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RV *Investigator* CTD Data Processing Report

Voyage ID	**IN2024_V01**
Voyage Title	Multidisciplinary Investigations of the Southern Ocean (MISO): Linking Physics, Biochemistry, Plankton, Aerosols, Clouds, And Climate
Depart	Hobart TAS, Monday 1st January 2024 21:00 UTC
Return	Freemantle WA, Monday 4th March 2024 02:20 UTC
Chief Scientist	Dr Steve Rintoul (CSIRO)
Data Processor	Vito Dirita (CSIRO – E&T Data Acquisition & Processing)

Document History

Date	Version	Author	Comments
6 May 2024	1.0	Vito Dirita	Initial version
15 May 2024	1.1	Vito Dirita	Final version

Contents

1 Summary

The objective of this voyage was to improve the understanding of how the Southern Ocean region influences the Earth system and use this knowledge to improve models. This voyage characterised the properties of aerosols, clouds, radiation, and precipitation over the Southern Ocean south of Australia and investigate how they are shaped by interactions between the ocean, atmosphere, and biosphere. Repeat observations were used to discover how and why the region is changing and the consequences of Southern Ocean change for climate, biogeochemical cycles, biological productivity, and the future of the Antarctic Ice Sheet. The voyage sought new insights into the processes controlling the availability of iron and other trace elements and their role in regulating productivity in the Southern Ocean and the production of marine organic aerosols that can drive cloud nucleation. The observations and insights gained from the voyage will be used to develop, test, and implement new parameterisations for models used for weather forecasts and climate projections This report describes the production of quality controlled, calibrated CTD data from RV *Investigator* voyage IN2024_V01.

Data for 103 CTD deployments were acquired using the Sea-Bird SBE9+V2 CTD unit #25 (S/N 1354), 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 configuration of the CTD for casts 1-103 is shown in table 1 below.

The final conductivity calibration was based on a single deployment grouping. The final calibration from the primary sensor had a standard deviation (SD) of 0.0012679 PSU, within our target of 'better than 0.002 PSU'. The standard product of 1-decibar binned averages were produced using data from the primary sensors.

The dissolved oxygen data (primary) calibration fit had a SD of 0.94146 (Casts: 1-52) and 0.94773 (Casts: 53-103) µM. The agreement between the CTD and bottle data was good.

Additional sensors include: Altimeter (Tritech PA500), Transmissometer (Wetlabs C-Star), CDOM, Chlorophyll-a, Scattering (Wetlabs ECO FLCDRTD) were installed on the auxiliary A/D channels of the CTD.

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

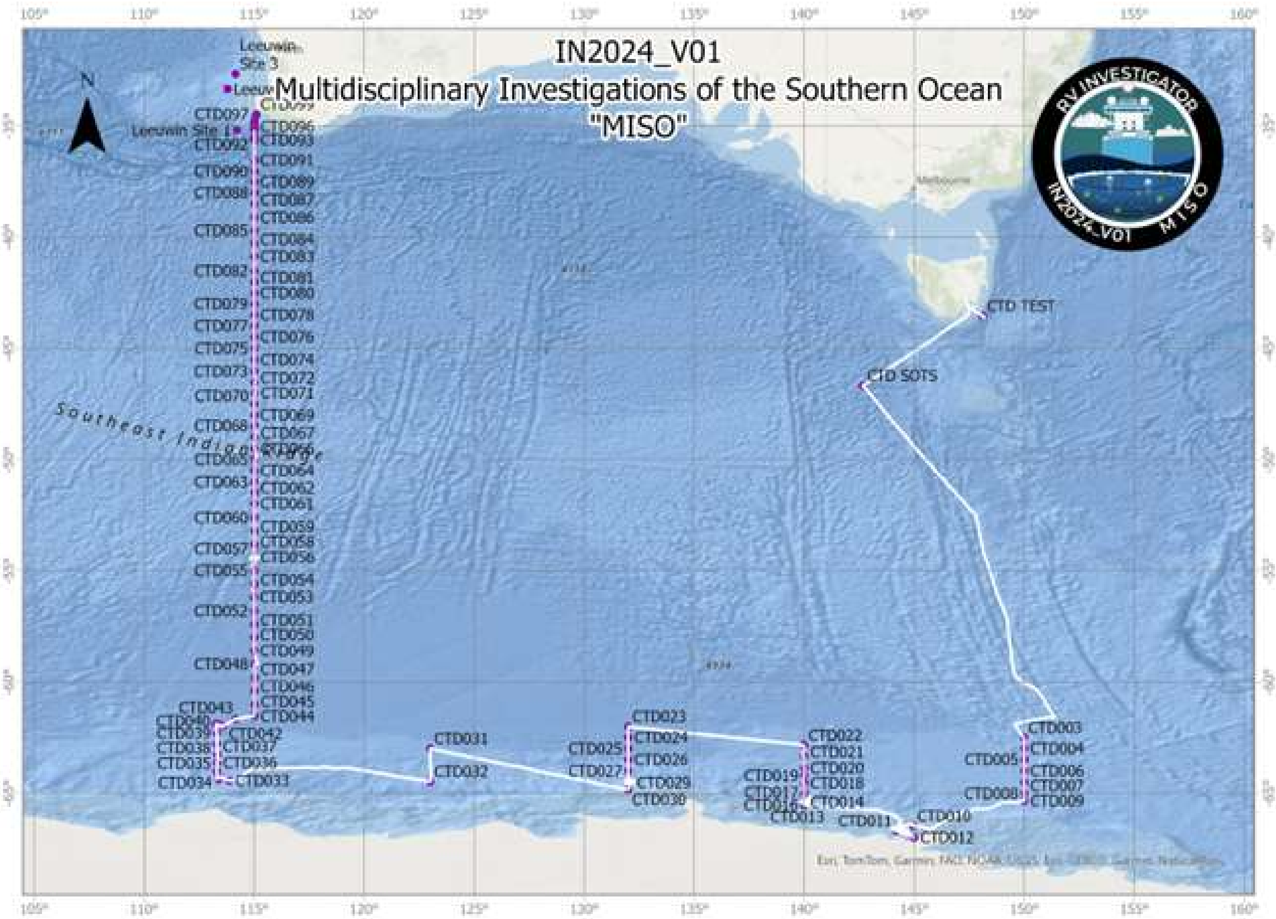


Figure 1: Voyage track

2 Data Processing

2.1 Background Information

103 CTD deployments were conducted on this voyage. The data were acquired with the CSIRO CTD unit #25 (S/N 1354), a Sea-Bird SBE911 with dual conductivity and temperature sensors.

The CTD was additionally fitted with SBE43 dissolved oxygen sensors including Altimeter, PAR, CDOM-Fluorometer, Transmissometer, Chlorophyll-a, and Turbidity. These sensors are described in Table 1 below including instrument serial numbers and calibration dates.

103 CTD casts were performed following the SR-3 southern transit to the ice edge and then the I09S transit north from the ice edge to the Australian continental shelf.

On the first two casts, there was a significant difference between the primary and secondary dissolved oxygen sensor readings. The secondary dissolved oxygen sensor was replaced after cast 2 to a sensor with a more recent membrane service. This configuration was kept till the end of the voyage, refer to Table 1.

Furthermore, both primary and secondary oxygen sensor calibrations have been divided into two sets: 1-52 and 53-103, to account for gradual sensor drift from by a relatively long voyage.

Sensor Description	Model	Serial No.	A/D Channel	Calibration Date	Calibration Source
Pressure	Digiquartz 410K-134	CTD25#1354	P	25-Jul-2023	Sea-Bird
Primary Temperature	Sea-Bird SBE3*plus*	2751	T0	28-Feb-2023	Sea-Bird
Secondary Temperature	Sea-Bird SBE3*plus*	4682	T1	28-Feb-2023	Sea-Bird
Primary Conductivity	Sea-Bird SBE4C	4774	C0	10-Oct-2023	Sea-Bird
Secondary Conductivity	Sea-Bird SBE4C	4683	C1	2-Oct-2023	Sea-Bird
Primary Oxygen	SBE43	3155	A0	7-Feb-2023	Sea-Bird
Secondary Oxygen (cast #1) **(cast #2)** **(cast#3-103)**	SBE43	3647 3646 3198	A1	10-Aug-2023 10-Aug-2023 10-Aug-2023	Sea-Bird
Altimeter	Tritech PA500	228403	A2	26-May-2022	Tritech
PAR	Biospherical QCP2300HP	70562	A3	13-Jan-2023	
CDOM Fluorometer CDOM	Wetlabs ECO FLBBRTD	7138	A4	1-Feb-2024	Wetlabs
Transmissometer	Wetlabs C-Star (DR)	1421	A5	9-Aug-2022	Wetlabs
Chlorophyll-a	Wetlabs ECO FLBBRTD	6765	A6	10-Apr-2023	Wetlabs/Sea-Bird
Scattering / Turbidity	Wetlabs ECO FLBBRTD	6765	A7	4-Oct-2023	Wetlabs/Sea-Bird
Midas SVX2 sound velocity probe	Valeport	73429			

Table 1: CTD Sensor configuration on IN2024_V01

Water samples were collected using a Sea-Bird SBE32, 12-litre 36-bottle rosette sampler which was fitted to the frame. 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 files with CNV_to_Scan (cnv_to_scan_ui2.py, from the CSIRO MNF Data Acquisition and Processing “marinetech” git repository) for processing using the MATLAB-based CapPro software.

The CapPro software version 2.11 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).

