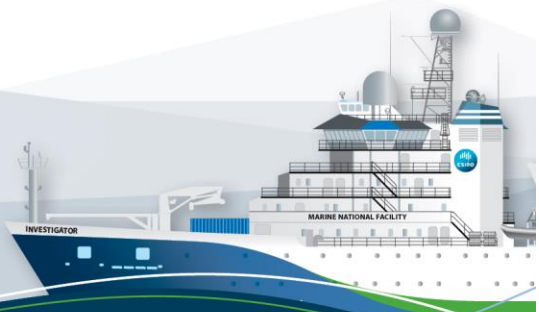
RV *Investigator*

CTD Processing Report

Voyage #:	IN2016_V05
Voyage title:	The Great Barrier Reef as a significant source of climatically relevant aerosol particles
Depart:	Brisbane, 0800 Wednesday, 28 September 2016
Return:	Brisbane, 1700 Monday, 24 October 2016
Report compiled by:	Francis Chui & Anoosh Sarraf



Contents

1 Summary

These notes relate to the production of quality controlled, calibrated CTD data from RV Investigator voyage IN2016_V05, from 28 Sep 2016 – 24 Oct 2016.

Data for 62 deployments were acquired using the Seabird SBE911 CTD 21 and CTD 20, 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 (S.D) of 0.0014061 PSU, well within our target of 'better than 0.002 PSU'. The standard product of 1 dBar binned averaged were produced using data from the primary sensors.

The dissolved oxygen data calibration fit had a S.D. of 0.67142 µM. The agreement between the CTD and bottle data was good.

Altimeter, PAR, CDOM, Fluorometer, Transmissometer, Nephelometer, ISUS Nitrate were also installed on the auxiliary A/D channels of the CTD.

2 Voyage Details

2.1 Title

The Great Barrier Reef as a significant source of climatically relevant aerosol particles.

2.2 Principal Investigators

Chief Scientist Zoran Ristovski (Queensland University of Technology), Principal Investigator Karen Wild-Allen.

2.3 Voyage Objectives

The scientific objectives for IN2016_V05 were outlined in the Voyage Plan.

For further details, refer to the Voyage Plan and/or summary which can be viewed on the CSIRO Oceans & Atmosphere web site.

