RV *Investigator*

CTD Processing Report

Voyage ID:	in2020_v10
Voyage title:	IN2020_v10 CTD Processing Report: Storm Bay Modelling
Depart:	Hobart, 0000 Friday, 13 November 2020
Return:	Hobart, 0000 Sunday, 22 November 2020

Document History

Date	Version	Author	Comments
5th May 2021	1.0	Steven van Graas	Initial version

Contents

1 Summary

These notes relate to the production of quality controlled, calibrated CTD data from RV Investigator voyage in2020_v10, from 13 Nov 2020 – 22 Nov 2020.

Data for 9 deployments were acquired using the Sea-Bird SBE911 CTD 24, 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.

The final conductivity calibration was based on a single deployment grouping. The final calibration from the secondary sensor had a standard deviation (SD) of 0.0011549 PSU, well within our target of 'better than 0.002 PSU'. The standard product of 1 decibar binned averaged were produced using data from the secondary sensors.

The dissolved oxygen primary sensor data calibration fit had a SD of 0.38919µM. The agreement between the CTD and bottle data was good.

A PAR, Transmissometer, Chelsea Fluorometer, and Wetlabs Fluorometer were also installed on the auxiliary A/D channels of the CTD.

2 Voyage Details

2.1 Title

IN2020_v10 CTD Processing Report: Storm Bay Modelling

2.2 Principal Investigators

Dr Karen Wild-Allen

2.3 Voyage Objectives

The scientific objectives for in2020_v10 were outlined in the Voyage Plan.

For further details, refer to the Voyage Plan and/or summary which can be viewed on the Marine National Facility web site.

2.4 Area of operation

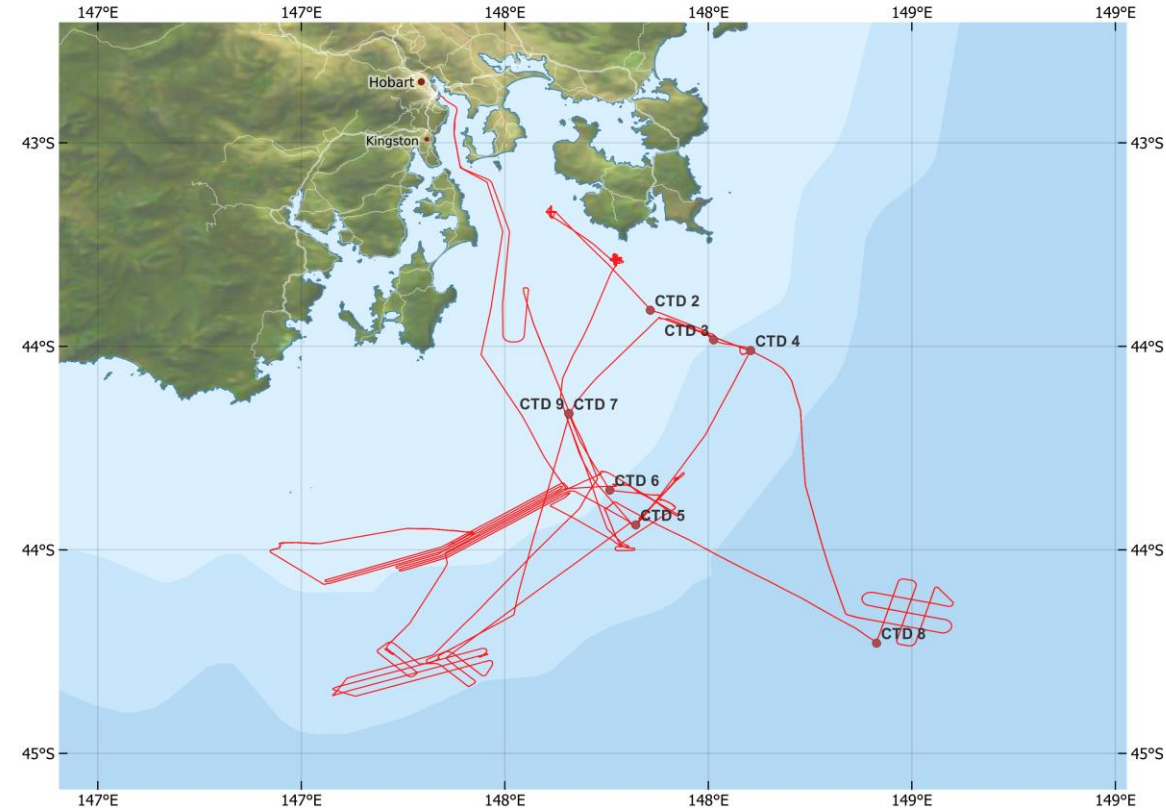


Figure 1 Area of operation for in2020_v10

3 Processing Notes

3.1 Background Information

The data for this voyage were acquired with the CSIRO CTD unit 24, a Sea-Bird SBE911 with dual conductivity and temperature sensors.

The CTD was additionally fitted with SBE43 dissolved oxygen sensors, Par, Transmissometer, Chelsea Fluorometer, and Wetlabs Fluorometer. These sensors are described in Table 1 below.

Description	Sensor	Serial No.	A/D	Calibration Date	Calibration Source
Pressure	Digiquartz 410K-134	1332	P	2-Jul-2020	CSIRO
Primary Temperature	Sea-Bird SBE3*plus*	6189	T0	25-Sep-2020	CSIRO
Secondary Temperature	Sea-Bird SBE3*plus*	6285	T1	25-Sep-2020	CSIRO
Primary Conductivity	Sea-Bird SBE4C	4773	C0	21-Sep-2020	CSIRO
Secondary Conductivity	Sea-Bird SBE4C	4774	C1	21-Sep-2020	CSIRO
Primary Dissolved Oxygen	SBE43	3155	A0	14-Oct-2020	CSIRO
Secondary Dissolved Oxygen	SBE43	3199	A1	24-Mar-2020	CSIRO
Altimeter	PA500	316739	A2	7-May-2019	Manufacturer
PAR	QCP2300HP	70111	A3	20-Oct-2020	Manufacturer
Transmissometer	C-Star	1735	A4	4-May-2020	Manufacturer
Chelsea Fluorometer	Aquatracka	11-8206-01	A5	11-Dec-2018	Manufacturer
Wetlabs Fluorometer	CDOM	4367	A6	18-May-2020	Manufacturer

Table 1 CTD Sensor configuration on in2020_v10

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

There was a total of 9 deployments. During the first cast an SBE11 modification to send serial data to the SBE9 Plus Serial Uplink port caused the SBE32 to cease handling bottle firing commands, which prevented water sampling for the first cast. Data for primary conductivity and oxygen sensors on cast 8 was adversely affected from approximately 1000 Dbar onwards. Subsequent casts did not present this issue.

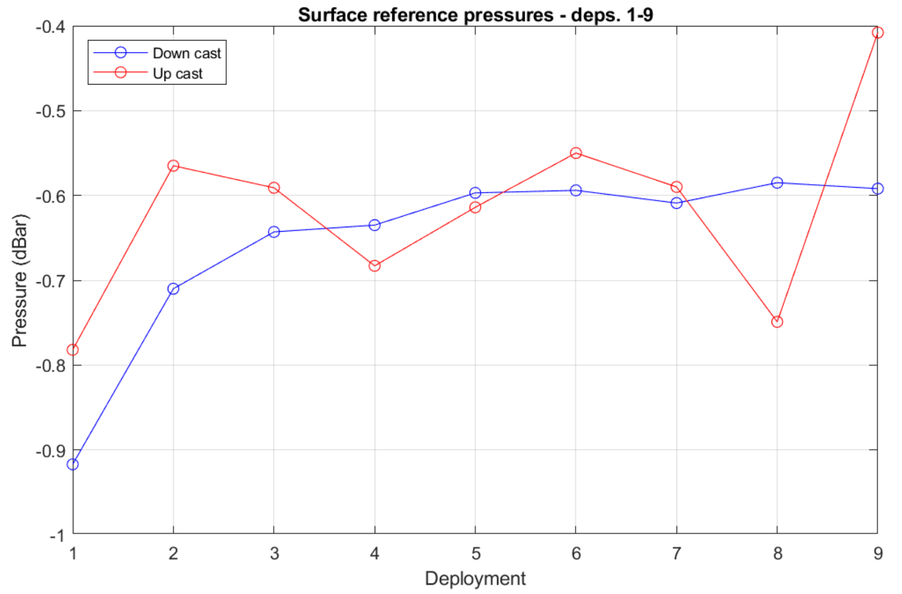
The raw CTD data were collected in SBE SeaSave version 7.26.7.110, converted to scientific units using SBE Data Processing version 7.26.7.129 and written to NetCDF format files with CNV_to_Scan for processing using the Matlab-base, CapPro package version 2.11.