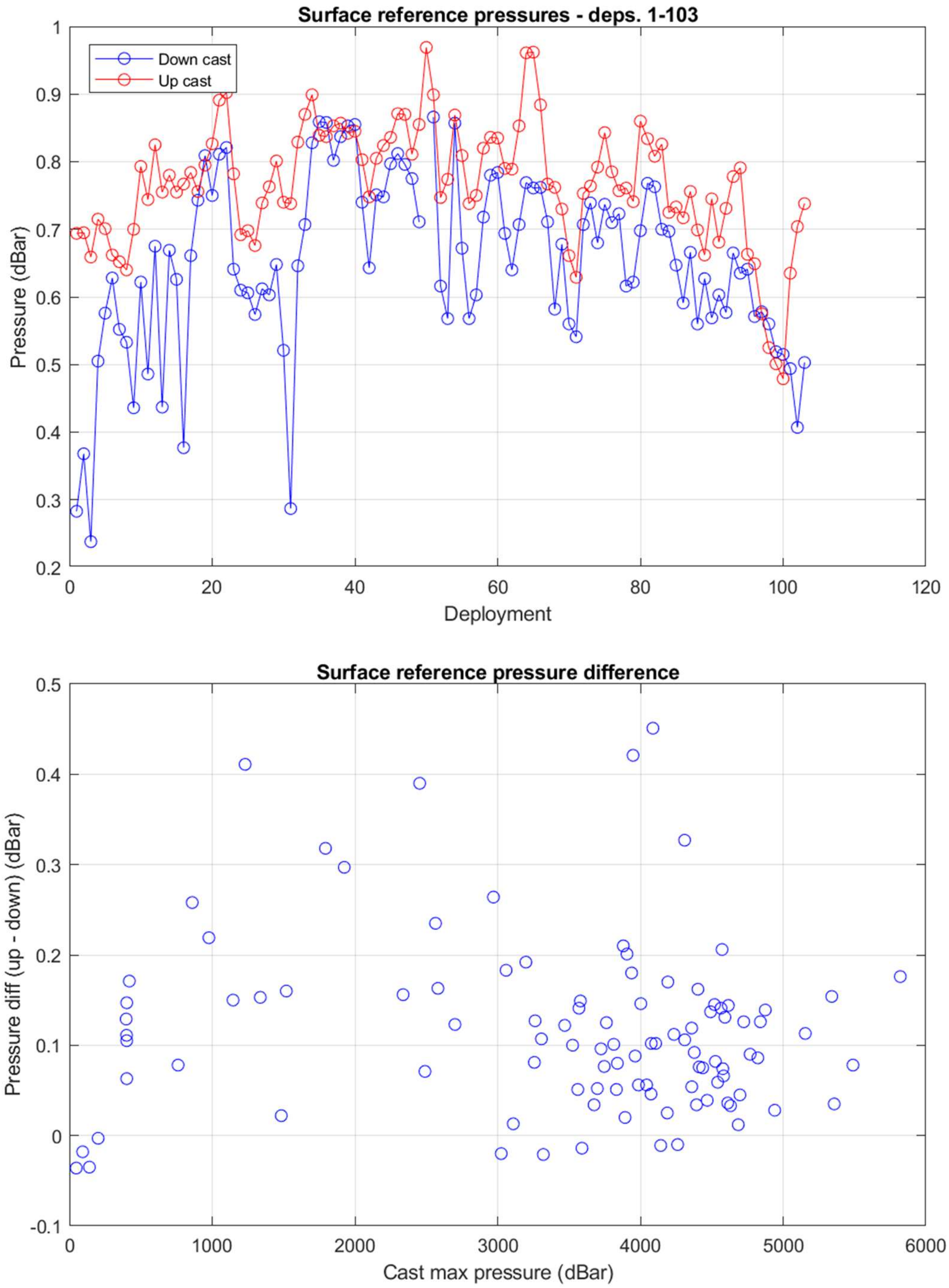


Figure 2: CTD pressure offsets

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. The consistent mean difference (red +

markers) between the primary and secondary temperature from deployment to deployment indicates neither sensor has drifted significantly from its calibration. Higher fluctuations in difference presented in the plots represents shallower casts, where the high gradient is present throughout most of the cast.

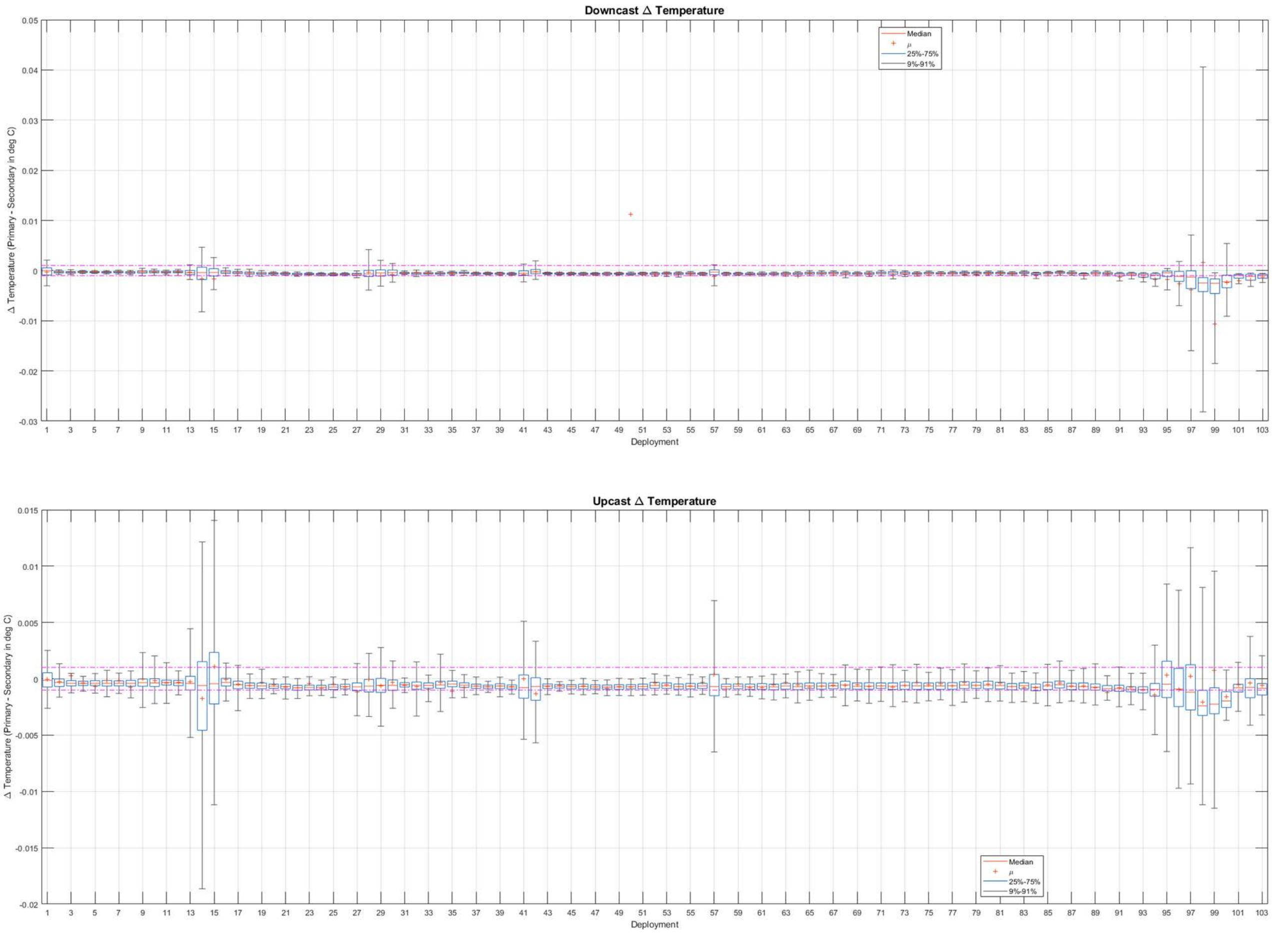


Figure 3: Difference (primary - secondary) between temperature sensor values on downcast (left) and upcast (right)

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 minor 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, 1642 of 2227 (73.7%) good samples from the primary unit and 1638 of 2227 (73.5%) good samples from the secondary unit. 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 0.003 (primary) and 0.003 (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.

