RV *Investigator*

CTD Processing Report

Voyage ID:	in2020_v09
Voyage title:	SOTS: Southern Ocean Time Series automated moorings for climate and carbon cycle studies southwest of Tasmania
Depart:	Hobart, 1200 Thursday, 27 August 2020
Return:	Hobart, 1730 Saturday, 12 September 2020
Report compiled by:	Francis Chui
Version:	1.0
Date:	6 October 2020
Comments:	Initial version

Contents

1 Summary

These notes relate to the production of quality controlled, calibrated CTD data from RV Investigator voyage in2020_v09, from 29 Aug 2020 – 11 Sep 2020.

Data for 6 deployments were acquired using the Sea-Bird SBE911 CTD 25, fitted with 24 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 primary sensor had a standard deviation (SD) of 0.0008174 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 primary sensors.

The dissolved oxygen data calibration fit had a SD of 0.89571 µM. The agreement between the CTD and bottle data was good.

Transmissometer, Wetlabs Eco-FLBB and Altimeter were also installed on the auxiliary A/D channels of the CTD. It should be noted that the transmissometer signal below 700 decibar should be treated as suspect.

2 Voyage Details

2.1 Title

SOTS: Southern Ocean Time Series automated moorings for climate and carbon cycle studies southwest of Tasmania

2.2 Principal Investigators

Elizabeth Shadwick, CSIRO

Tom Trull, CSIRO

2.3 Voyage Objectives

The scientific objectives for in2020_v09 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