The CapPro software 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. The automatically determined pressure offsets and in-water points were inspected.

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.

3.2 Pressure and temperature calibration

The pressure offsets are plotted in Figure 2 below.   The blue circles refer to initial out-of-water values and the red circles the final out-of-water values.



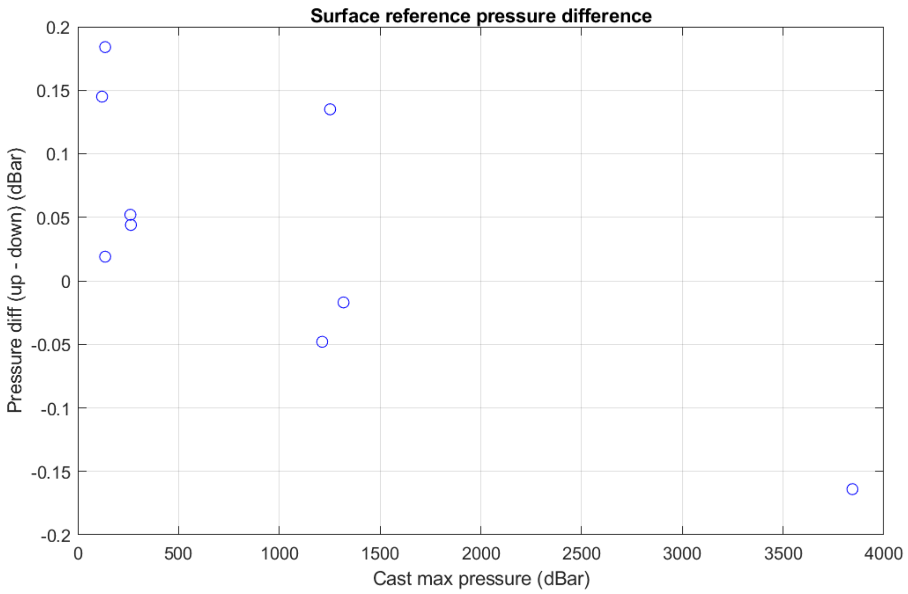


Figure 2 CTD pressure offsets

The difference between the primary and secondary temperature sensors for the downcast is plotted below. Most deployments plot within ±0.001°C of zero – outliers result from sampling in regions of high vertical temperature gradient as supported by the similarity between the temperature and conductivity difference shown in Figure 3. This indicates neither sensor has drifted significantly from its calibration.

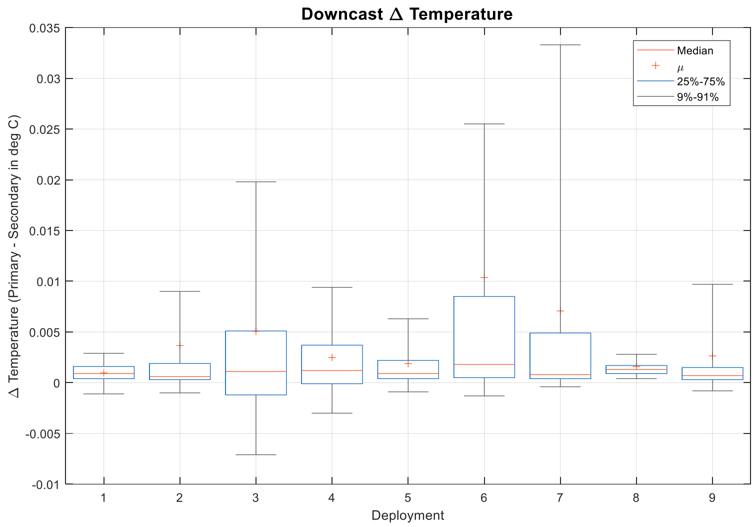


Figure 3 Difference between primary and secondary temperature sensors

3.3 Conductivity Calibration

Discrepancies and possible sampling problems between bottle and CTD salinities for the primary conductivity sensor would show in Figure 4; the plot of calibrated (CTD - Bottle) salinity below. The calibration was based upon the sample data (primary/secondary) for 29/28 of the total of 40 samples taken during deployments which are above our target of 70%.

The outliers marked in Figure 4 below with magenta dots are excluded from the calibration, the outliers marked with blue dots are used in the calibration but are weighted based on their distance from the mean. Any outliers marked with red crosses or dots are also excluded from the calibration.

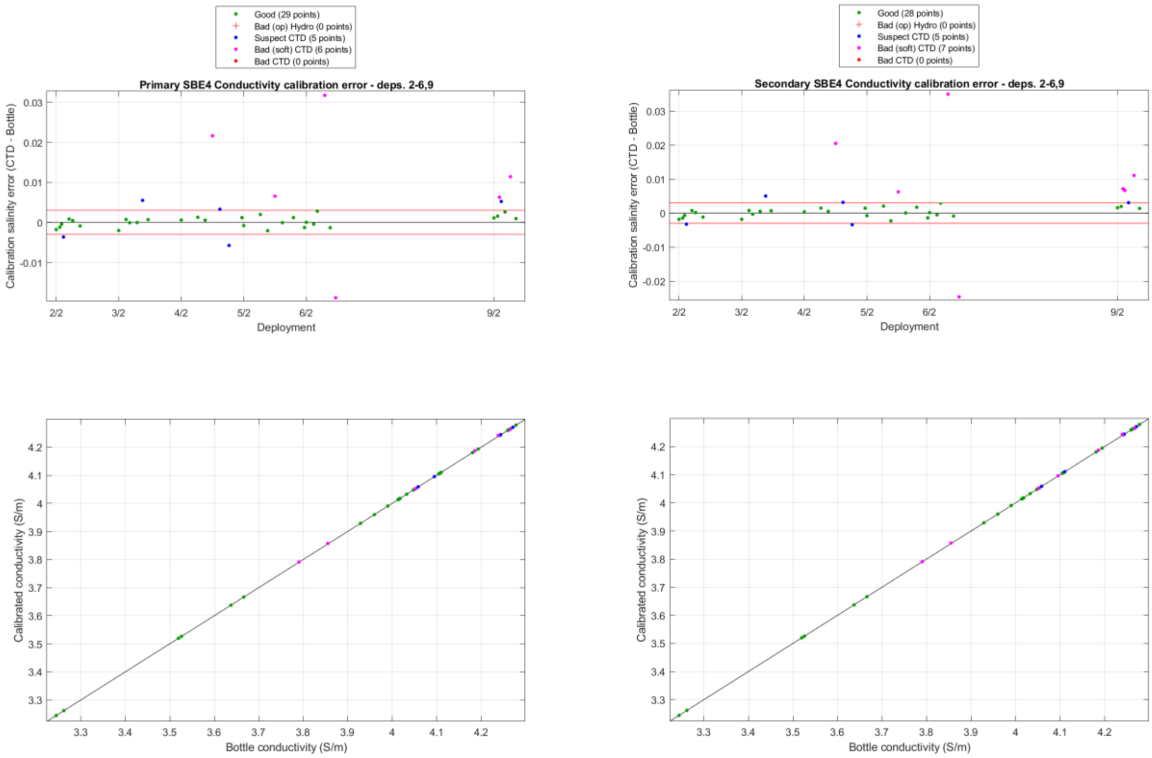


Figure 4 CTD - bottle salinity plot

The box plot of calibrated downcast conductivities (primary - secondary) for all deployments in Figure 5 shows that the calibrated conductivity cell responses corresponded very well.