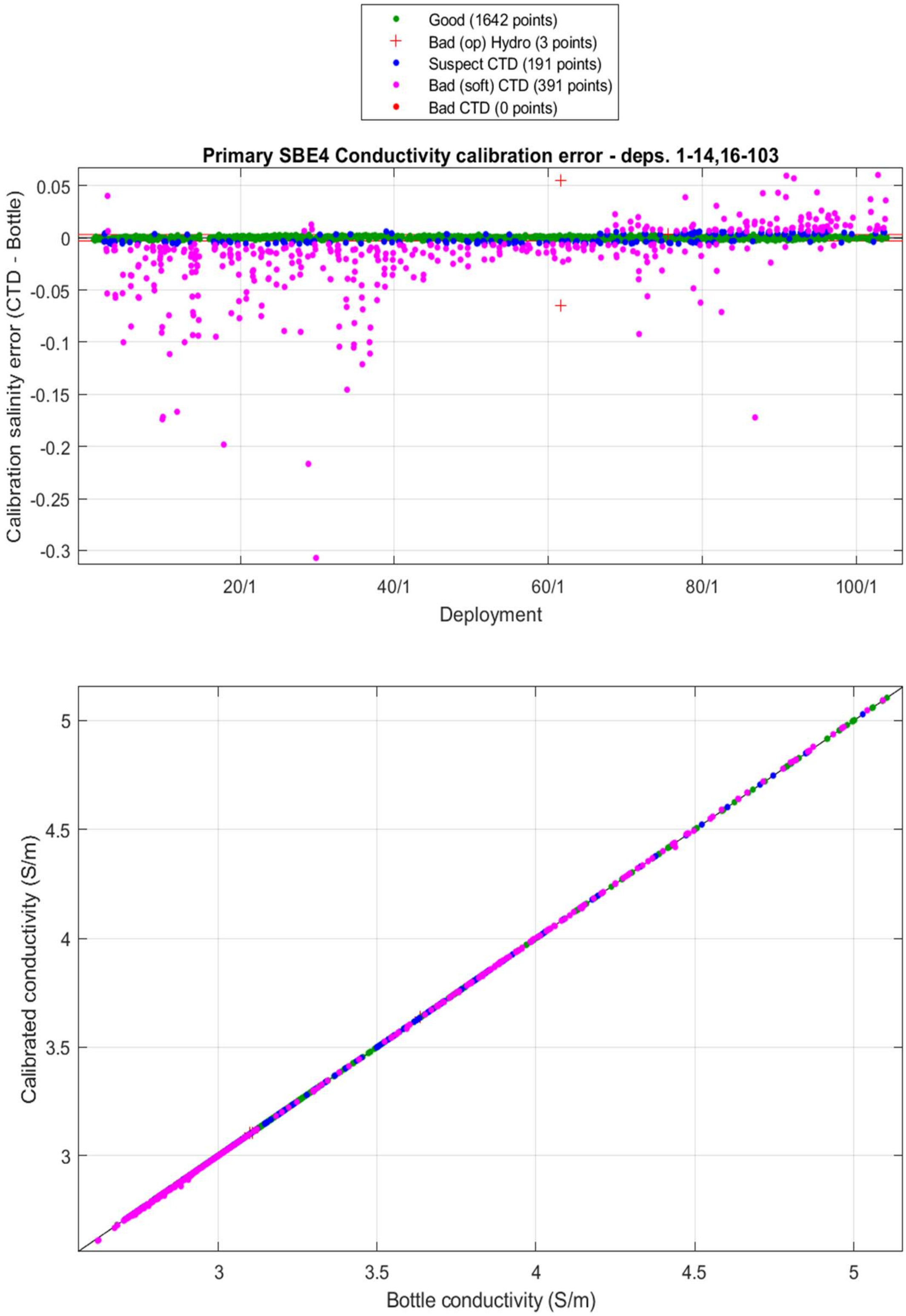


Figure 4a: CTD - bottle conductivity difference and salinity calibration error (primary)

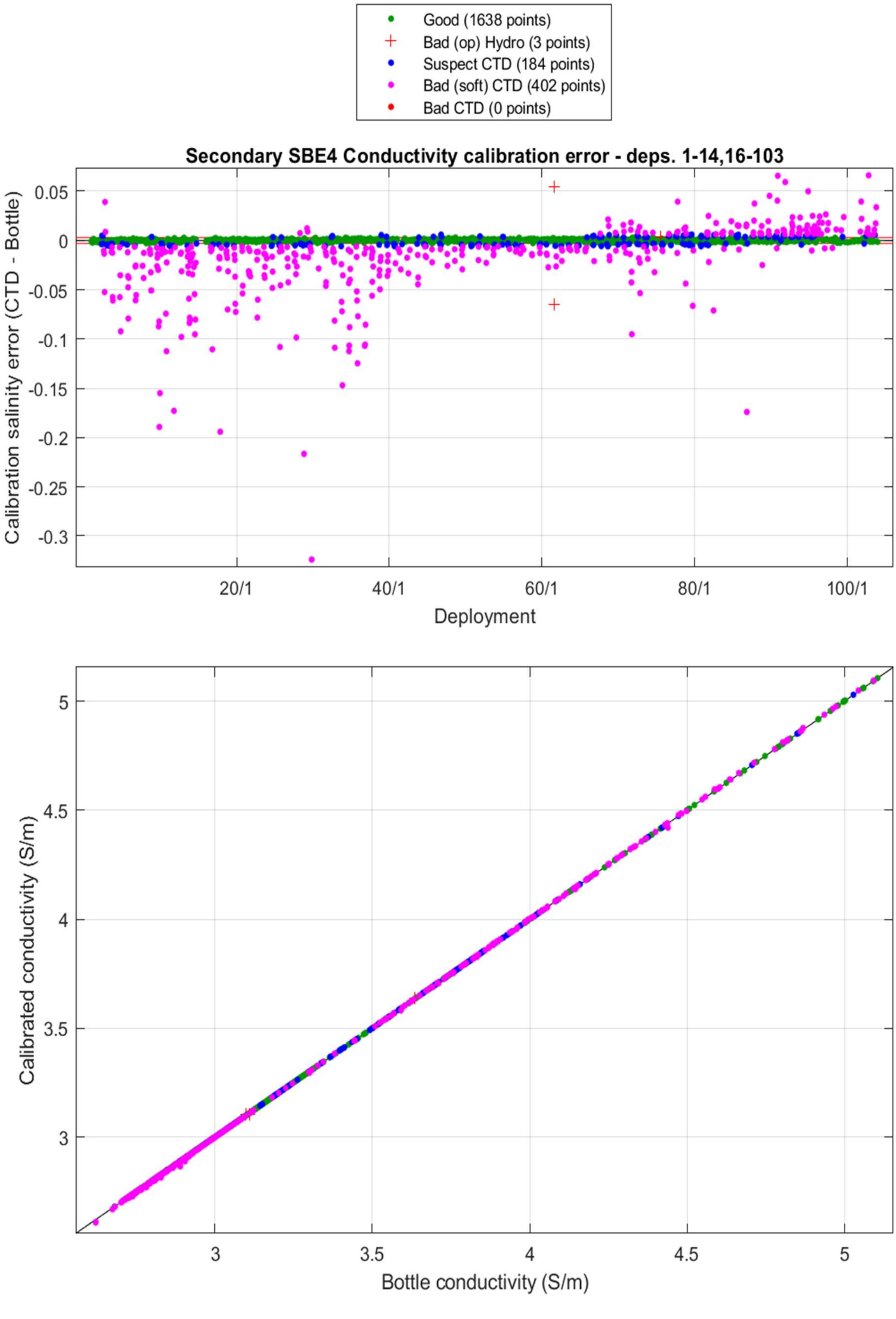


Figure 4b: CTD - bottle conductivity difference and salinity calibration error (secondary)

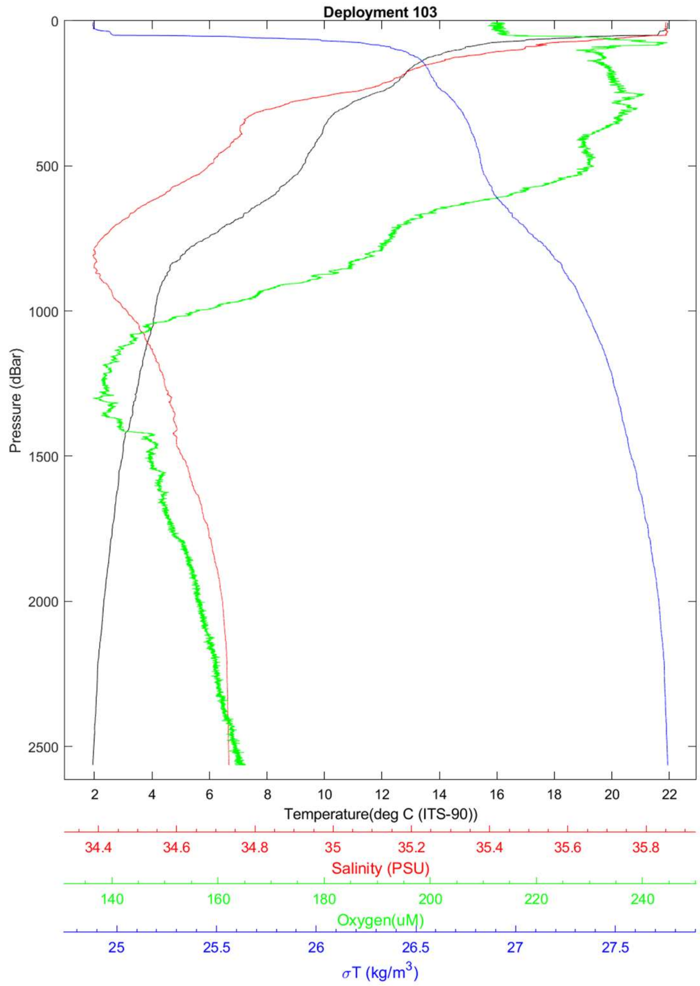


Figure 5: Temperature, salinity, dissolved oxygen and σT profiles

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 well to each other.