2.4 Area of operation

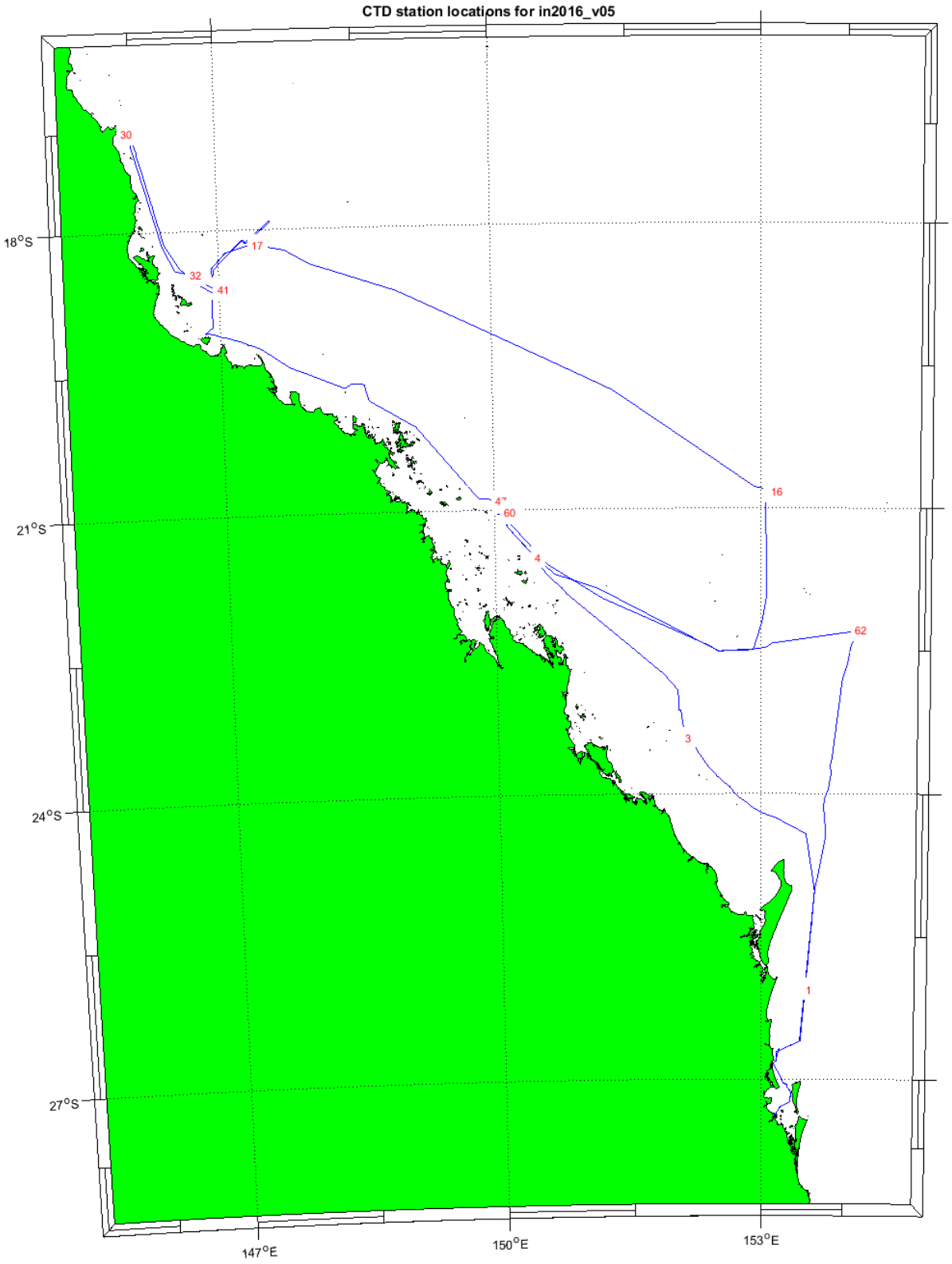


Figure 1 Area of operation for IN2016_V05

3 Processing Notes

3.1 Background Information

The data for this voyage were acquired with the CSIRO CTD unit 21 for deployment 1 and CTD unit 20 for the remaining deployments, both units were Seabird SBE911 with dual conductivity and temperature sensors. There were issues with pressure readings returned from CTD unit 21 and it was replaced with CTD unit 20 which was mounted on the Triaxus.

Subsequent to the voyage it was discovered the calibration values for pressure were incorrectly entered in CAP for deployment 1 in PSI when they should have been in dBar. The data was corrected by regenerating the scan netCDF file and reprocessed.

The CTD was additionally fitted with a SBE43 dissolved oxygen sensor, Altimeter, Fluorometer, PAR, CDOM, Transmissometer, Nephelometer and ISUS Nitrate sensors. These sensors are described in Table 1, Table 2, Table 3 and Table 4.

Description	Sensor	Serial No.	A/D	Calibration Date	Calibration Source
Pressure	SBE9+ V1	858	P	2016-03-10	Seabird cal report 3826P
Primary Temperature	SBE3T	5450	T0	2016-03-10	CSIRO Calibration Lab report #3831T
Secondary Temperature	SBE3T	5422	T1	2016-03-10	CSIRO Cal Lab report 3830T
Primary Conductivity	SBE4C	3309	C0	2016-03-10	CSIRO Calibration report 3835C
Secondary Conductivity	SBE4C	3169	C1	2016-03-10	CSIRO Calibration Lab report 3832C
Primary Dissolved Oxygen	SBE43	3154	A0	2016-03-10	CSIRO report 3837 DO.
Secondary Dissolved Oxygen	SBE43	3159	A1	2016-03-10	CSIRO Cal Report for 3839 SBE-43 DO sensor
Altimeter	PA 500	5301	A2	2016-09-07	
PAR	QCP2300HP	70111	A3	2016-08-01	Manufacturer's cal job R12719
CDOM	FLCDRTD	4367	A4	2016-02-05	Manufacturer's
Transmissometer	CSTAR	CST-1735DR	A5	2015-07-16	Wet Labs 25cm
Nitrate	MBARI-ISUS V3	236	A6	2016-08-11	

Table 1 CTD Sensor configuration for deployment 1 of IN2016_V05

Description	Sensor	Serial No.	A/D	Calibration Date	Calibration Source
Pressure	SBE9+ V2	552	P	2016-07-27	Seabird Cal Report 4127 P -dBar
Aquatracka Fluorometer	088-3598C	06-5941-001	A1	2014-02-06	Manufacturer's

Table 2 CTD Sensor configuration alterations for deployment 2-12 of IN2016_V05

Description	Sensor	Serial No.	A/D	Calibration Date	Calibration Source
Nephelometer	Seapoint Turbidity meter	13142	A5	2016-01-10	