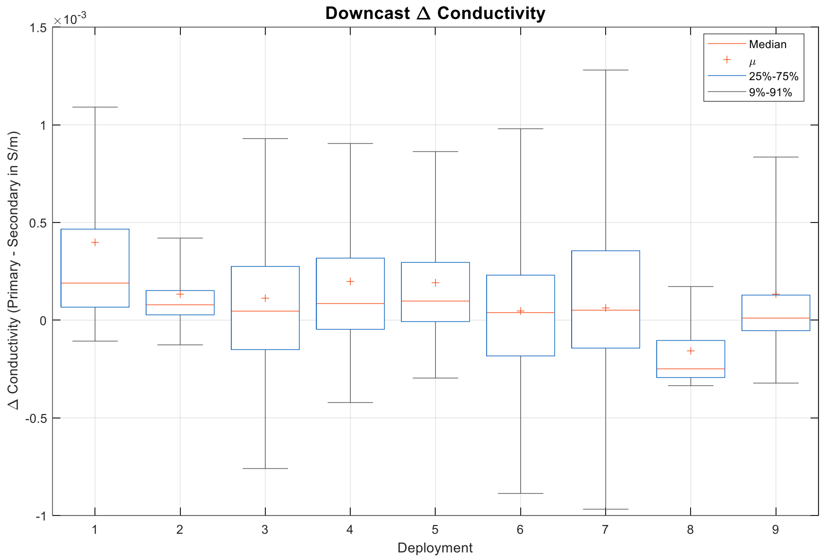


Figure 5 Difference between primary and secondary conductivity sensors

The final result 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	1-9	1.001	0.0090463	-0.00038008	0.037842	0.0015179	0.0011753
Secondary	1-9	1.003	0.0085518	-0.0018944	0.035787	0.0011549	0.0013915

Table 2 Conductivity calibration with respect to manufacturers' calibration coefficients and post-calibration results

Conductivity Sensor	Deployments	CPcor	±
Primary	1-9	-1.1864-07	2.1667e-06
Secondary	1-9	-1.6868e-07	2.0503e-06

Table 3 Calculated CPcor for primary and secondary compared to the manufacturer nominal value of -9.5700e-08

This is a good calibration. We normally aim for a S.D. of 0.002 PSU for 'typical' oceanographic voyages. The above calibration factors were applied to all deployments. Full plots of residuals before and after calibration are available in Conductivity Calibration Residual Plots. Data from the secondary conductivity and temperature sensors were used to produce the averaged salinities with primary sensors included with a suffix '_1'.

3.4 Dissolved Oxygen Sensor Calibration

3.4.1 SBE calibration procedure

AN64: SBE 43 Dissolved Oxygen Sensor - Background Information, Deployment Recommendations, and Cleaning and Storage (Sea-Bird, 2013) describes the SBE43 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 *AN64-2: SBE 43 Dissolved Oxygen Sensor Calibration and Data Corrections* (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.

3.4.2 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 *AN64-3: SBE 43 Dissolved Oxygen (DO) Sensor - Hysteresis Corrections* (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 up-cast data to compute the new *Soc* and *Voffset* coefficients. The plot below is of CTD - bottle oxygen differences for both upcast and downcast data (red indicates 'bad' data; + for upcast and square for downcast).

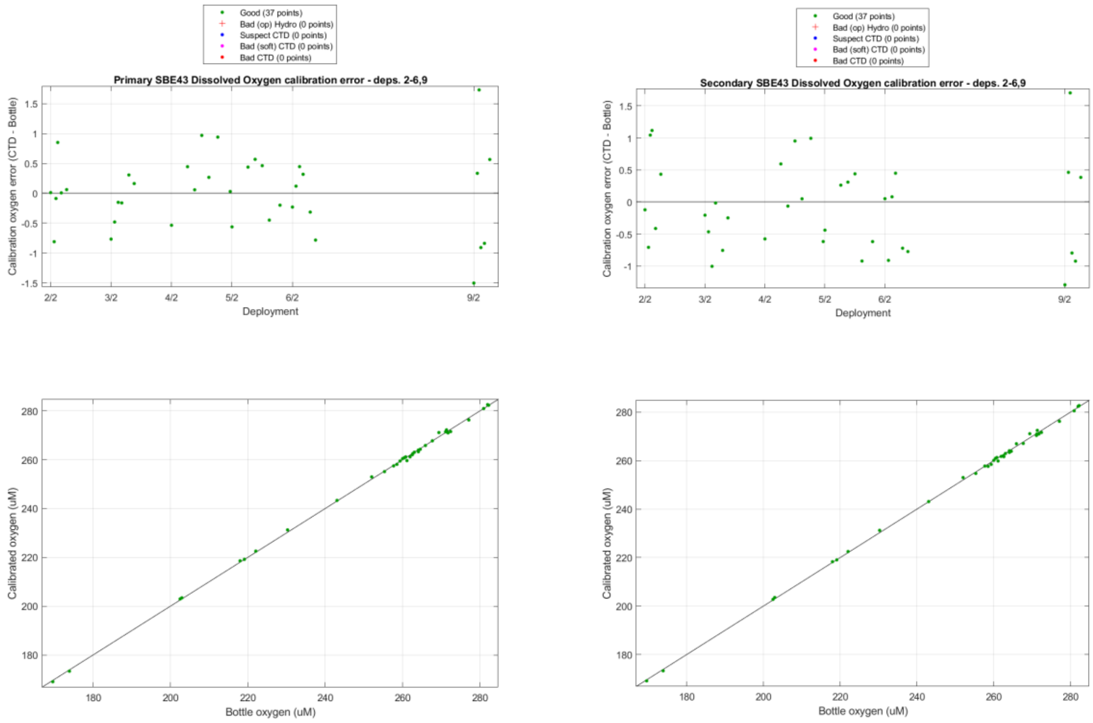


Figure 6 Dissolved Oxygen Difference with upcast CTD data (SBE43 - Bottle)

The box plot of calibrated downcast Dissolved Oxygen readings (primary - secondary) for all deployments in Figure 7 shows that the calibrated Dissolved Oxygen sensor responses corresponded well, excepting for cast 8 where an issue with the primary oxygen sensor caused drift and noise in the sensor readings. Flushing the sensor post-cast resolved the issue.

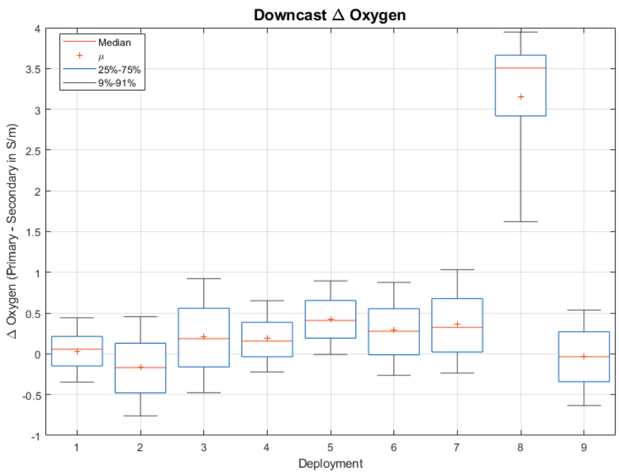


Figure 7 Difference between primary and secondary Dissolved Oxygen sensors

The old and new *Soc* and *Voffset* values for DO sensors are listed in Table 2 below. The Soc value is a linear slope scaling coefficient; *Voffset* is the fixed sensor voltage at zero oxygen. As expected, over time, the increasing *Soc* scale factors show the SBE43 sensor is losing sensitivity. Full plots of residuals before and after calibration are available in Dissolved Oxygen Calibration Residual Plots.

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

Sensor	Calibration Source	Deployments	Calibration Coefficients				Dissolved Oxygen (µM)	
			Voffset	±	*Soc*	±	Residual SD	M.A.D.
Primary DO	CapPro	1-9	-0.48081	0.005226	0.52419	0.001581	0.39835	0.44386
	CSIRO	1-9	-0.5054		0.52968			
Secondary DO	CapPro	1-9	-0.4537	0.0064721	0.51883	0.001907	0.38919	0.57693
	CSIRO	1-9	-0.4901		0.52027			

Figure 7 Dissolved oxygen calibrations

3.5 Other sensors

The Chelsea fluorometer was used for all deployments. The fluorometer has been calibrated with manufacturer supplied formula derived from various concentrations of Chlorophyll-a dissolved in acetone in addition to pure water and pure acetone. The coefficients in the formula are used in the SBE Data Processing software to convert the raw counts to fluorophore concentration in µg/L with a range of 0 – 100 micrograms per litre with an uncertainty of 0.02 micrograms per litre plus 3% of value. Please refer to the calibration certificate for more details.