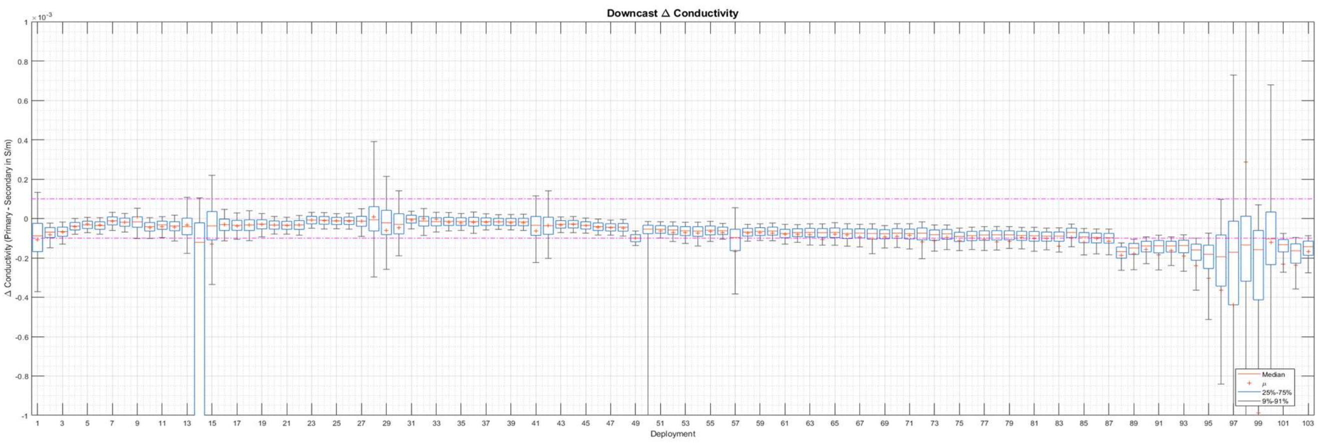


Figure 6: Difference (primary - secondary) between conductivity sensor values on downcast

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	1-103	0.99964	0.00015681	0.00073884	0.00052973	0.0012679	0.00088842
Secondary	1-103	0.99967	0.00015132	0.00074918	0.00050985	0.0012645	0.00080845

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

Conductivity Sensor	Deployments	CPcor	±
Primary	1-103	-8.2025e-08	1.4091e-08
Secondary	1-103	-7.6901e-08	1.339e-08

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 good calibration. We normally aim for a SD of 0.002 PSU 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

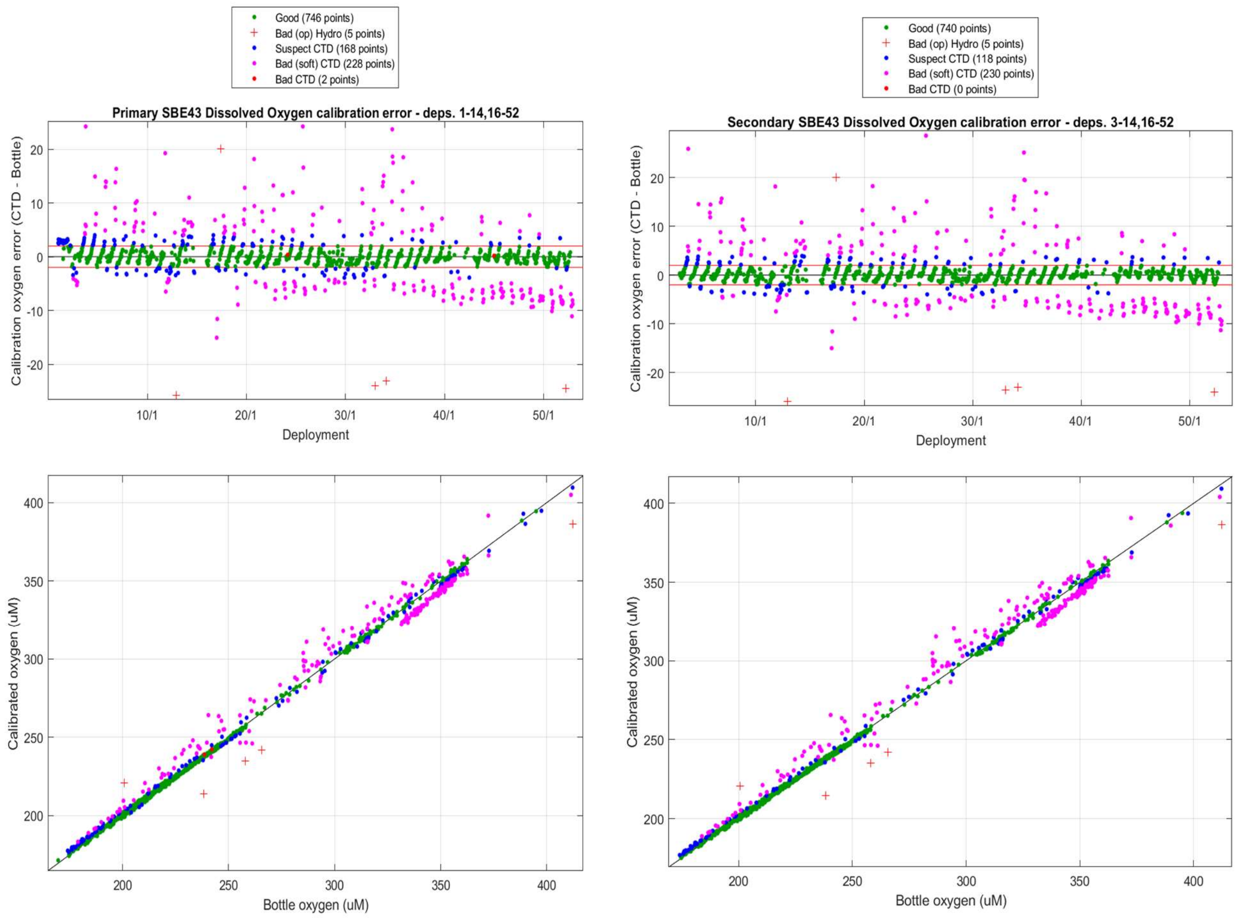
AN64: SBE 43 Dissolved Oxygen Sensor - Background Information, Deployment Recommendations, and Cleaning and Storage (Sea-Bird, 2013) describes the SBE43 dissolved oxygen sensor as "a polarographic membrane oxygen sensor having a single output signal of 0 to +5 volts, which is proportional to the temperature-compensated 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 *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.

On the first two casts, there was a significant difference between the primary and secondary dissolved oxygen sensor readings. The secondary dissolved oxygen sensor was replaced after cast 2 to a sensor with a more recent membrane service. This configuration was kept till the end of the voyage, refer to Table 1. For the secondary oxygen, four calibration groups were used with the associated SBE43 upcast data to compute the new *Soc* and *Voffset* coefficients and two calibration groups for the primary. 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. 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 well to each other. Both primary and secondary oxygen sensor calibrations have been further divided into two sets: 1-52 and 53-103, to account for gradual sensor drift from by a relatively long voyage.



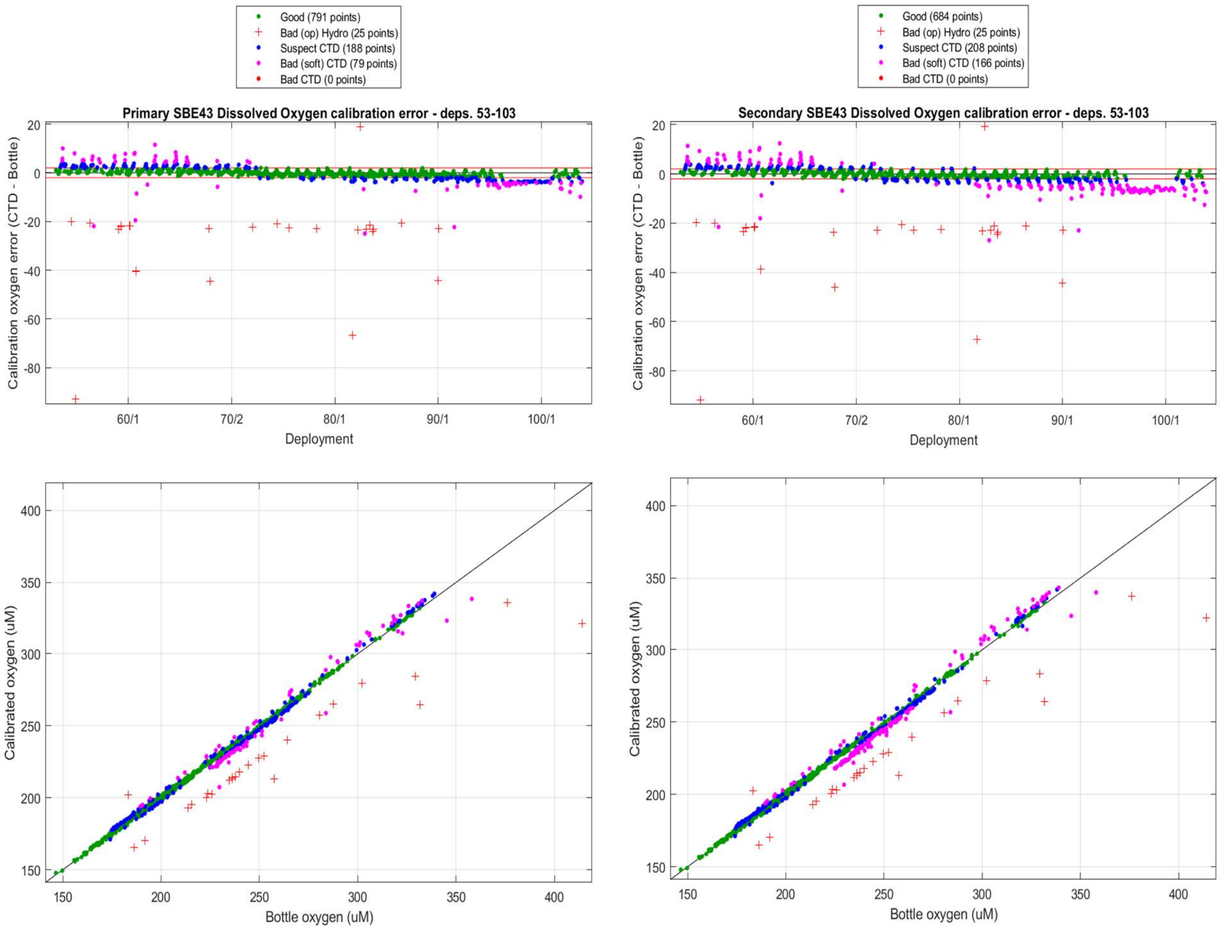


Figure 7: CTD SBE43 - bottle dissolved oxygen difference and calibration error (left: primary, right: secondary)

