e-03 | 0.019912 | 0.0024925 | 0.0023744 |
| Secondary | 1 | 1.0003 | 0.0037898 | -1.786e-03 | 0.019444 | 0.0024157 | 0.002389 |

Table 2: Conductivity calibration with respect to manufacturer’s calibration coefficients and post-calibration results

| Conductivity Sensor | Deployments | CPcor | ± |
|---------------------|-------------|-------------|------------|
| Primary | 1 | -2.8937e-07 | 1.8059e-06 |
| Secondary | 1 | -2.6996e-07 | 1.7627e-06 |

Table 3: Calculated CPcor (the correction for pressure effects on the conductivity cell) for primary and secondary conductivity units compared to the manufacturer’s nominal value of -9.5700e-08 (for pressure in decibars) (Sea-Bird, 2017)

This is a marginal calibration. We normally aim for a SD of 0.002 PSU (or less) for ‘typical’ oceanographic voyages. The above calibration factors were applied to the indicated deployments. Full plots of residuals before and after calibration are available in A.1.

Data from the secondary conductivity and temperature sensors were used to produce the averaged salinities (these data variables have no suffix) with primary sensors included with a suffix ‘_2’.

2.4 Dissolved Oxygen Sensor Calibration

2.4.1 SBE Calibration Procedure

(Sea-Bird, 2013) describes the SBE43 dissolved oxygen sensor as “a polarographic membrane oxygen sensor having a single output signal of 0 to +5 volts, which is proportional to the temperature-compensated current flow occurring when oxygen is reacted inside the membrane. A Sea-Bird CTD that is equipped with an SBE43 oxygen sensor records this voltage for later conversion to oxygen concentration, using a modified version of the algorithm by Owens and Millard (1985).”

Calibration involves performing a linear regression, as per (Sea-Bird, 2012) to produce new estimates of the calibration coefficients Soc and $Voffset$. These new coefficients are used, along with the other, manufacturer-supplied coefficients, to derive oxygen concentrations from the sensor voltages.

2.4.2 Results

Deeper casts (>1000m) are known to be affected by pressure-induced hysteresis with this sensor. This is corrected automatically within CapPro using the method discussed in (Sea-Bird, 2014).

There is a small mismatch between downcast and upcast dissolved oxygen due to the response time of the sensor. No correction for the sensor lag effect has been applied.

A single calibration group was used with the associated SBE43 upcast data to compute the new Soc and $Voffset$ coefficients. Figure 7 plots CTD SBE43 - bottle oxygen differences for both upcast (Hydro bottle) and downcast (CTD SBE43) data. The ‘bad’ outliers (magenta dots, red dots and red + markers) are excluded from the calibration, the ‘suspect’ outliers (blue dots) are used in the calibration but are weighted based on their distance from the mean. All green dots are considered ‘good’ data points and are not weighted based on distance from the mean.