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.

The Biospherical PAR sensor was also used for all deployments. The output is a nominal 0-5 volts which is converted to the unit µEinsteins/m2/second using 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. Clearly, time of day and environmental factors such as sea state and cloud cover impact on 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.

3.6 Bad data detection

The 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 4 below. 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
Oxygen	-1	500	0.5
Fluorometer	0	100	0.5

PAR	-5	2000	0.5
Transmissometer	0	100	0.5

Table 4 Sensor limits for bad data detection

3.7 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.

3.8 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 QC flag. Our quality control flagging scheme is described in *Data Quality Control Flags* (Pender, 2000).

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 are taken to be the worst of the estimates for the parameters from which they are derived.

4 References

Dr Karen Wild-Allen. (2020). *The RV Investigator. Voyage Plan* in2020_v10. Retrieved from Marine National Facility: Voyage Plans and summaries: https://mnf.csiro.au/en/Voyages/Voyage-Catalogue

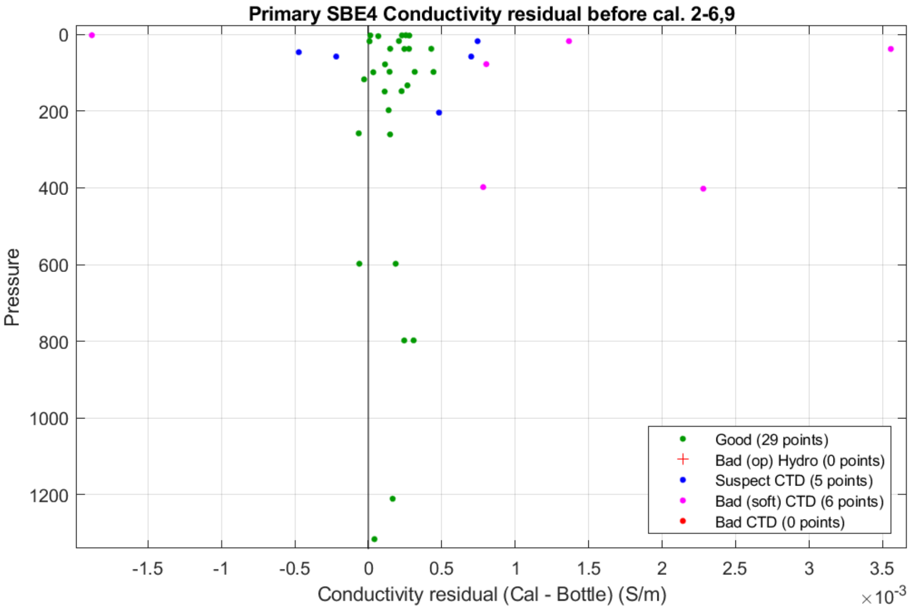
Pender, L. (2000). *Data Quality Control Flags.* Retrieved from Oceans & Atmosphere Information and Data Centre: http://www.cmar.csiro.au/datacentre/ext_docs/DataQualityControlFlags.pdf

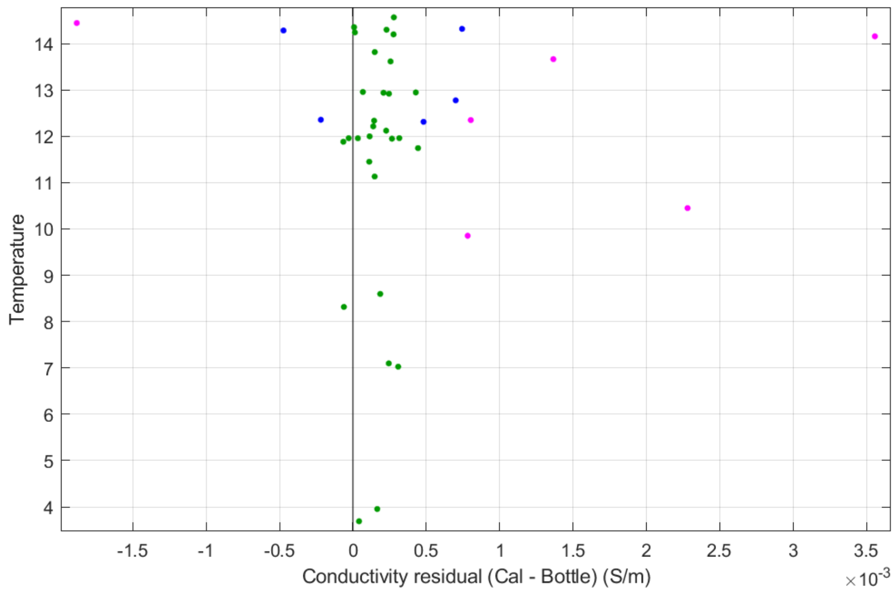
Sea-Bird. (2012). *AN64-2: SBE 43 Dissolved Oxygen Sensor Calibration and Data Corrections.* Retrieved from Sea-Bird Electronics: https://www.seabird.com/asset-get.download.jsa?code=251034

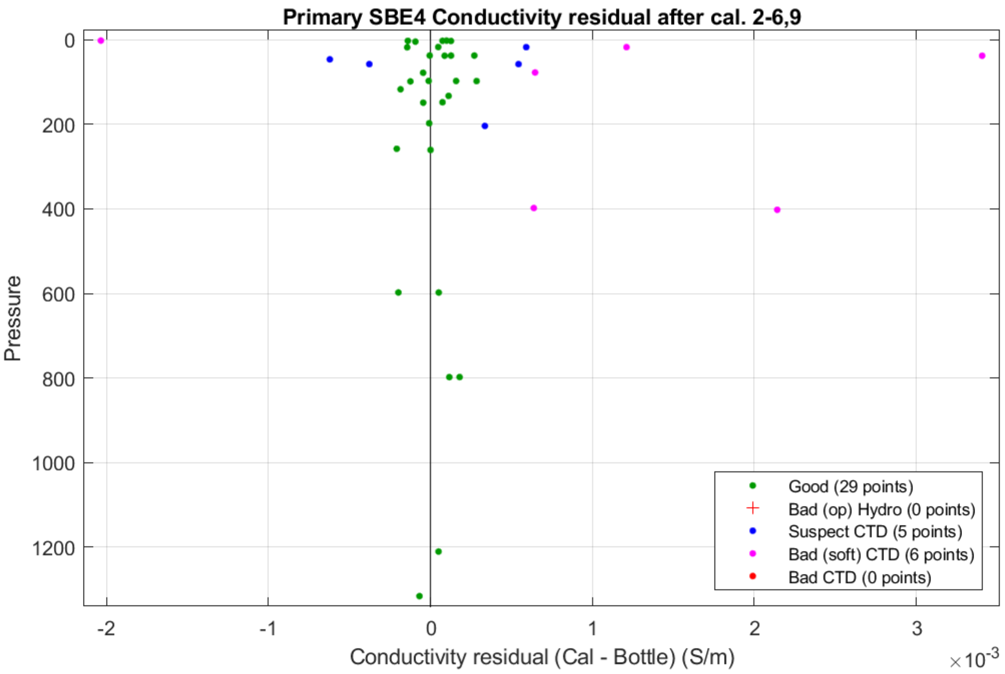
Sea-Bird. (2013). *AN64: SBE 43 Dissolved Oxygen Sensor - Background Information, Deployment Recommendations, and Cleaning and Storage.* Retrieved from Sea-Bird Electronics: https://www.seabird.com/asset-get.download.jsa?code=251036

Sea-Bird. (2014). *AN64-3: SBE 43 Dissolved Oxygen (DO) Sensor - Hysteresis Corrections.* Retrieved from Sea-Bird Electronics: https://www.seabird.com/asset-get.download.jsa?code=251035