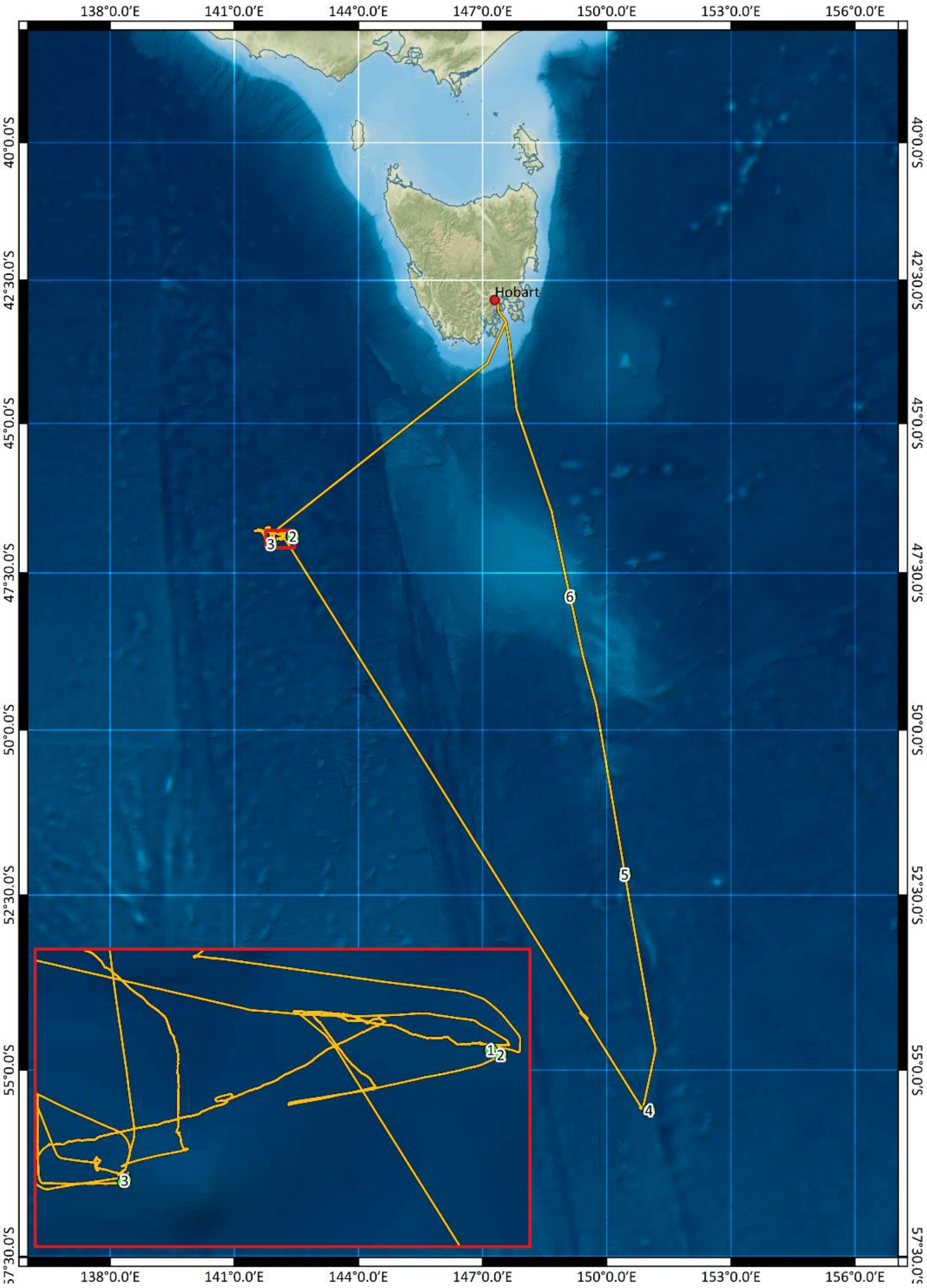


Figure 1 Area of operation for in2020_v09

3 Processing Notes

3.1 Background Information

The data for this voyage were acquired with the CSIRO CTD unit 25, a Sea-Bird SBE911 with dual conductivity and temperature sensors.

The CTD was additionally fitted with SBE43 dissolved oxygen sensors, transmissometer, photosynthetically active radiation, ECO fluorometer and Backscatter. These sensors are described in Table 1 below.

Description	Sensor	Serial No.	A/D	Calibration Date	Calibration Source
Pressure	Digiquartz 410K-134	1354	P	1-Nov-2019	Calibration Facility
Primary Temperature	Sea-Bird SBE3*plus*	4718	T0	31-Oct-2019	Calibration Facility
Secondary Temperature	Sea-Bird SBE3*plus*	6022	T1	31-Oct-2019	Calibration Facility
Primary Conductivity	Sea-Bird SBE4C	3868	C0	29-Oct-2019	Calibration Facility
Secondary Conductivity	Sea-Bird SBE4C	4664	C1	29-Oct-2019	Calibration Facility
Primary Dissolved Oxygen	SBE43	3198	A0	12-Aug-2019	Calibration Facility
Secondary Dissolved Oxygen	SBE43	3155	A1	1-Nov-2019	Calibration Facility
Altimeter	PA-500	5301.316739	A2	7-May-2019	Tri-tech
PAR	QCP-2300HP	70111	A3	14-Aug-2019	Biospherical Instruments
Transmissometer	Wetlabs CSTAR 25cm	CST-2009DR	A4	30-Oct-2019	Wet Labs
Wet labs ECO - Chlorophyll	FLBBNTU	4799	A6	24-Aug-2018	Wet Labs
Wet labs ECO - Scattering	FLBBNTU	4799	A7	24-Aug-2018	Wet Labs

Table 1 CTD Sensor configuration on in2020_v09

Water samples were collected using a Sea-Bird SBE32, 24-bottle rosette sampler. Sampling was from 24 twelve litre bottles which were fitted to the frame.

There were 6 deployments and of these, deployments 0 were on-deck TSG calibration runs.

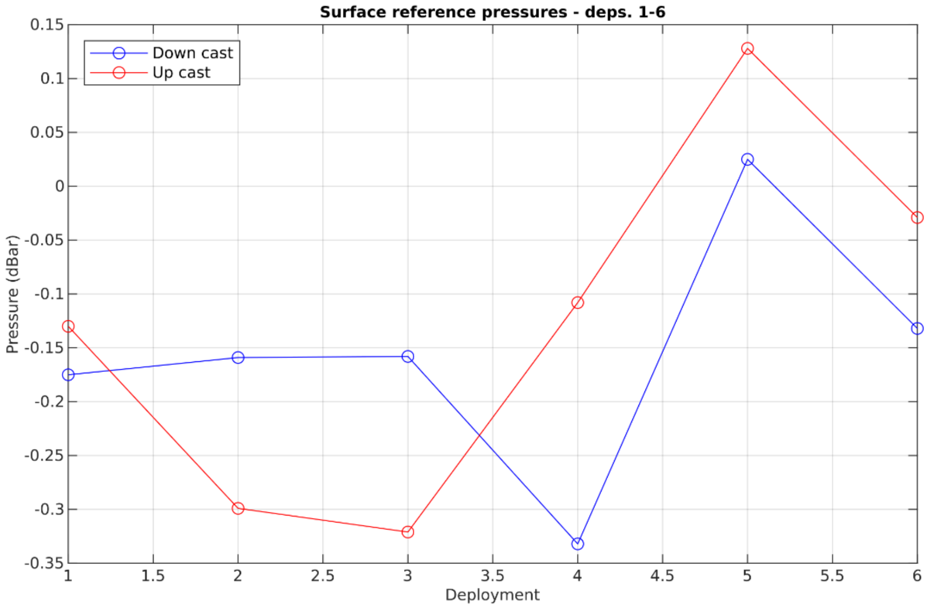
The raw CTD data were collected in SBE SeaSave version 7.26.7.129, converted to scientific units using SBE Data Processing version 7.26.7.129 and written to NetCDF format files with CNV_to_Scan for processing using the Matlab-base, CapPro package version 2.11.