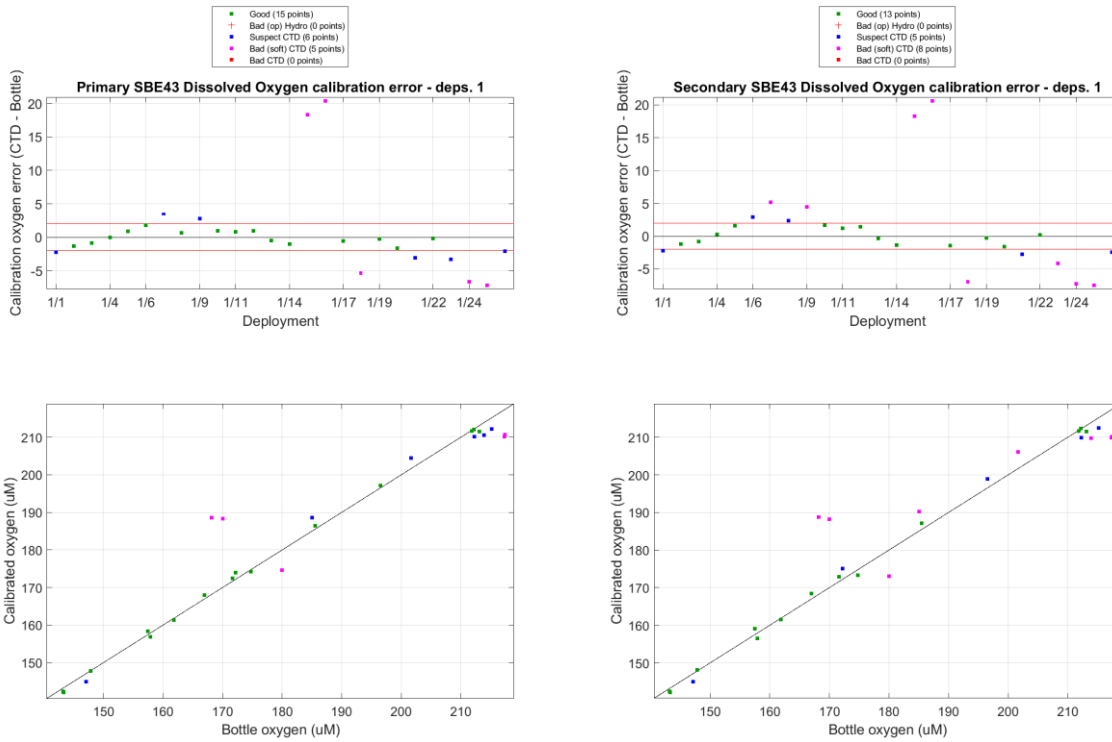


Figure 7: CTD SBE43 - bottle dissolved oxygen difference and calibration error (left: primary, right: secondary)

The box plot (Figure 8) of calibrated downcast dissolved oxygen readings (primary - secondary) at the bottle sampling depths for all deployments shows that the calibrated primary and secondary dissolved oxygen sensor responses corresponded very well to each other.

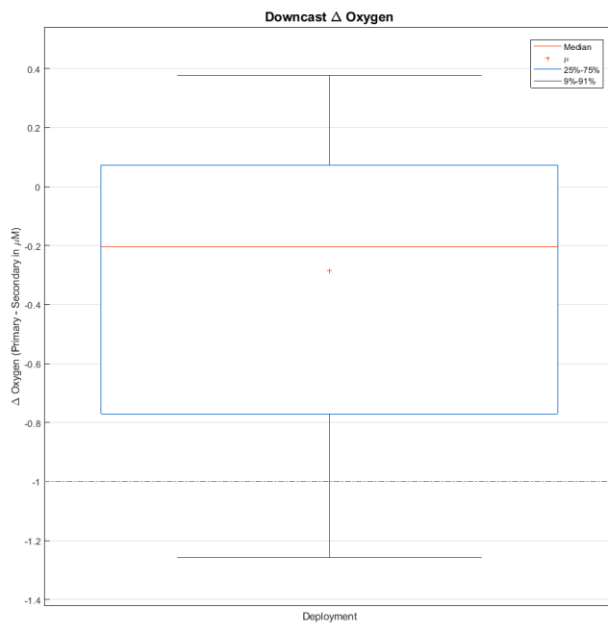


Figure 8: Difference (primary - secondary) between dissolved oxygen sensor values on downcast

The old and new *Soc* and *Voffset* values for DO sensors are listed in Table 4. The *Soc* value is a linear slope scaling coefficient; *Voffset* is the fixed sensor voltage at zero oxygen. Full plots of residuals before and after calibration are available in A.2.

The calibrations were applied for each sensor and the averaged files were created using the result from the secondary sensor.

| Sensor | Calibration Source | Deployments | Calibration Coefficients | | | | Dissolved Oxygen (μM) | |
|--------------|--------------------|-------------|--------------------------|----------|------------|-----------|------------------------------------|---------|
| | | | <i>Voffset</i> | \pm | <i>Soc</i> | \pm | Residual SD | M.A.D. |
| Primary DO | CapPro | 1 | -0.49821 | 0.011703 | 0.50197 | 0.0048796 | 1.0613 | 0.95748 |
| | Sea-Bird | 1 | -0.4772 | | 0.47054 | | | |
| Secondary DO | CapPro | 1 | -0.5392 | 0.011146 | 0.56592 | 0.0060009 | 0.85269 | 1.4313 |
| | Sea-Bird | 1 | -0.5105 | | 0.50954 | | | |

Table 4: Dissolved oxygen calibrations

2.5 Other Sensors

2.5.1 C-Star Transmissometer

The C-Star transmissometer was used on all deployments. It was calibrated by the manufacturer with meter outputs with the beam blocked, in air with a clear beam path and with clean water in the path. These values are used to determine a scale and offset for use in SBE Data Processing software to convert the raw counts to a beam transmittance output of 0 - 100 percent.