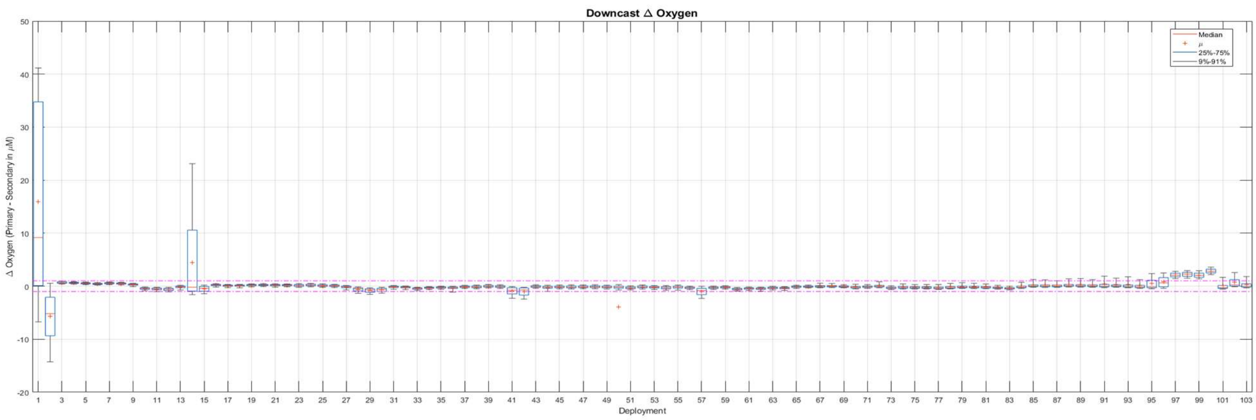


Figure 8: Difference (primary - secondary) between dissolved oxygen sensor values on downcast

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. 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 A.2. The calibrations were applied for each sensor and the averaged files were created using the result from the primary sensor. Note that an anomaly was observed on the primary oxygen sensor at cast #53 at around 2160 dbar (blockage or fault) lasting over several dbars which was not detected by CapPro (see appendix A.3)

Sensor	Calibration Source	Casts:	Calibration Coefficients				Dissolved Oxygen (µM)	
			Voffset	±	*Soc*	±	Residual SD	M.A.D.
Primary	CapPro	1-52 53-103	-0.44717 -0.48291	0.0012128 0.00085716	0.49553 0.52217	0.00055687 0.00043486	0.94146 0.94773	0.97618 1.0056
	Sea-Bird 3155	1-103	-0.5007		0.50630			
Secondary	CapPro	1 2 3-52 53-103	0.40292 -0.44787 -0.42158 -0.47502	3.0362 0.0069257 0.0013967 0.0012259	0.24629 0.44502 0.39158 0.41515	0.36852 0.0025269 0.00040188 0.00040842	0.57144 1.0061 0.91316 0.98538	0.16003 0.77762 0.7985 1.109
	Sea-Bird 3647 Sea-Bird 3646 Sea-Bird 3198	1 2 3-103	-0.5234 -0.4616 -0.4947		0.52803 0.53156 0.41235			

Table 4: Dissolved oxygen calibrations

2.5 Other Sensors

2.5.1 WET Labs C-Star Transmissometer

The C-Star transmissometer was used on all deployments. It was calibrated by the manufacturer by measuring the output 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 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 (= µg/L). The scattering (optical backscatter, OBS) has been calibrated with manufacturer supplied coefficients to give volume scattering outputs in $m^{-1}sr^{-1}$.

2.5.4 Chlorophyll-a Chelsea Aquatracka Fluorometer

The instrument operated without fault or issue throughout the voyage.

2.5.5 Sea-Bird Scientific Deep SUNA V2 nitrate sensor

The Sea-Bird Scientific Deep SUNA V2 nitrate sensor was not used on this voyage.

2.5.6 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 µEinsteins/m2/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 **Error! Reference source not found.**. The rejection rate is recorded in the CapPro processing log file.

Sensor	Range minimum	Range maximum	Maximum Second
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
Altimeter	0	50	0.5
PAR	-5	2000	0.5
Transmissometer	0	100	0.5
CDOM	-5	515	0.5
OBS	0	0.008	0.5
Nitrate	0	100	10

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 **Error! Reference source not found.**. 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)
1-103	-0.073	-0.55	-0.0229

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)
1-103	-0.073	-1.70	-0.0708

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 & NCMI 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

Tim O'Hara. (2022). *The RV Investigator. Voyage Plan* IN2024_V01. Retrieved from Marine National Facility: Voyage Plans and summaries: https://mnf.csiro.au/en/Voyages/Voyage-Catalogue

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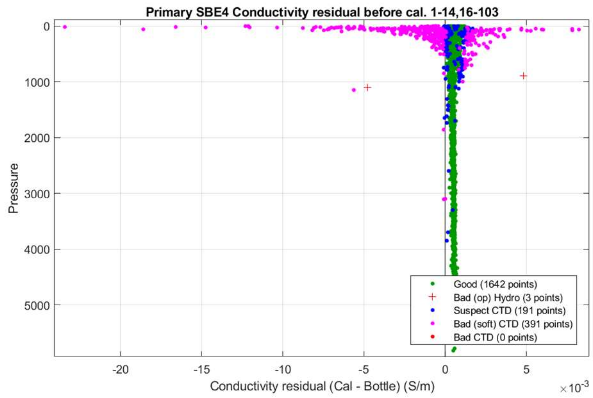
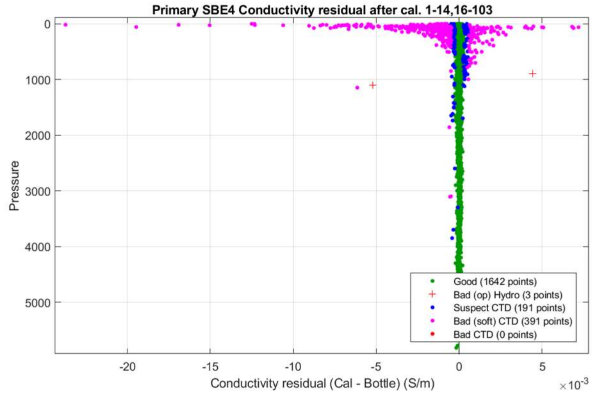
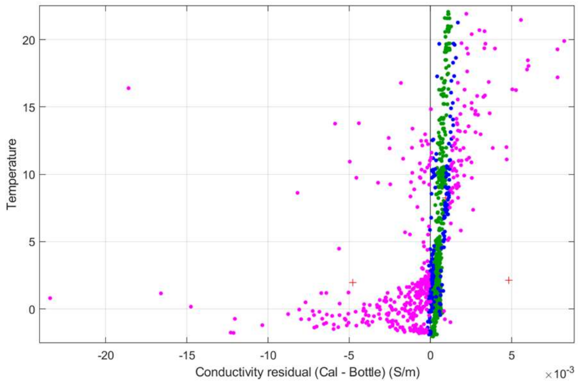
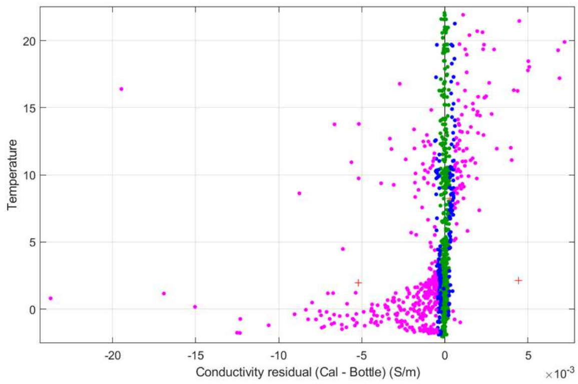
4 Appendices

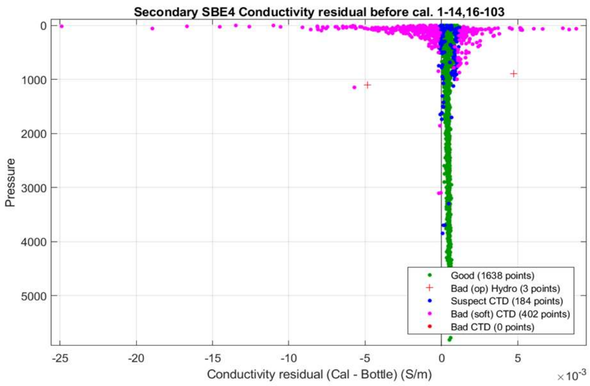
A.1 Conductivity Calibration Residual Plots