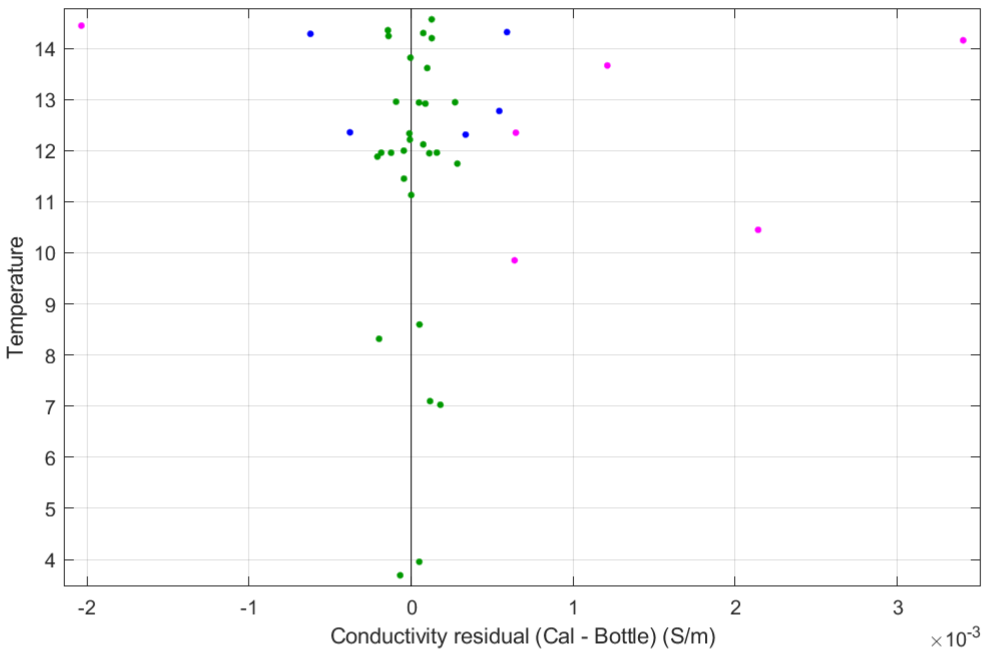
Appendix I: Conductivity Calibration Residual Plots



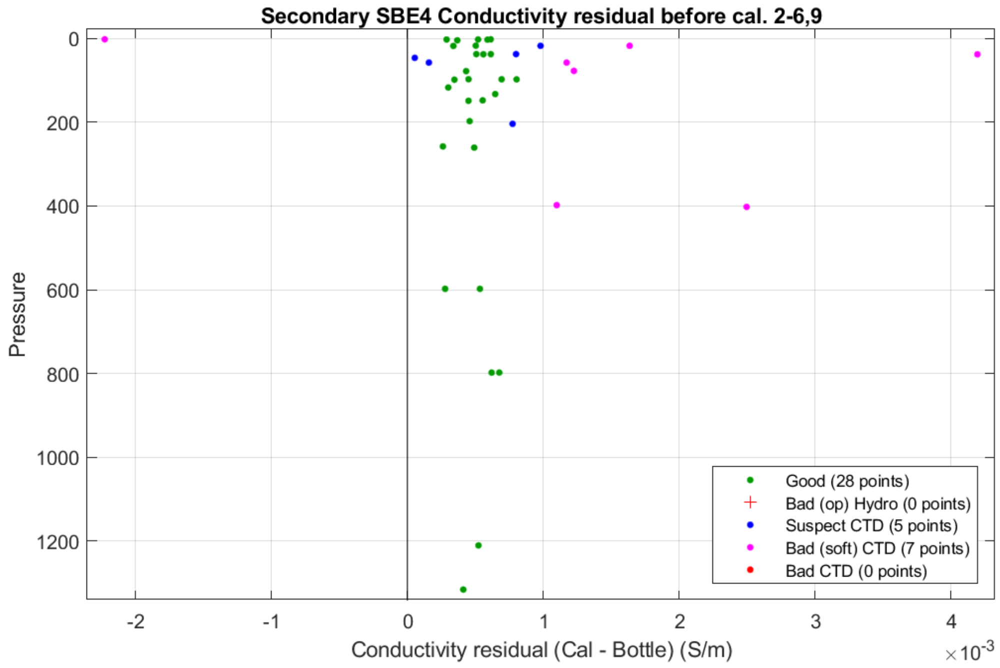


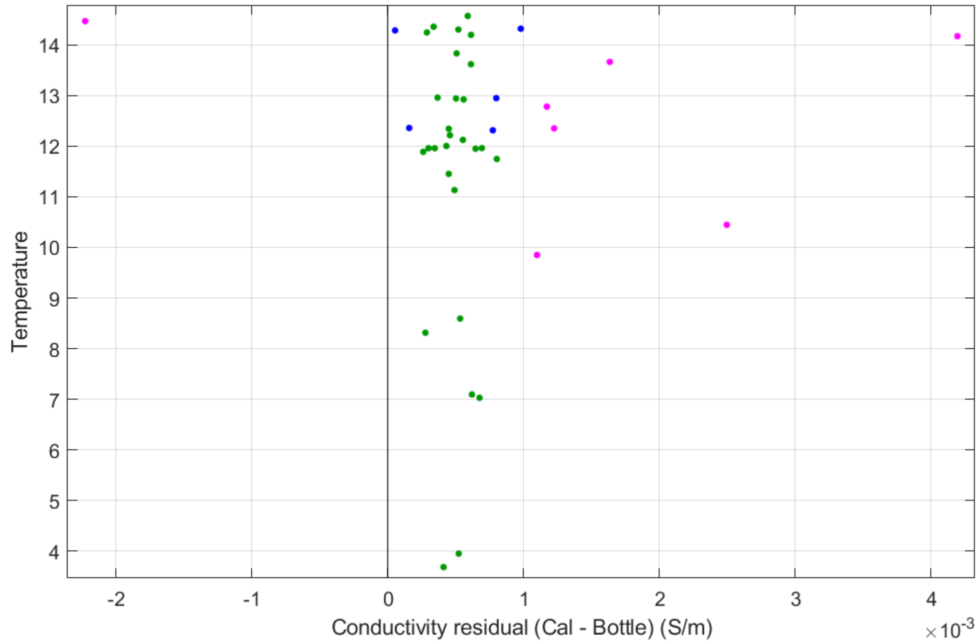


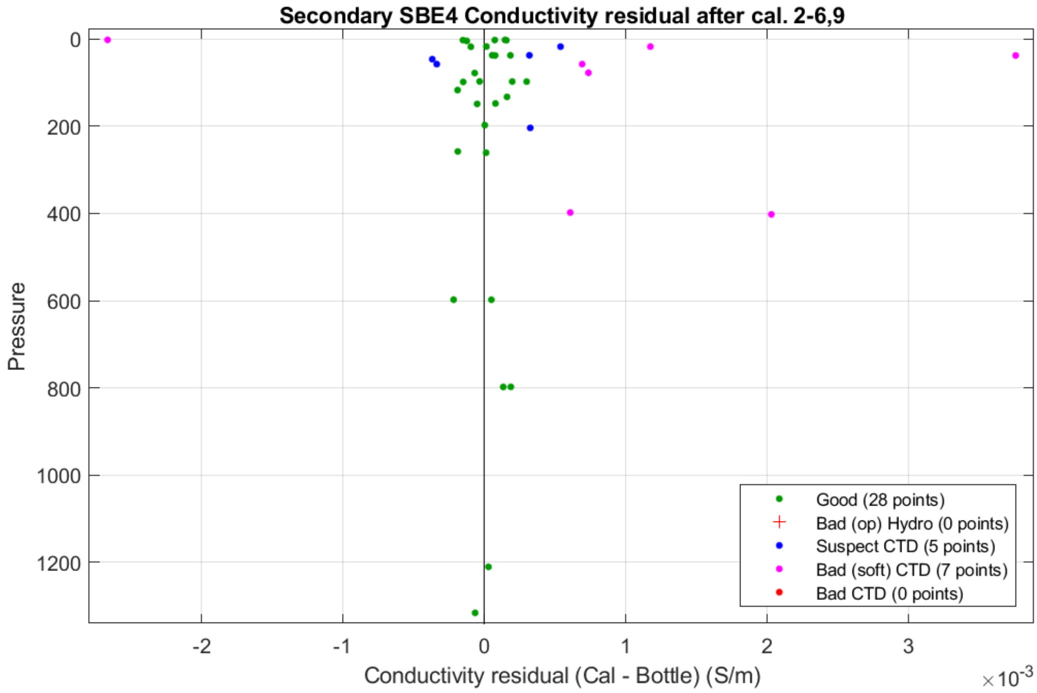
Primary SBE4 Conductivity residual after cal. 2-6,9
Pressure
0
200
400
600
800
1000
1200
-2
-1
0
1
2
3
Conductivity residual (Cal - Bottle) (S/m)
×10-3
Good (29 points)
Bad (op) Hydro (0 points)
Suspect CTD (5 points)
Bad (soft) CTD (6 points)
Bad CTD (0 points)