This sensor worked as expected during this voyage.

2.5.2 WET Labs ECO CDOM Sensor

The WET Labs ECO CDOM (coloured dissolved organic matter) sensor was used for all deployments. The CDOM has been calibrated with manufacturer supplied coefficients.

This sensor worked as expected during this voyage.

2.5.3 WET Labs ECO Fluorometer-Scattering Sensor

The WET Labs ECO Fluorometer-Scattering sensor was used for all deployments. The fluorometer (Chlorophyll-*a*) has been calibrated with manufacturer supplied coefficients to give outputs in mg/m^3 ($= \mu\text{g}/\text{L}$). The scattering (optical backscatter, OBS) has been calibrated with manufacturer supplied coefficients to give volume scattering outputs in $\text{m}^{-1}\text{sr}^{-1}$.

This sensor worked as expected during this voyage.

2.5.4 Biospherical PAR Sensor

The Biospherical PAR (photosynthetically active radiation) sensor was used for all deployments. The output is a nominal 0 - 5 volts which is converted to the unit $\mu\text{Einsteins}/\text{m}^2/\text{second}$ using a manufacturer supplied wet calibration factor and the dark voltage determined at calibration. This data channel has been included in the output files for all deployments. Time of day and environmental factors such as sea state and cloud cover impact these readings. If most or all of the values for a deployment are near zero it indicates a night-time cast. In deployments where the PAR profiles have sub-surface maxima the CTD may have been shaded by the ship.

This sensor worked as expected during this voyage.

2.6 Bad-Data Detection

The value limits for each sensor are configured in CNV_to_Scan conversion software and are written to the NetCDF scan file. Typical limits used for the sensor range and maximum second difference are in Table 5. The rejection rate is recorded in the CapPro processing log file.

| Sensor | Range minimum | Range maximum | Maximum Second Difference |
|------------------|---------------|---------------|---------------------------|
| Pressure | -7 | 6500 | 0.5 |
| Temperature | -2 | 40 | 0.05 |
| Conductivity | -0.01 | 7 | 0.01 |
| Dissolved Oxygen | -1 | 500 | 0.5 |
| Fluorometer | 0 | 100 | 0.5 |
| PAR | -5 | 2000 | 0.5 |
| Transmissometer | 0 | 100 | 0.5 |

Table 5: Sensor limits for bad-data detection

2.7 Heave Filtering

Sensor data impacted by ship heave impeding the CTD deployment is filtered out in three stages and applied during data binning. The first stage detects negative acceleration of the CTD which can cause trailing mixed water to be pumped through the sensors. The second stage looks at all negative density gradients and flags readings which are above 10 times the standard deviation of all negative gradients, for 2 seconds. The third stage flags any pressure reversals which are greater than the height of the CTD sensor pump inlet above the frame.

2.8 Temperature-Conductivity Lag

To precisely align the temperature and conductivity measurements for a sample of water a temporal offset can be applied. A manufacturer-recommended nominal offset (Δt_{C_SBE9+}) of -0.073 seconds is initially applied at time of acquisition by the SBE9+ deck unit on both primary and secondary conductivity channels. This offset advances the conductivity sensor readings in time to

compensate for the amount of time it takes for the measured water sample to move from the temperature sensor through into the conductivity sensor cell.