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.



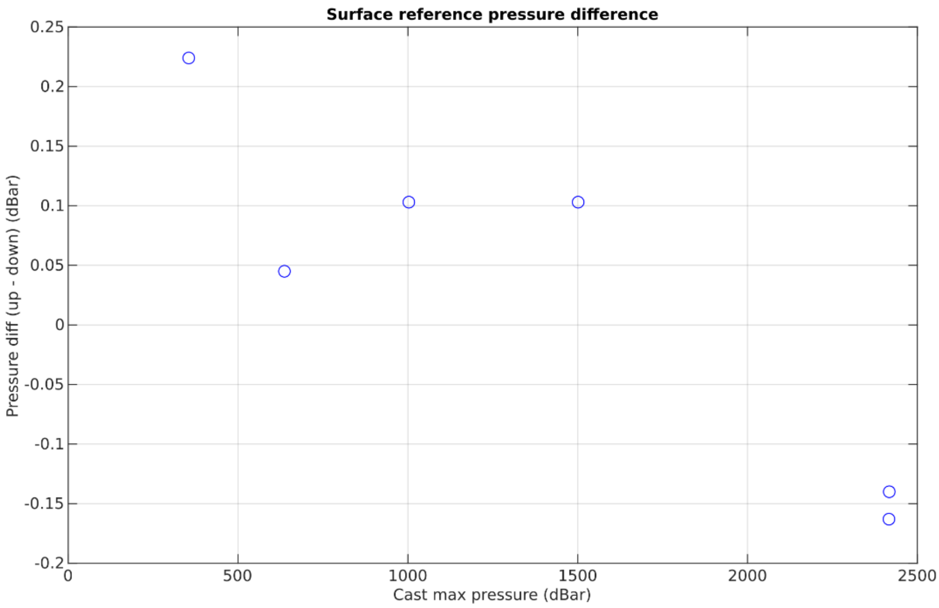


Figure 2 CTD pressure offsets

The differences between the primary and secondary temperature sensors at the bottle sampling depths is plotted below in Figure 3. Deployments 1-3 plot within ±0.001°C of zero with only outliers above the 91st percentile outside this region. Deployments 4 and 5 had means outside this region which may have been a result of sampling in regions of high vertical temperature gradient. The similarity between sensors can be seen on the downcast temperature difference from the full resolution data as shown in. This indicates neither sensor has drifted significantly from its calibration.

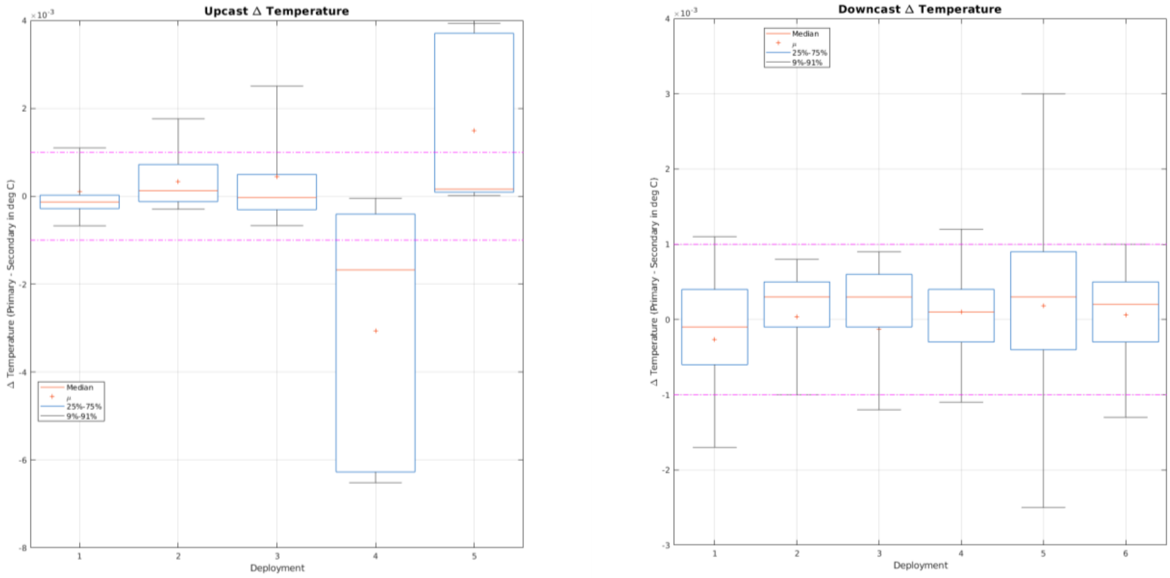


Figure 3 Differences between primary and secondary temperature sensors at bottle sampling (left) and the full resolution downcast (right)

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 70/72 of the total of 75 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.