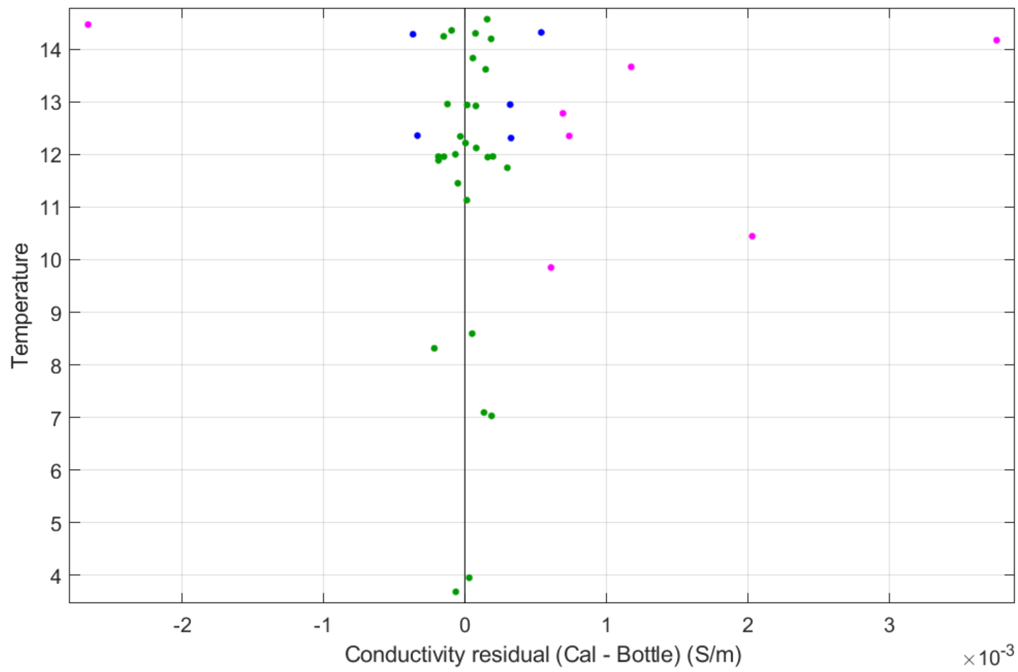


Temperature
14
13
12
11
10
9
8
7
6
5
4
-2
-1
0
1
2
3
Conductivity residual (Cal - Bottle) (S/m)
×10-3

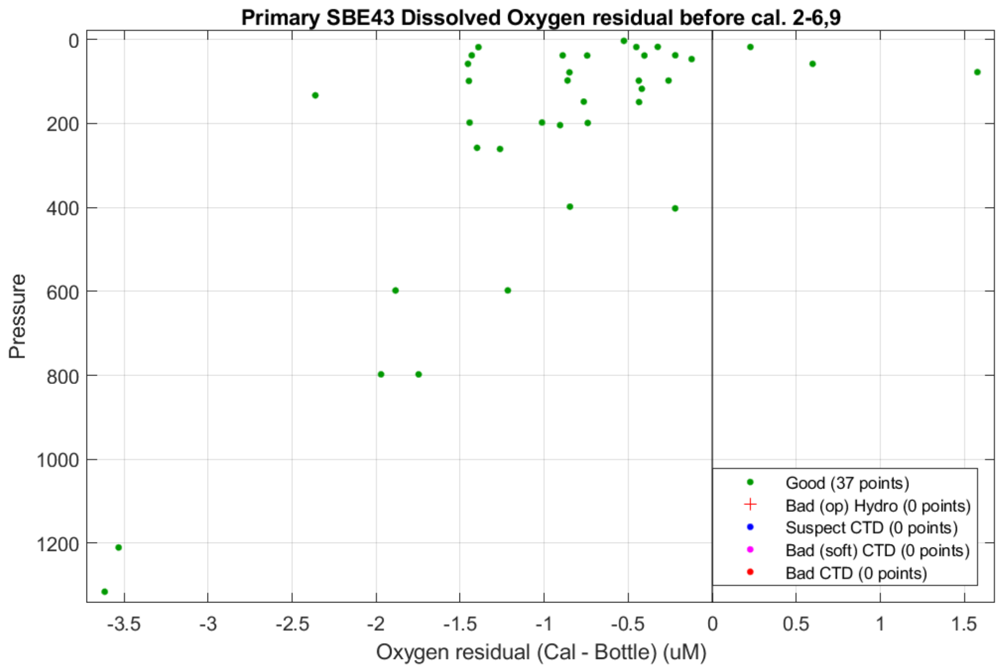

Secondary SBE4 Conductivity residual before cal. 2-6,9
Pressure
0
200
400
600
800
1000
1200
-2
-1
0
1
2
3
4
Conductivity residual (Cal - Bottle) (S/m)
×10-3
Good (28 points)
Bad (op) Hydro (0 points)
Suspect CTD (5 points)
Bad (soft) CTD (7 points)
Bad CTD (0 points)

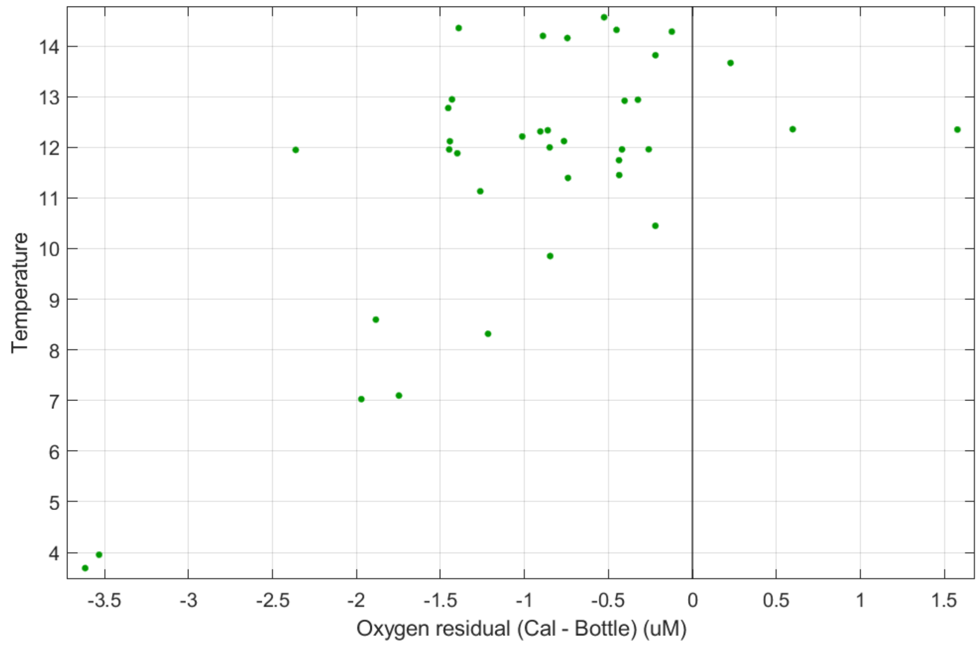

Temperature
14
13
12
11
10
9
8
7
6
5
4
-2
-1
0
1
2
3
4
Conductivity residual (Cal - Bottle) (S/m)
×10-3