Table 3 CTD Sensor configuration alterations for deployment 14 of IN2016_V05

Description	Sensor	Serial No.	A/D	Calibration Date	Calibration Source
Nitrate Uncertainty	MBARI-ISUS V3	236	A7	-	

Table 4 CTD Sensor configuration alterations for deployments 13, 15-62 of IN2016_V05

Water samples were collected using a Seabird SBE32, 24-bottle rosette sampler. Sampling was from 24 ten litre bottles which were fitted to the frame. There were 62 deployments (deployments 9, 15 and 61 were for surface water collection only and deployment 10 was cancelled).

The raw CTD data were converted to scientific units and written to netCDF format files for processing using the Matlab-based, CapPro package.

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 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 dBar 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.

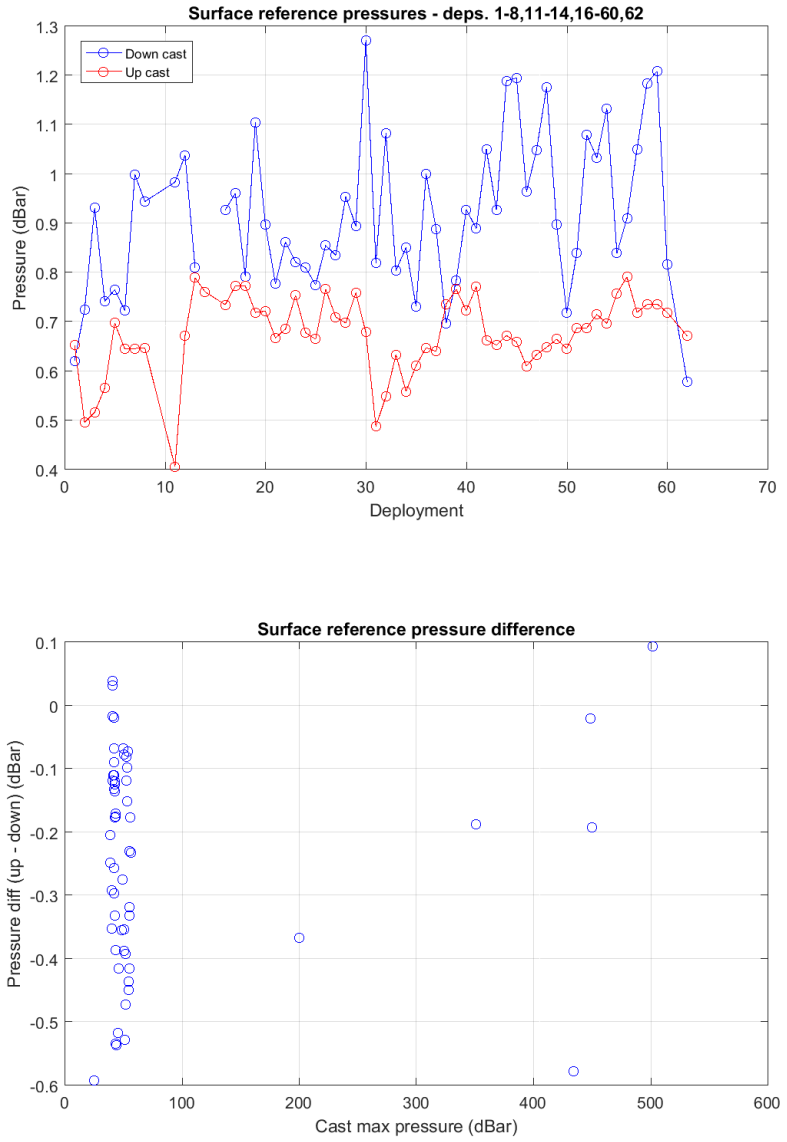


Figure 2 CTD pressure offsets

3.3 Conductivity Calibration

Discrepancies and possible sampling problems between bottle and CTD salinities for the primary conductivity sensor would show in Figure 3 and Figure 4, the plots of calibrated (CTD - Bottle) salinity below. The calibration was based upon the sample data for 150 (124 good and 26 suspect) of the total of 201 samples taken during deployments with a cut off of 0.003 S/m. The outliers marked with blue dots were used in the calibration but were weighted based on their distance from the mean while those marked with magenta dots have been excluded). Additional plots of residuals can be found in Appendix I: Conductivity Residuals.