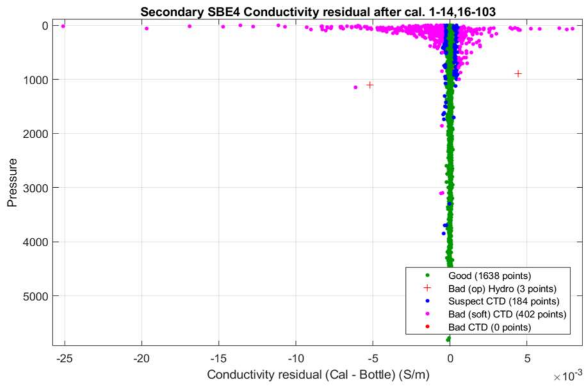


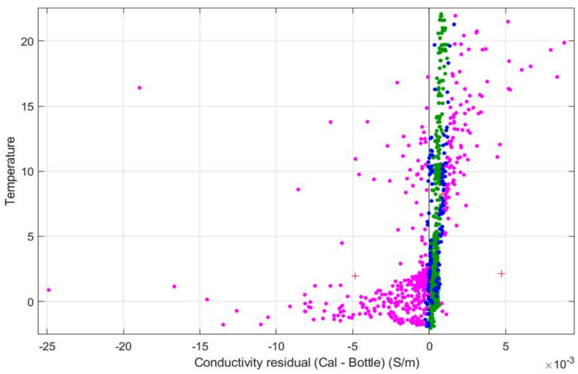


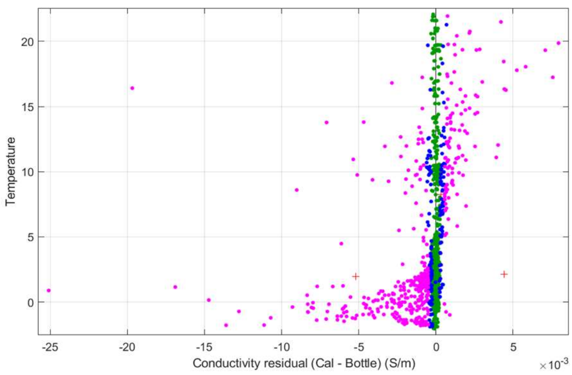




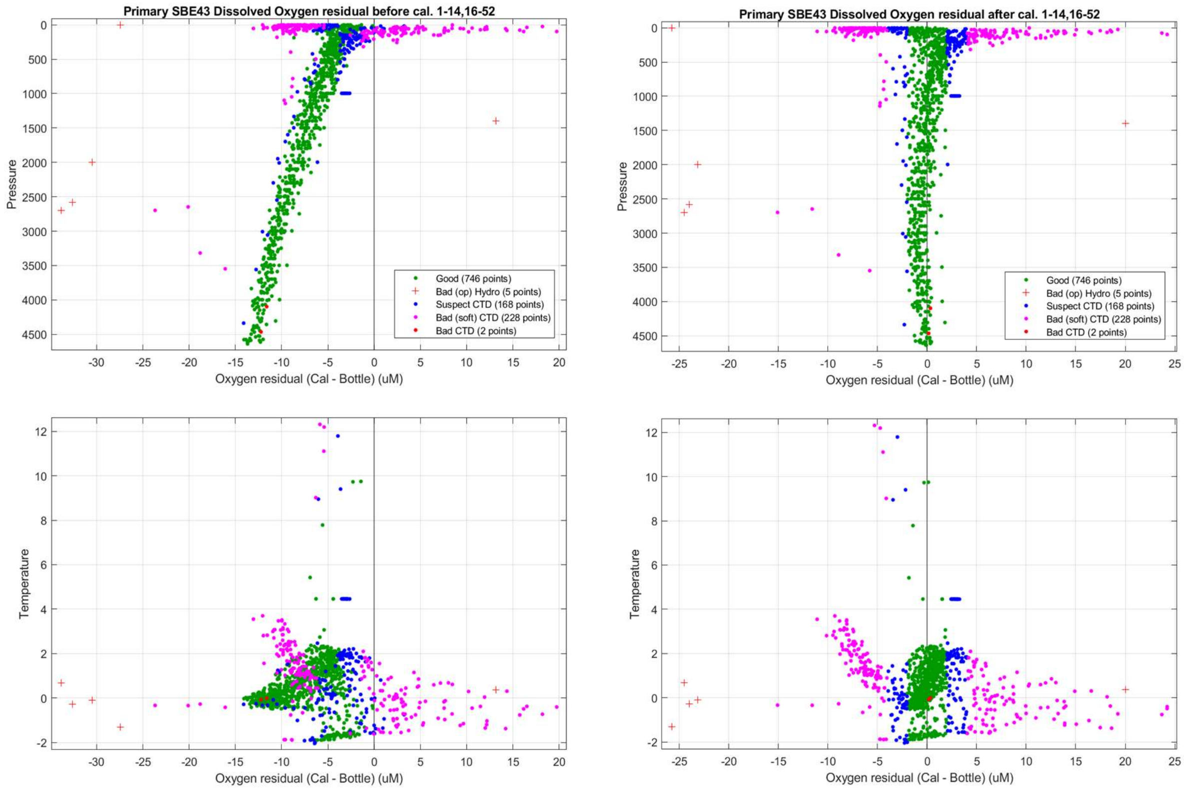


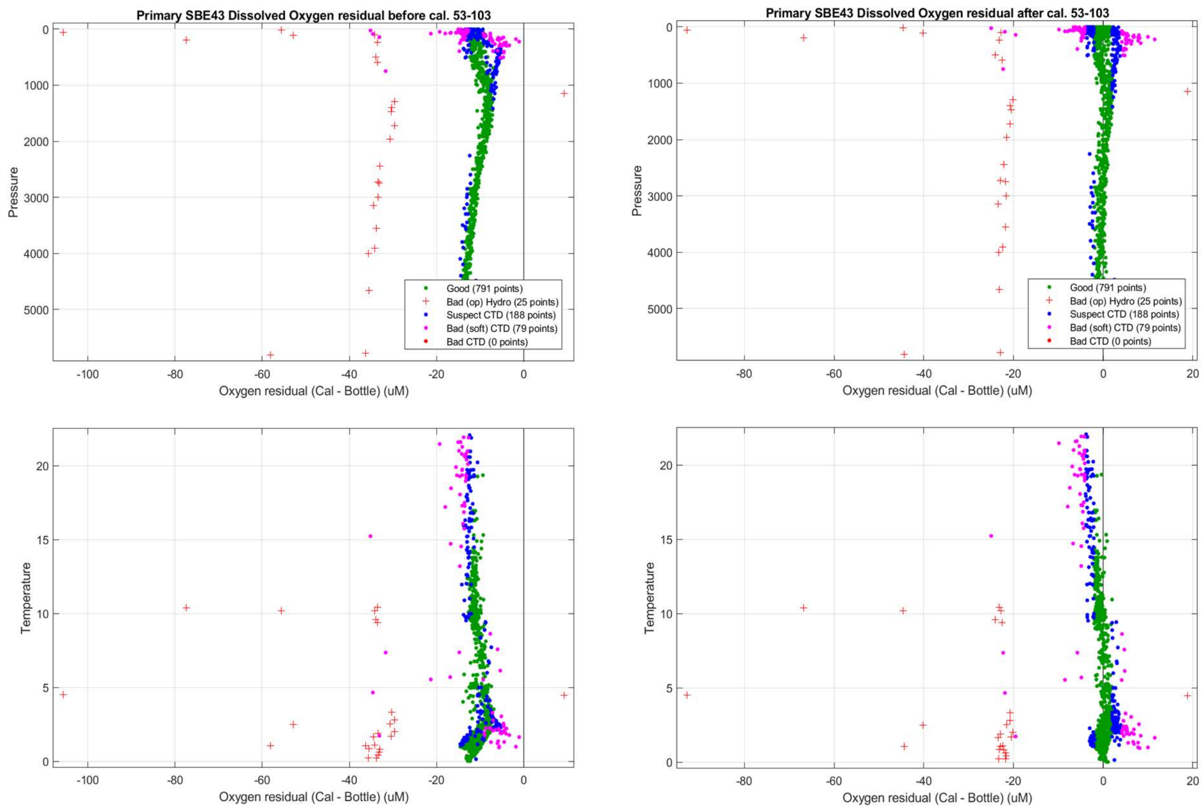


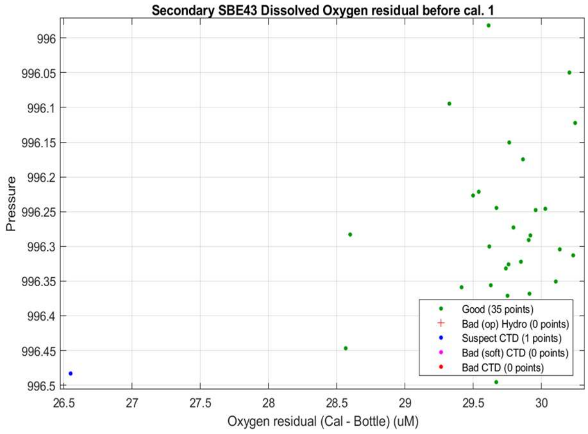


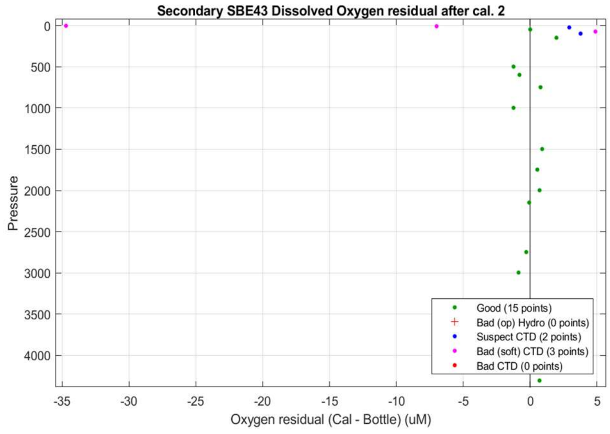


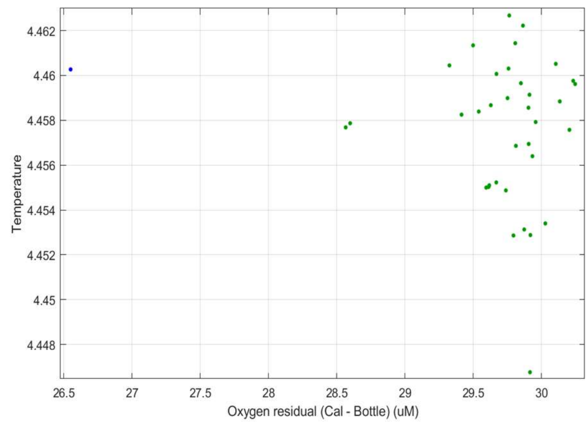
A.2 Dissolved Oxygen Calibration Residual Plots