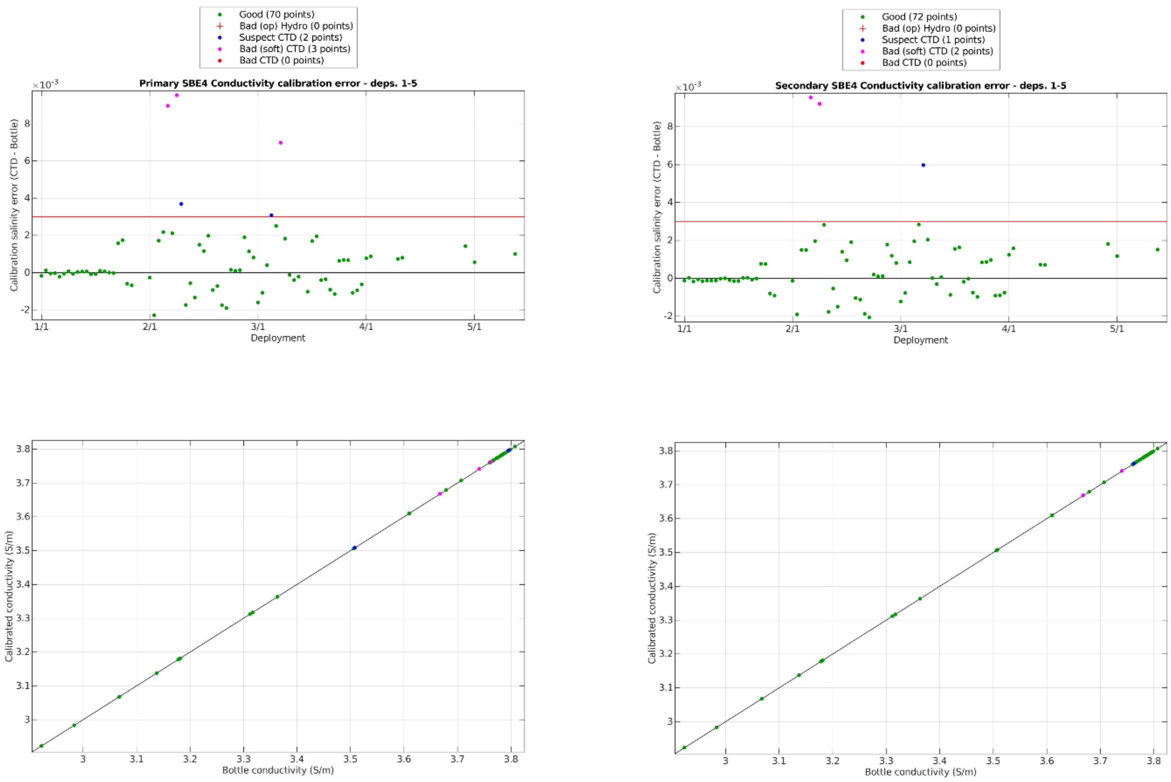


Figure 4 CTD - bottle salinity plot

The box plots of bottle sampling differences on the upcast and calibrated downcast conductivities (primary - secondary) for all deployments are shown in

Figure 5. The variance on the upcast for deployment 4 was significantly larger than other casts but the downcast showed that the calibrated conductivity cell responses corresponded very well.