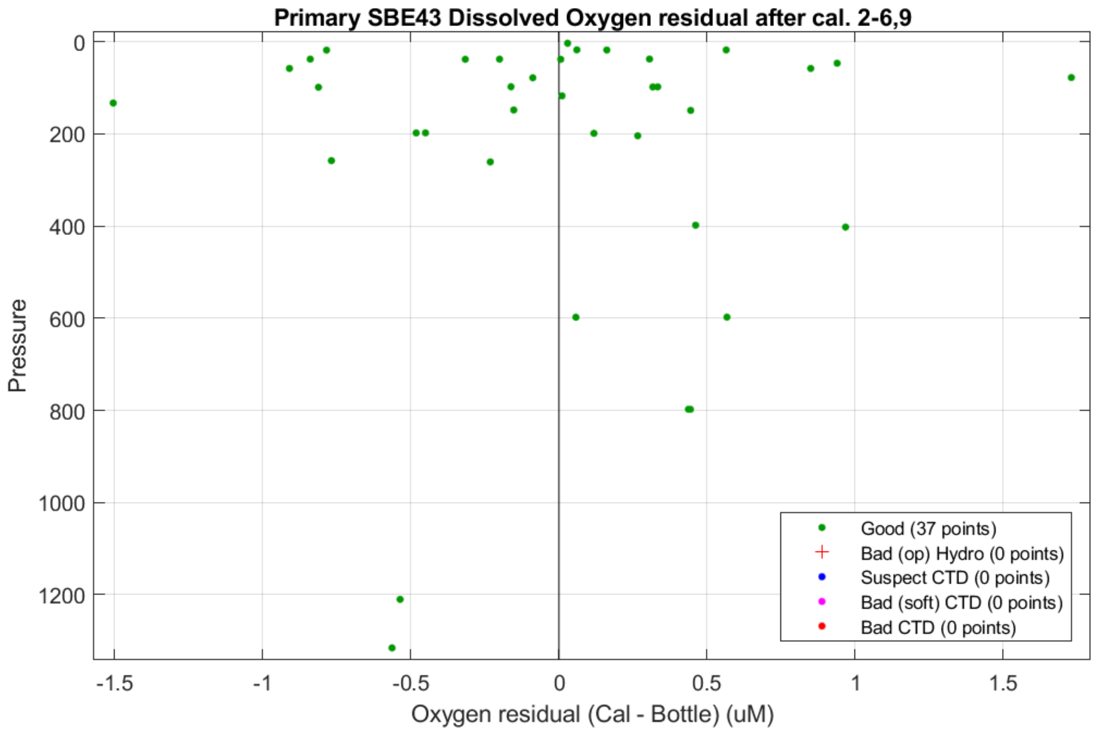

Secondary SBE4 Conductivity residual after cal. 2-6,9
Pressure
0
200
400
600
800
1000
1200
-2
-1
0
1
2
3
Conductivity residual (Cal - Bottle) (S/m)
×10-3
Good (28 points)
Bad (op) Hydro (0 points)
Suspect CTD (5 points)
Bad (soft) CTD (7 points)
Bad CTD (0 points)


Temperature
14
13
12
11
10
9
8
7
6
5
4
-2
-1
0
1
2
3
Conductivity residual (Cal - Bottle) (S/m)
×10-3

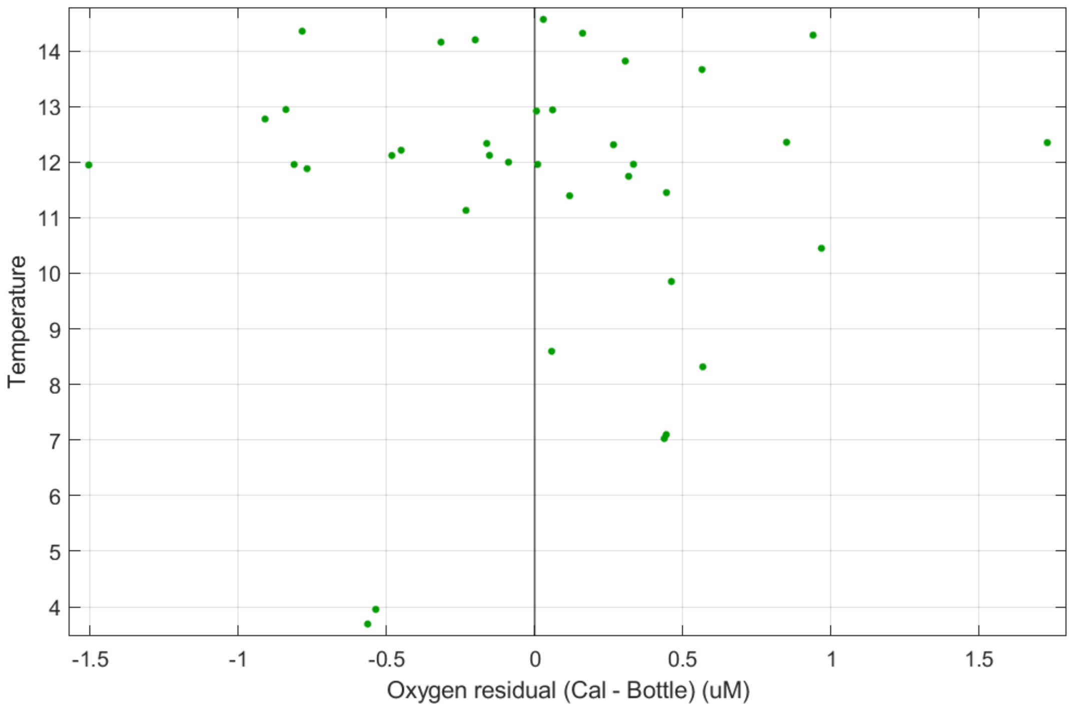
Appendix II: Dissolved Oxygen Calibration Residual Plots