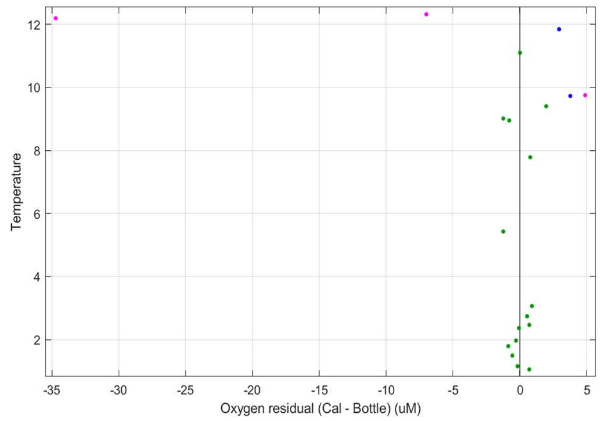


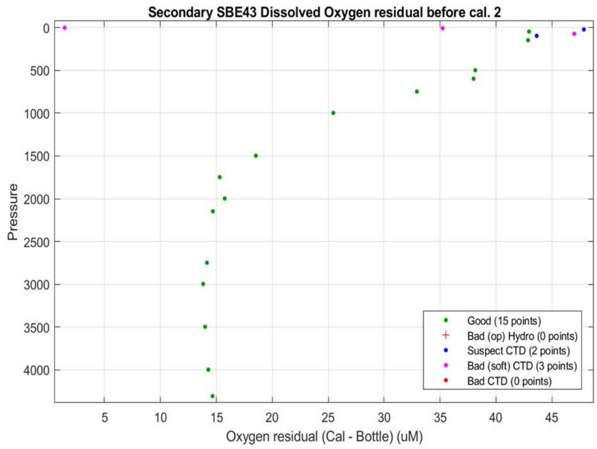


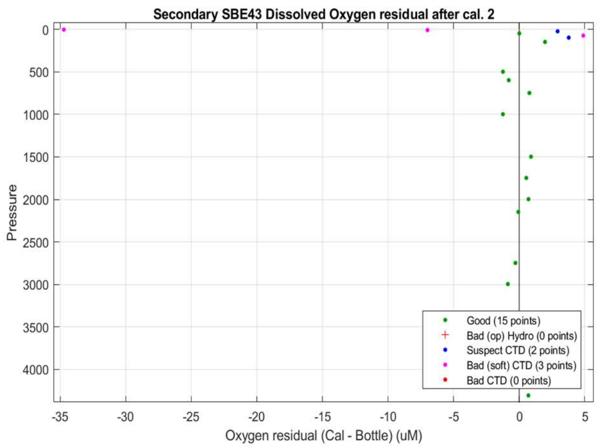

Secondary SBE43 Dissolved Oxygen residual before cal. 1
Pressure
Oxygen residual (Cal - Bottle) (uM)
Good (35 points)
Bad (op) Hydro (0 points)
Suspect CTD (1 points)
Bad (soft) CTD (0 points)
Bad CTD (0 points)

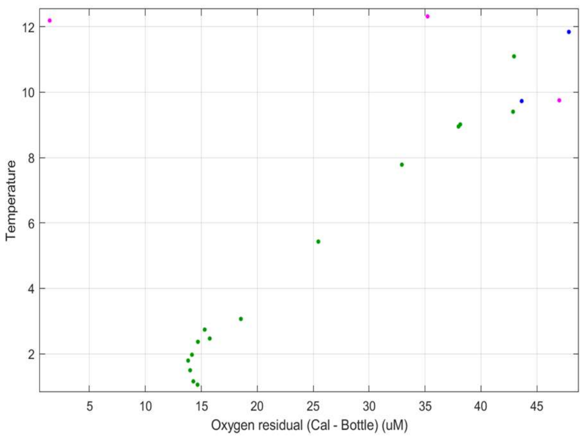

Secondary SBE43 Dissolved Oxygen residual after cal. 2
Pressure
Oxygen residual (Cal - Bottle) (uM)
Good (15 points)
Bad (op) Hydro (0 points)
Suspect CTD (2 points)
Bad (soft) CTD (3 points)
Bad CTD (0 points)

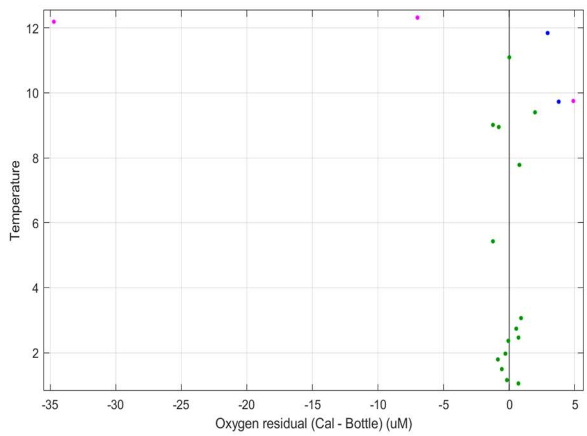

Temperature
Oxygen residual (Cal - Bottle) (uM)

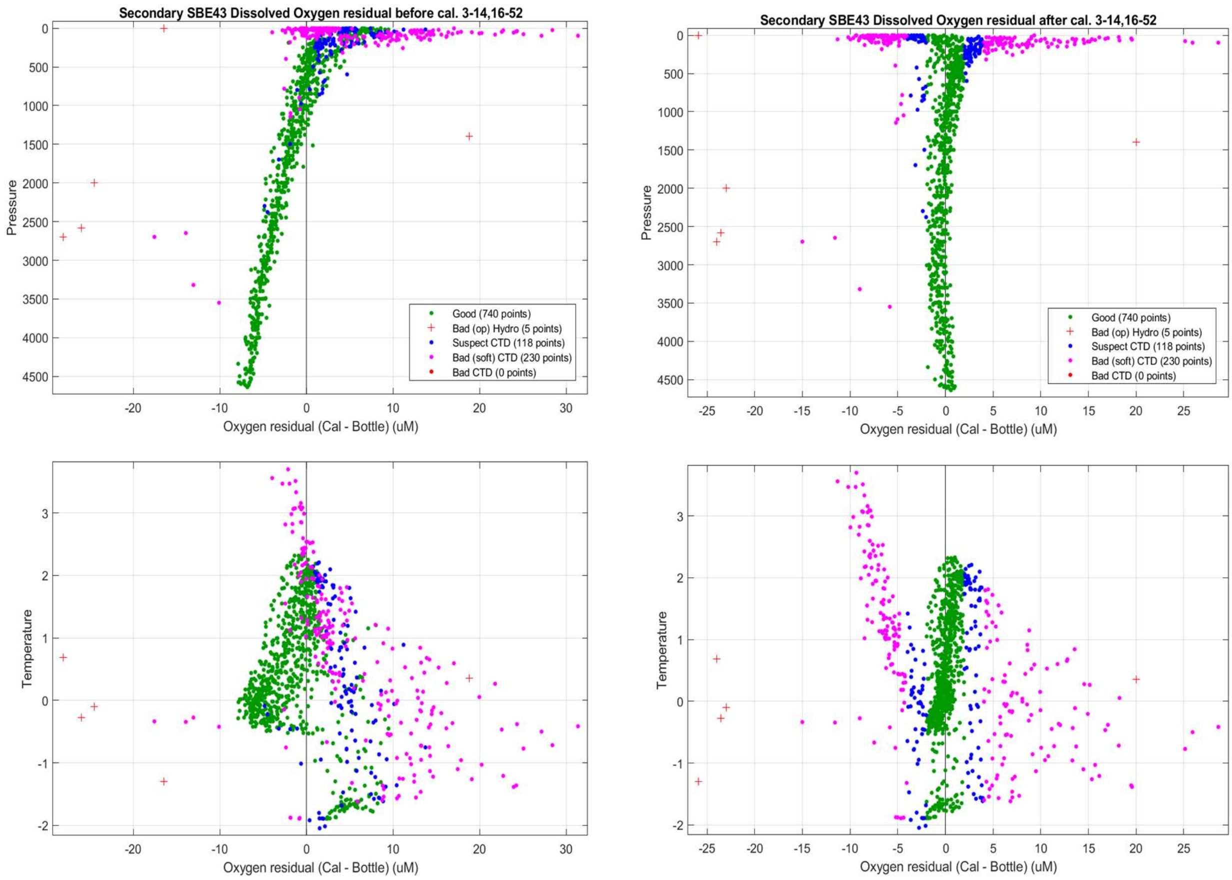

Temperature
Oxygen residual (Cal - Bottle) (uM)