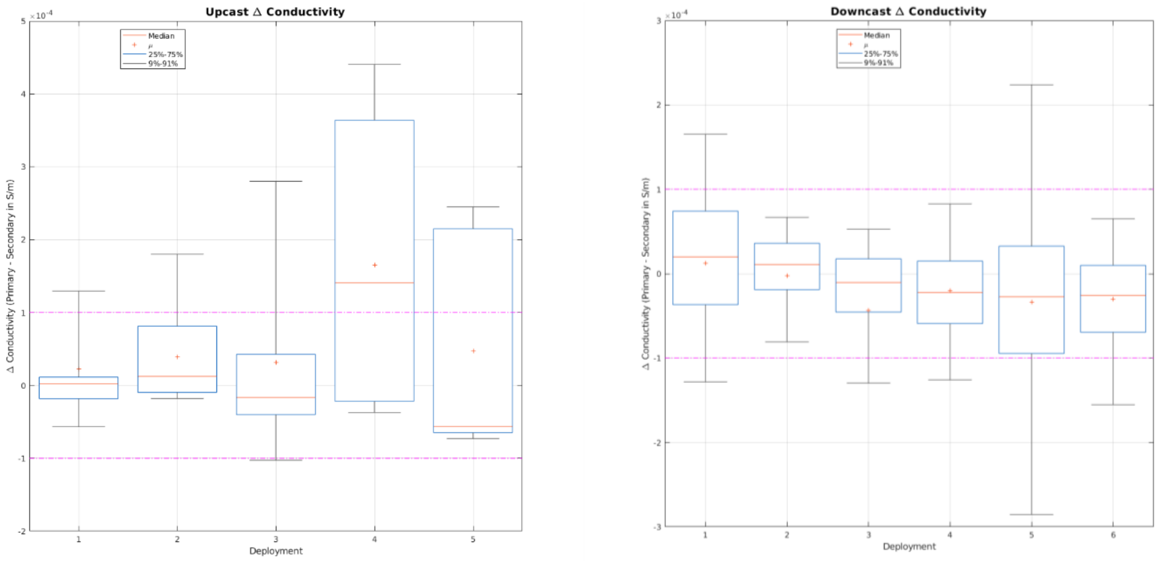


Figure 5 Difference between primary and secondary conductivity sensors at bottle sampling (left) and the full resolution downcast (right)

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	1-6	0.99954	0.0010669	1.2918e-03	0.0039841	0.00081740	0.00072604
Secondary	1-6	0.99952	0.0011019	1.3361e-03	0.0041170	0.00094275	0.00083636

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

Conductivity Sensor	Deployments	CPcor	±
Primary	1-6	-7.4859e-08	1.6941e-07
Secondary	1-6	-6.8666e-08	1.7536e-07

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 primary conductivity and temperature sensors were used to produce the averaged salinities with secondary sensors included with a suffix '_2'.

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).

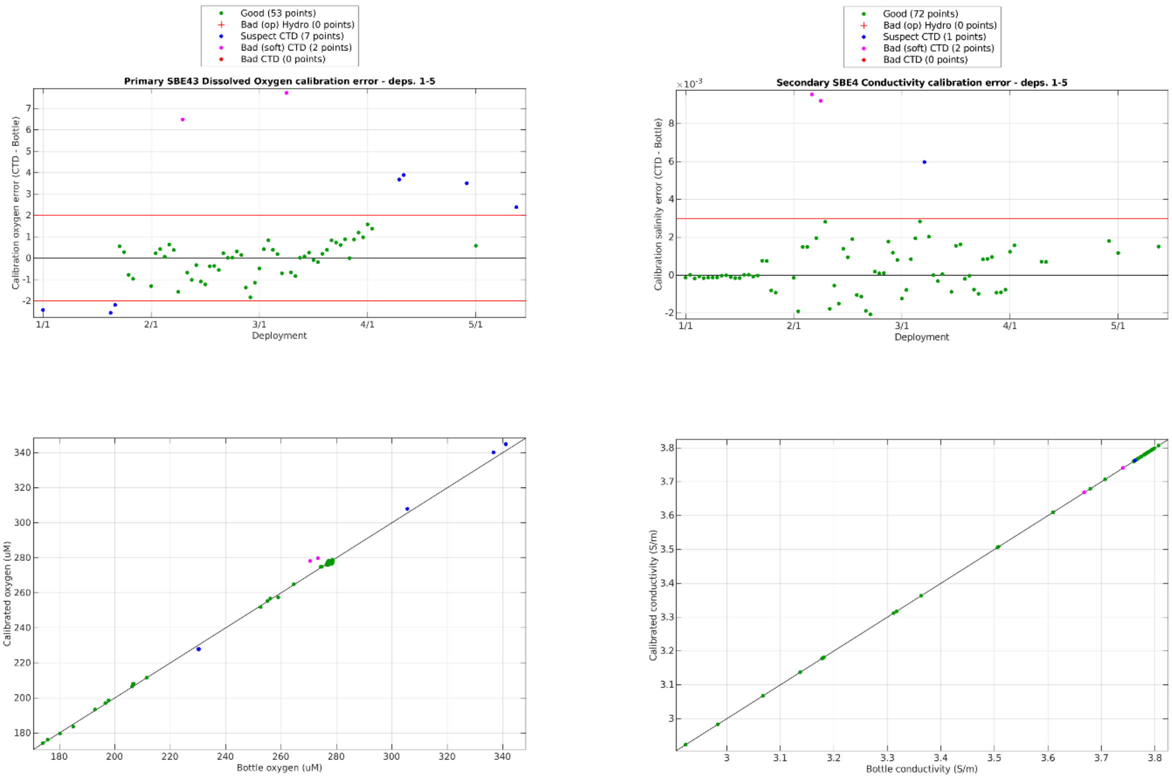
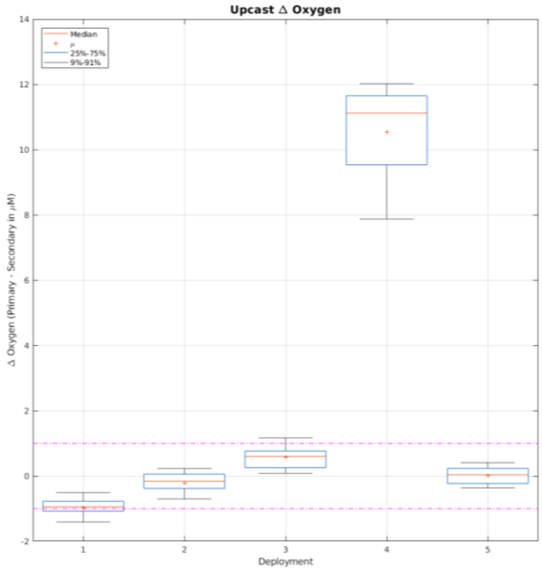