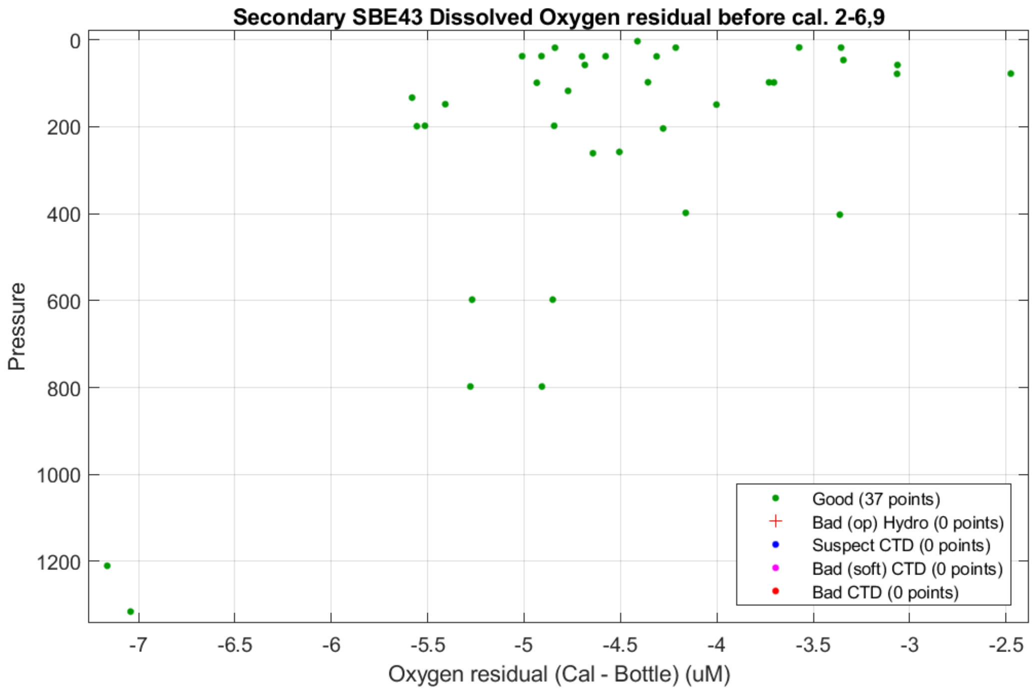


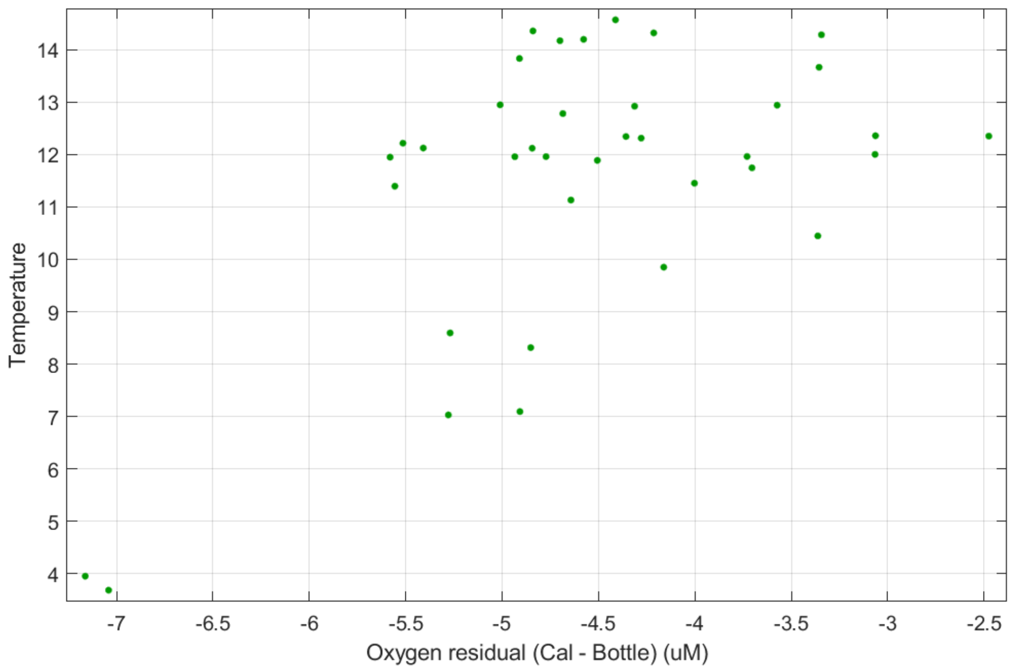


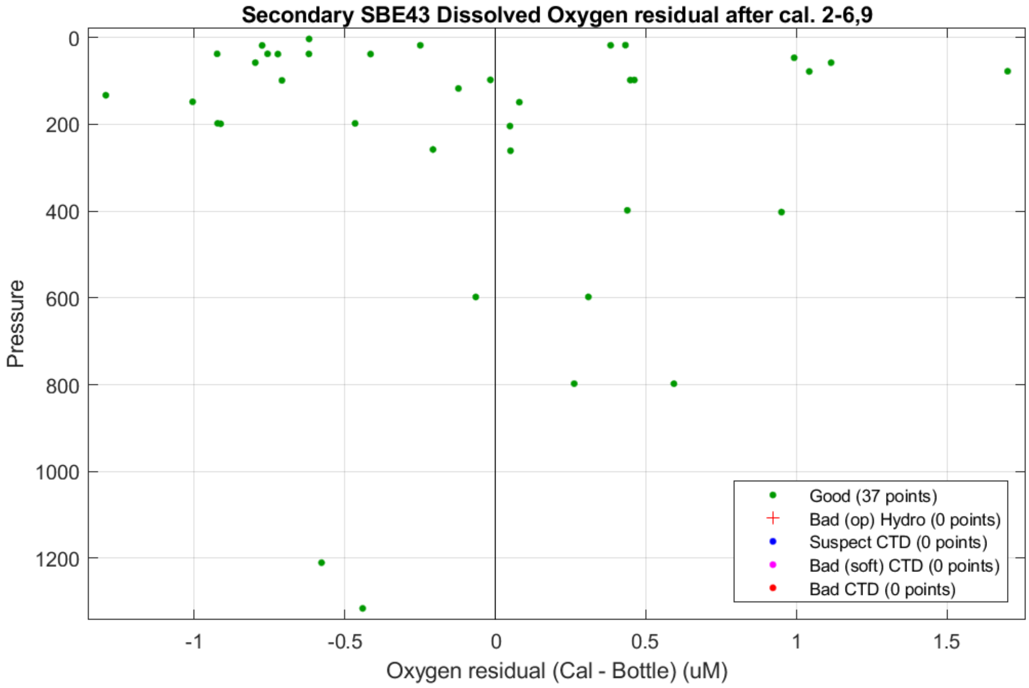
Primary SBE43 Dissolved Oxygen residual after cal. 2-6,9
Pressure
0
200
400
600
800
1000
1200
-1.5
-1
-0.5
0
0.5
1
1.5
Oxygen residual (Cal - Bottle) (uM)
Good (37 points)
Bad (op) Hydro (0 points)
Suspect CTD (0 points)
Bad (soft) CTD (0 points)
Bad CTD (0 points)

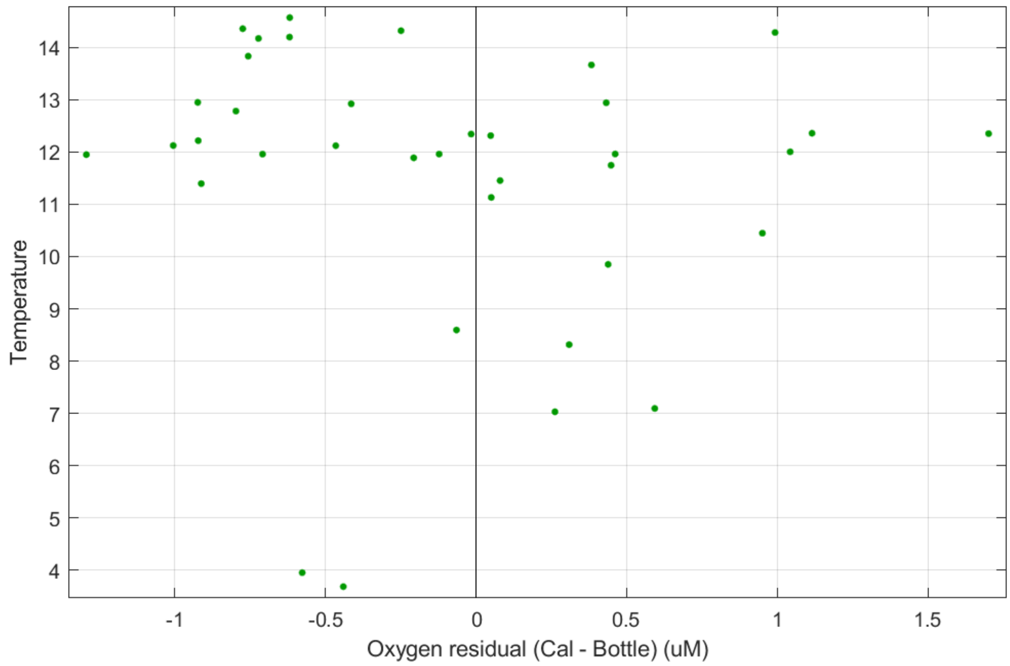


Temperature
14
13
12
11
10
9
8
7
6
5
4
-1.5
-1
-0.5
0
0.5
1
1.5
Oxygen residual (Cal - Bottle) (uM)


Secondary SBE43 Dissolved Oxygen residual before cal. 2-6,9
Pressure
0
200
400
600
800
1000
1200
-7
-6.5
-6
-5.5
-5
-4.5
-4
-3.5
-3
-2.5
Oxygen residual (Cal - Bottle) (uM)
Good (37 points)
Bad (op) Hydro (0 points)
Suspect CTD (0 points)
Bad (soft) CTD (0 points)
Bad CTD (0 points)


Temperature
14
13
12
11
10
9
8
7
6
5
4
-7
-6.5
-6
-5.5
-5
-4.5
-4
-3.5
-3
-2.5
Oxygen residual (Cal - Bottle) (uM)


Secondary SBE43 Dissolved Oxygen residual after cal. 2-6,9
Pressure
Oxygen residual (Cal - Bottle) (uM)
Good (37 points)
Bad (op) Hydro (0 points)
Suspect CTD (0 points)
Bad (soft) CTD (0 points)
Bad CTD (0 points)


Temperature
Oxygen residual (Cal - Bottle) (uM)