Post-voyage inspection of the temperature and conductivity data in CapPro can determine fine-tuning adjustments to the conductivity sample time (seconds) offset (Δt_{c_CP}) that will optimally align the data. The final adjustments applied to the conductivity sample time can be found in Table 6 and Table 7. Note that although CapPro can set an offset ('lag', in number of scans, with a scan frequency of 24 Hz) for both temperature and conductivity samples, DAP only sets a lag for the conductivity sample to maintain consistency with the nominal offset applied by the SBE9+ to the conductivity data. The equation governing this conductivity sample time adjustment is given below, where $t_{c_aligned}$ is the best-estimate of the conductivity measurement time (seconds) to align it with the temperature measurement from the same sample of water on the downcast, and t_{c_meas} is the original, uncorrected conductivity measurement time (seconds).

$$t_{c_aligned} = t_{c_meas} + \Delta t_{c_SBE9+} + \Delta t_{c_CP}$$

| Cast # | Nominal Offset Time Applied by SBE9+, Δt_{c_SBE9+} (sec) | Offset ('Cond lag') Set in CapPro (scans) | Calculated Offset Time from CapPro 'Cond lag', Δt_{c_CP} (sec = scans/24 Hz) |
|--------|---|---|---|
| 1 | -0.073 | -0.47 | -0.000019583 |

Table 6: Primary conductivity sensor offset adjustments

| Cast # | Nominal Offset Time Applied by SBE9+, Δt_{c_SBE9+} (sec) | Offset ('Cond lag') Set in CapPro (scans) | Calculated Offset Time from CapPro 'Cond lag', Δt_{c_CP} (sec = scans/24 Hz) |
|--------|---|---|---|
| 1 | -0.073 | -0.13 | -0.000005417 |

Table 7: Secondary conductivity sensor offset adjustments

2.9 Averaging

The calibrated data were 'filtered' to remove pressure reversals and binned into the standard product of 1-decibar averaged NetCDF files. The binned values were calculated by applying a linear, least-squares fit as a function of pressure to the sensor data for each bin, using this to interpolate the value for the bin mid-point. This method is used to avoid possible biases which would result from averaging with respect to time.

Each binned parameter is assigned a quality control (QC) flag (also in the NetCDF files). Our QC flagging scheme is described in (Pender & NCM Information & Data Centre, 2022).