Figure 6 Dissolved Oxygen Difference with upcast CTD data (SBE43 - Bottle)

The box plot for bottle sampling depths and downcasts are shown in Figure 7. Again the sampling data at bottle depths for deployment 4 showed significant differences between the primary/secondary oxygen sensor pair. The calibrated downcast Dissolved Oxygen readings (primary - secondary) for all deployments in shows that the calibrated Dissolved Oxygen sensor responses corresponded well.



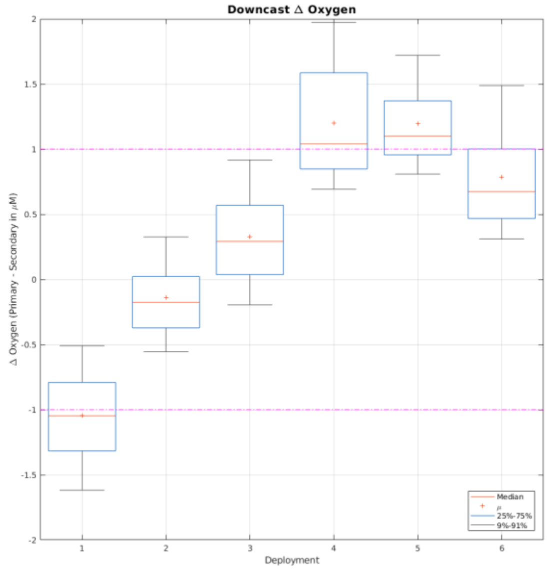


Figure 7 Difference between primary and secondary Dissolved Oxygen sensors at bottle sampling (left) and the full resolution downcast (right)

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	1-6	-0.47632	0.0072807	0.41349	0.0014536	0.89571	0.64972
	Oceanographic Calibration Facility	1-6	-0.50190482		0.40444623			
Secondary DO	CapPro	1-6	-0.49016	0.0036786	0.53129	0.0012174	0.48585	0.52622
	Oceanographic Calibration Facility	1-6	-0.50830889		0.52179013			

Figure 7 Dissolved oxygen calibrations

3.5 Other sensors

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 WET labs ECO Fluorometer-Scattering sensor was used for all deployments. The fluorometer has been calibrated with manufacturer supplied coefficients to give outputs in mg/m3. The scattering (OBS) has been calibrated with manufacturer supplied coefficients to give outputs in m-1/sr.

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
OBS	-5	5000	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.

3.9 Data Issues

For all deployments it was apparent there was a pressure dependant affect inducing a signal on the transmissometer starting between 700 and 1200 decibar which were particularly evident on deployments 2, 3 and 5. In plot below, it can be seen that the upcast profile does not follow the downcast on its return to the surface until 330 decibar.