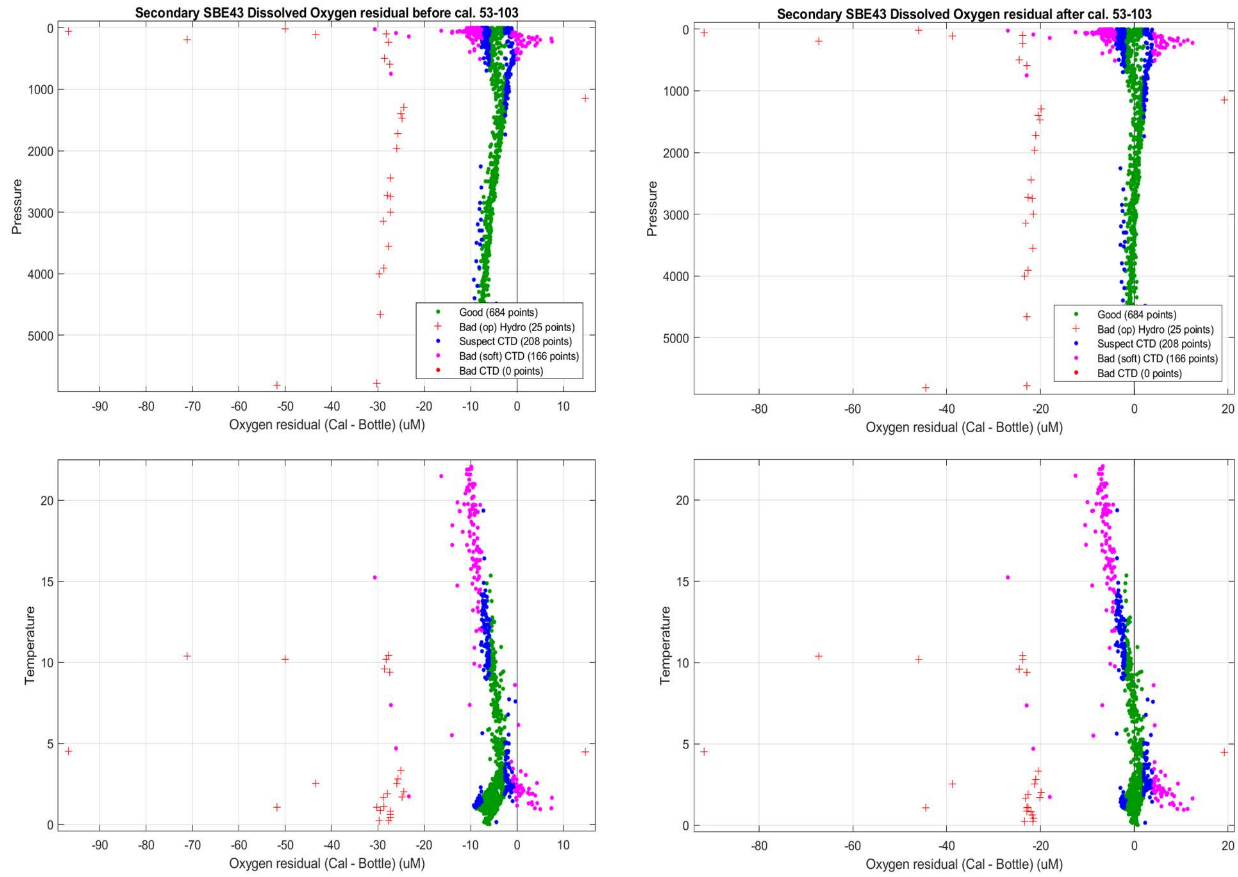

Secondary SBE43 Dissolved Oxygen residual before cal. 2
Pressure
Oxygen residual (Cal - Bottle) (uM)
Good (15 points)
Bad (op) Hydro (0 points)
Suspect CTD (2 points)
Bad (soft) CTD (3 points)
Bad CTD (0 points)


Secondary SBE43 Dissolved Oxygen residual after cal. 2
Pressure
Oxygen residual (Cal - Bottle) (uM)
Good (15 points)
Bad (op) Hydro (0 points)
Suspect CTD (2 points)
Bad (soft) CTD (3 points)
Bad CTD (0 points)


Temperature
Oxygen residual (Cal - Bottle) (uM)

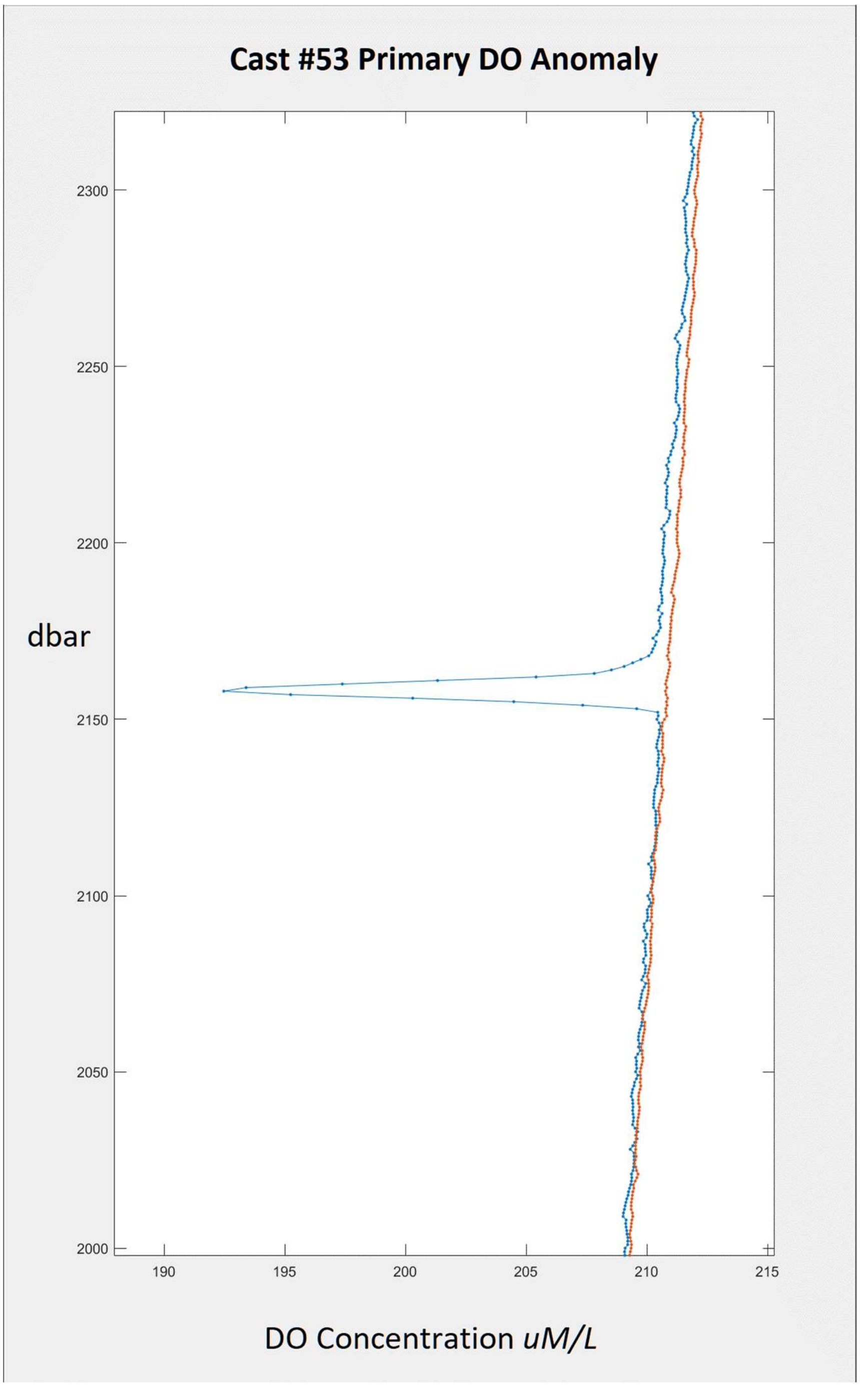

Temperature
Oxygen residual (Cal - Bottle) (uM)


Secondary SBE43 Dissolved Oxygen residual before cal. 3-14,16-52
Secondary SBE43 Dissolved Oxygen residual after cal. 3-14,16-52
Pressure
Temperature
Oxygen residual (Cal - Bottle) (uM)
Good (740 points)
Bad (op) Hydro (5 points)
Suspect CTD (118 points)
Bad (soft) CTD (230 points)
Bad CTD (0 points)


Secondary SBE43 Dissolved Oxygen residual before cal. 53-103
Secondary SBE43 Dissolved Oxygen residual after cal. 53-103
Pressure
Temperature
Oxygen residual (Cal - Bottle) (uM)
Good (684 points)
Bad (op) Hydro (25 points)
Suspect CTD (208 points)
Bad (soft) CTD (166 points)
Bad CTD (0 points)

A.3 Cast #53 Primary Dissolved Oxygen Anomaly

Anomaly observed on the primary oxygen sensor at cast #53 at around 2160 dbar (blockage or fault) not flagged using second differences filtering method by CapPro, this is illustrated below where the blue plot is the primary oxygen and the orange is the secondary oxygen.



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