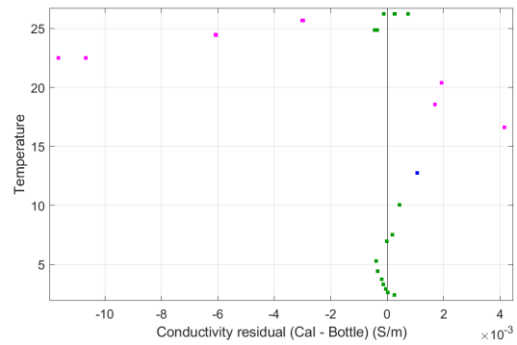
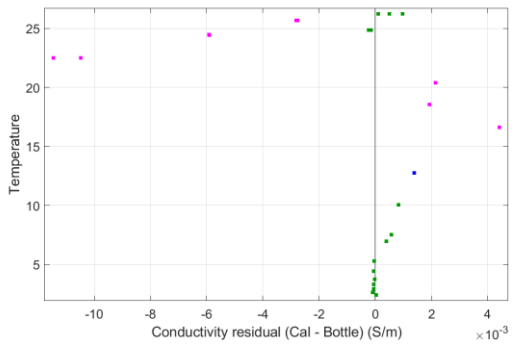
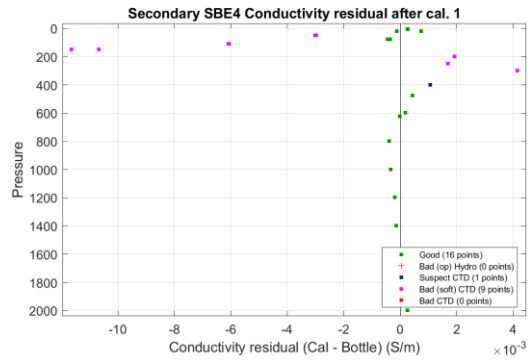
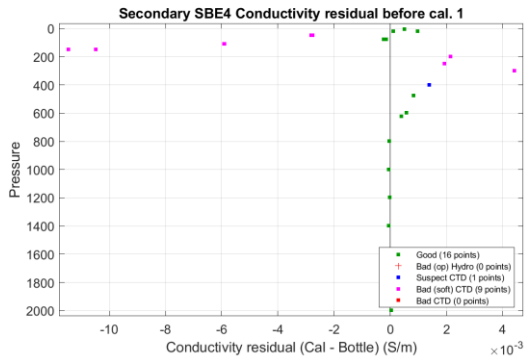
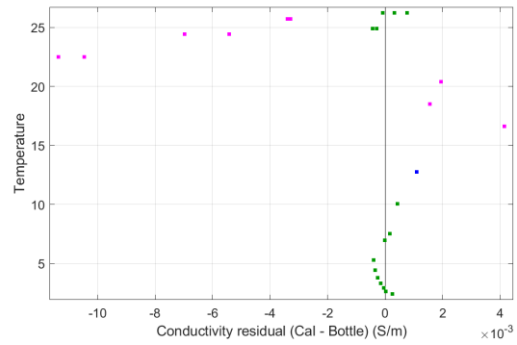
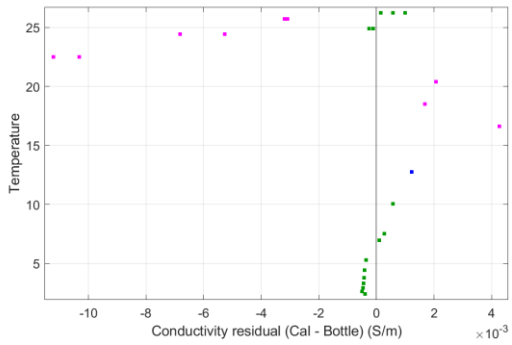
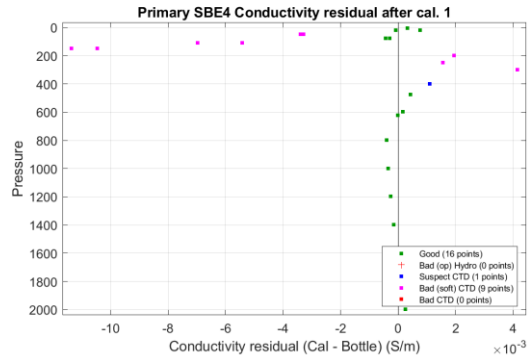
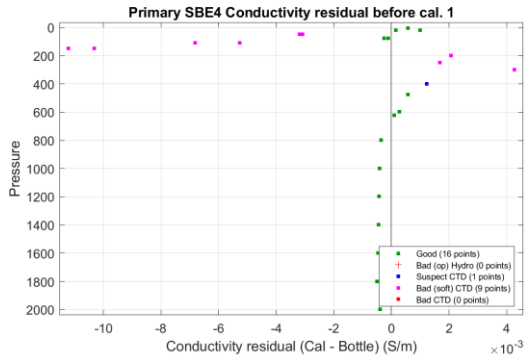
The QC Flag for each bin is estimated from the values for the bin components. The QC Flag for derived quantities, such as salinity and dissolved oxygen, is taken to be the worst of the estimates for the parameters from which they are derived.