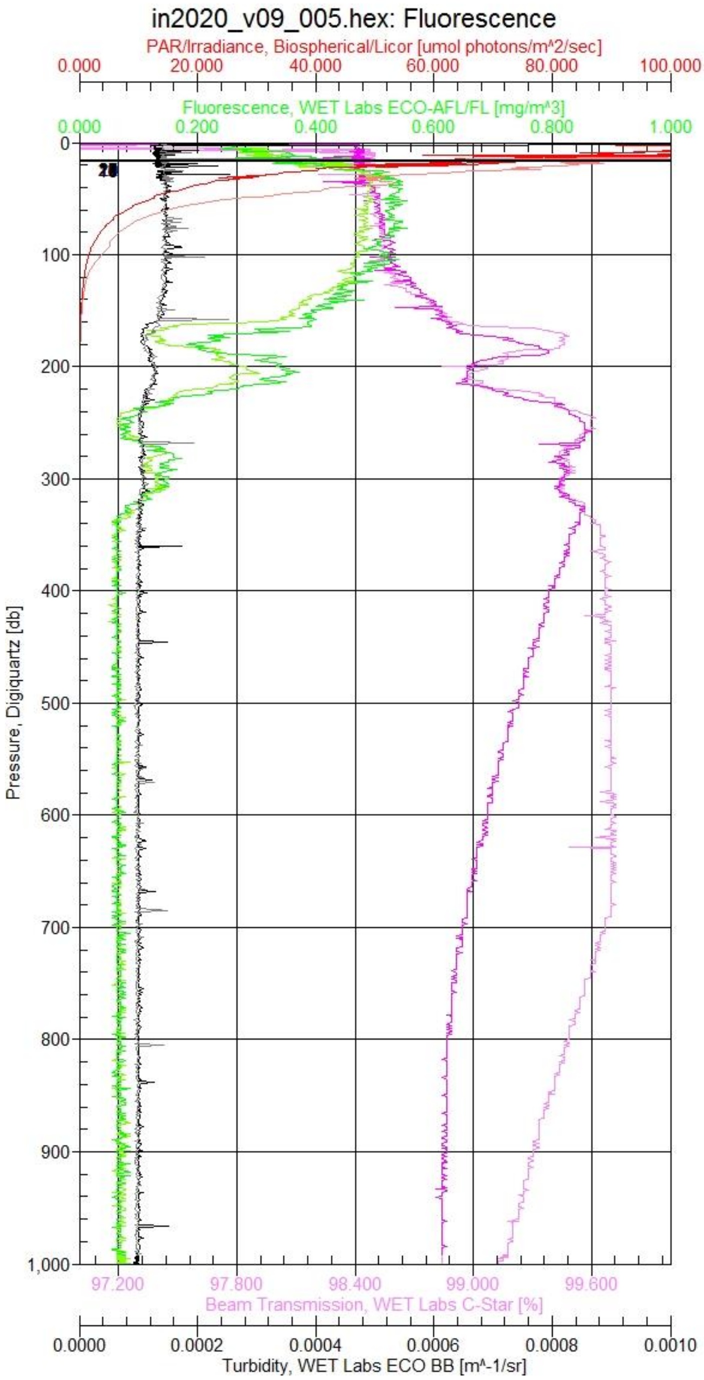


Figure 8 SeaSave plot from optical sensors on deployment 5 illustrating the pressure dependent signal induced on the transmissometer. Downcast trace is in light pink and upcast in dark pink.

4 References

Shadwick, E. (2020). *The RV Investigator. Voyage Plan* in2020_v09. Retrieved from Marine National Facility: Voyage Plans and summaries: https://www.marine.csiro.au/data/reporting/get_file.cfm?eov_pub_id=1418

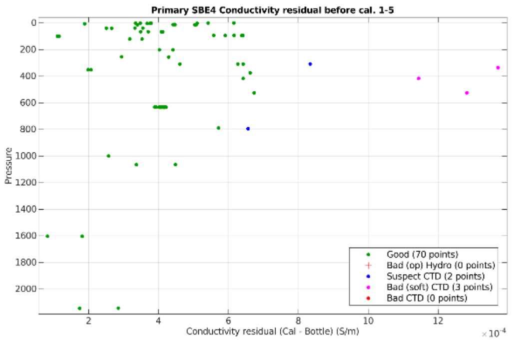
Pender, L. (2000). *Data Quality Control Flags.* Retrieved from Oceans & Atmosphere Information and Data Centre: http://www.cmar.csiro.au/datacentre/ext_docs/DataQualityControlFlags.pdf

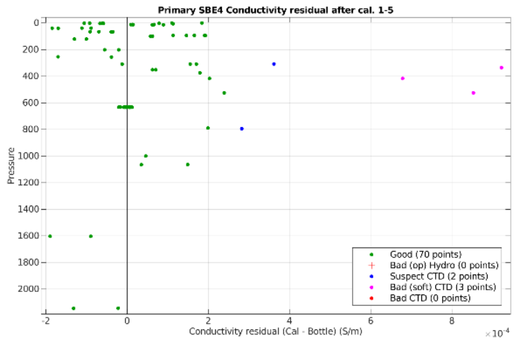
Sea-Bird. (2012). *AN64-2: SBE 43 Dissolved Oxygen Sensor Calibration and Data Corrections.* Retrieved from Sea-Bird Electronics: https://www.seabird.com/asset-get.download.jsa?code=251034

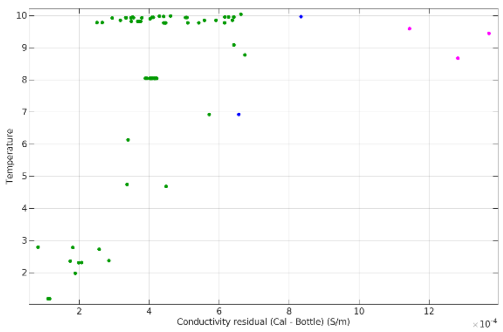
Sea-Bird. (2013). *AN64: SBE 43 Dissolved Oxygen Sensor - Background Information, Deployment Recommendations, and Cleaning and Storage.* Retrieved from Sea-Bird Electronics: https://www.seabird.com/asset-get.download.jsa?code=251036

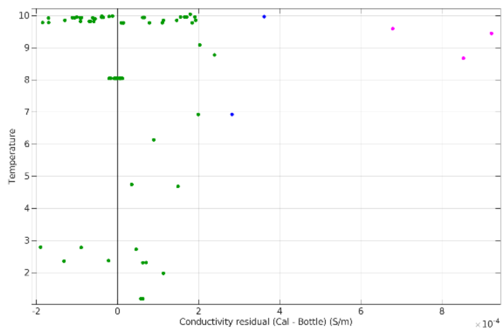
Sea-Bird. (2014). *AN64-3: SBE 43 Dissolved Oxygen (DO) Sensor - Hysteresis Corrections.* Retrieved from Sea-Bird Electronics: https://www.seabird.com/asset-get.download.jsa?code=251035

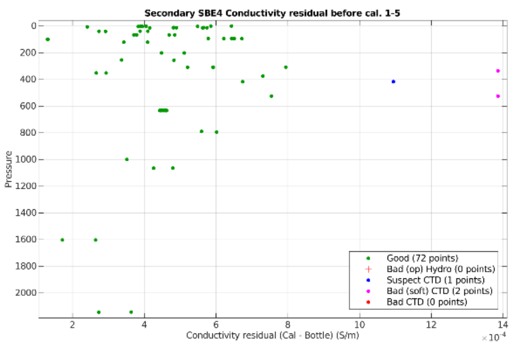
Appendix I: Conductivity Calibration Residual Plots

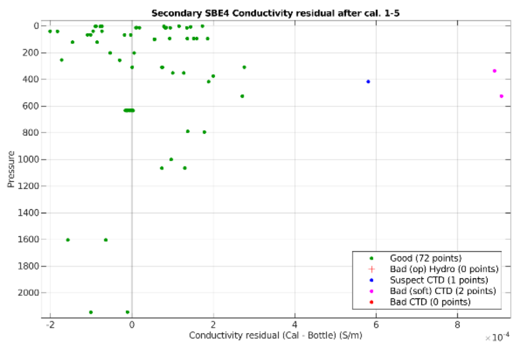


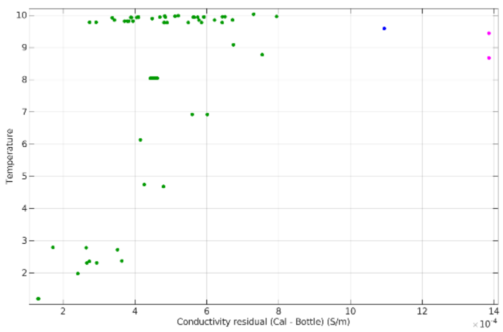


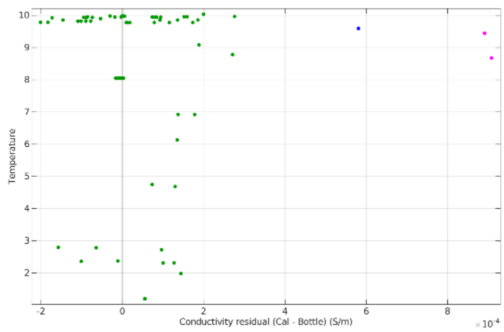












Appendix II: Dissolved Oxygen Calibration Residual Plots