3 References

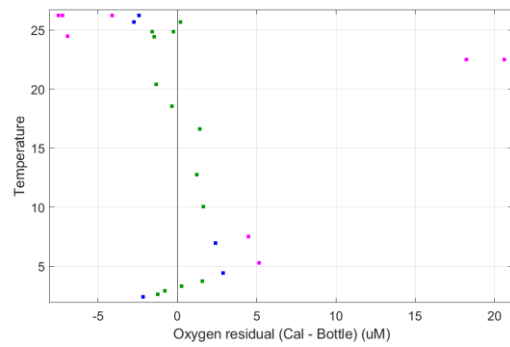
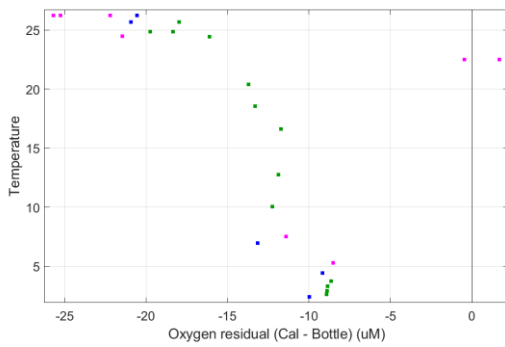
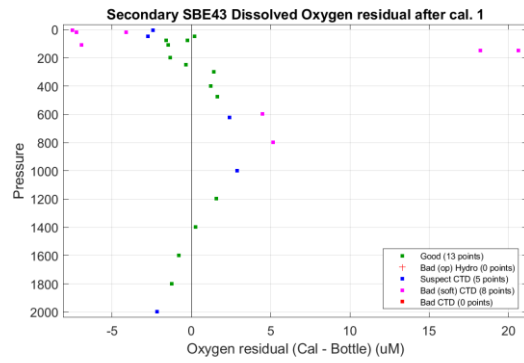
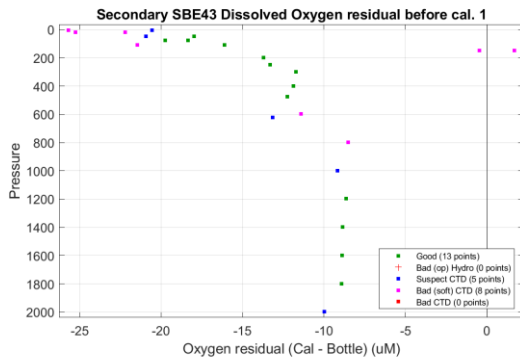
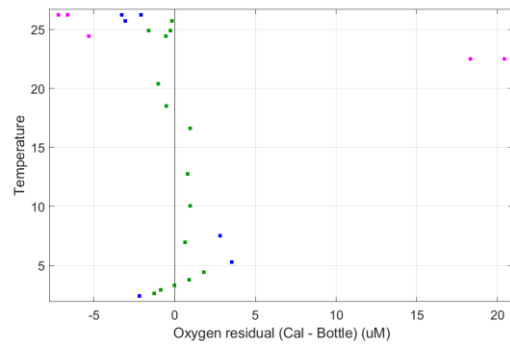
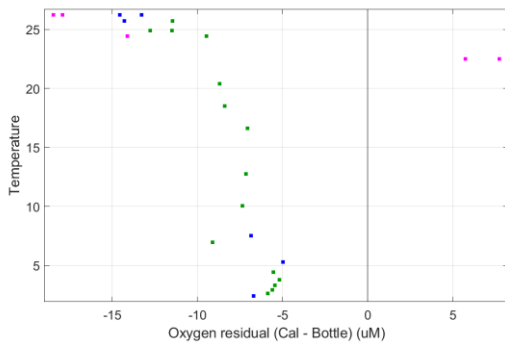
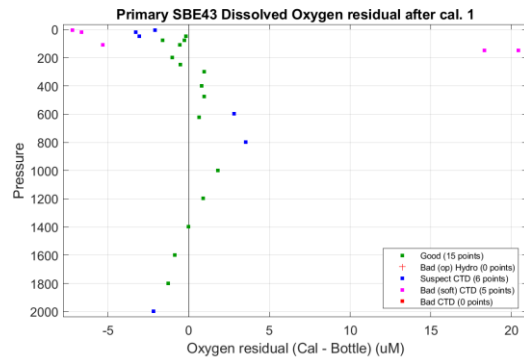
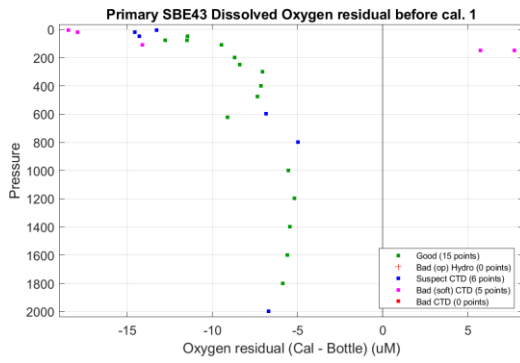
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4 Appendices

A.1 Conductivity Calibration Residual Plots



A.2 Dissolved Oxygen Calibration Residual Plots



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