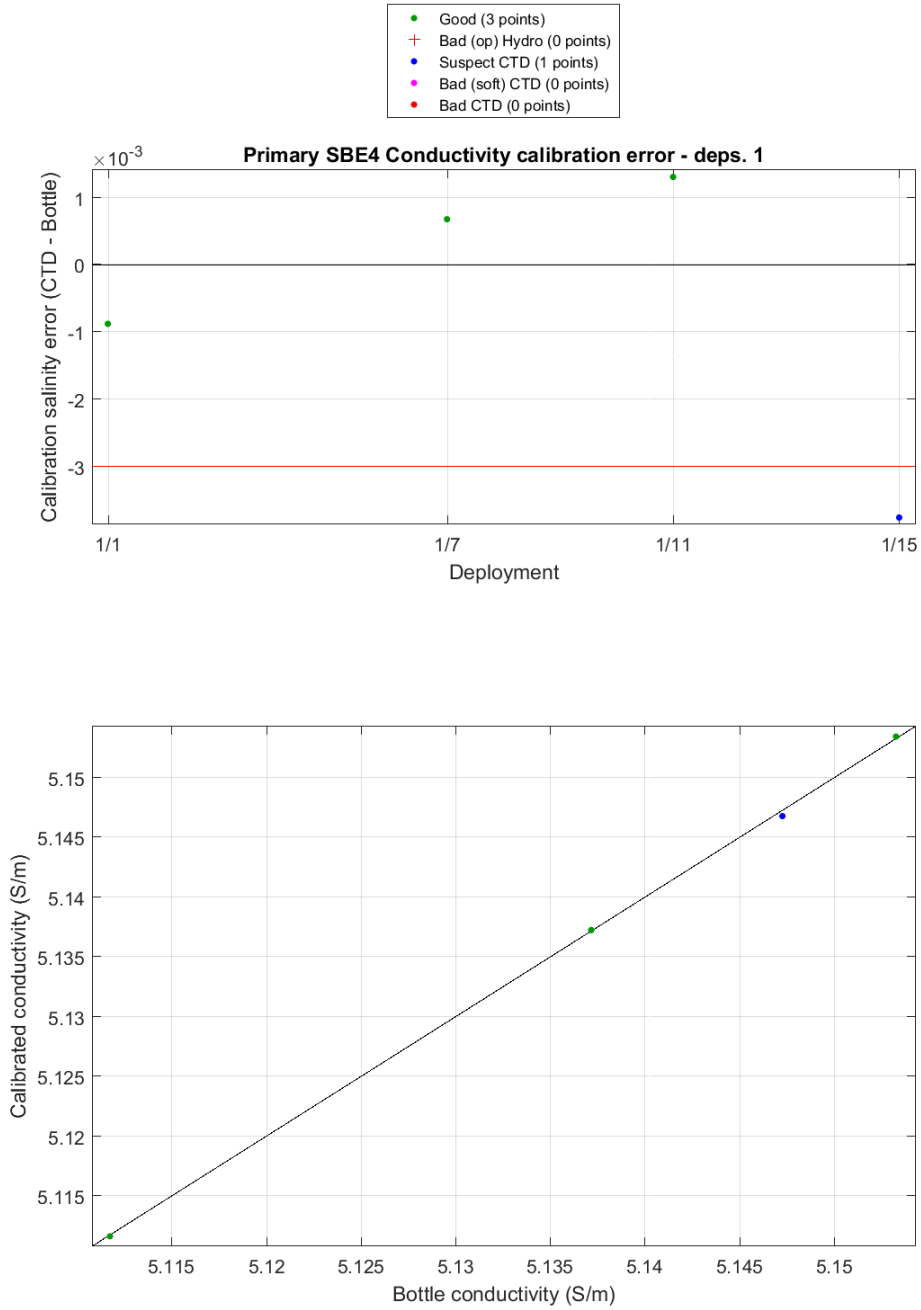


Figure 3 CTD - bottle salinity plot for cast 1

The final result for the primary conductivity sensor for cast 1 was –

Scale Factor (a1)	0.99964	wrt. Manufacturer's calibration
Offset (a0)	-0.000058515	ditto
Calibration S.D. (Sal)	0.0014262 PSU	

The calibration using the secondary conductivity sensor for cast 1 was –

Scale Factor (a1)	0.99927	wrt. Manufacturer's calibration
Offset (a0)	0.00071733	ditto
Calibration S.D. (Sal)	0.001772 PSU	

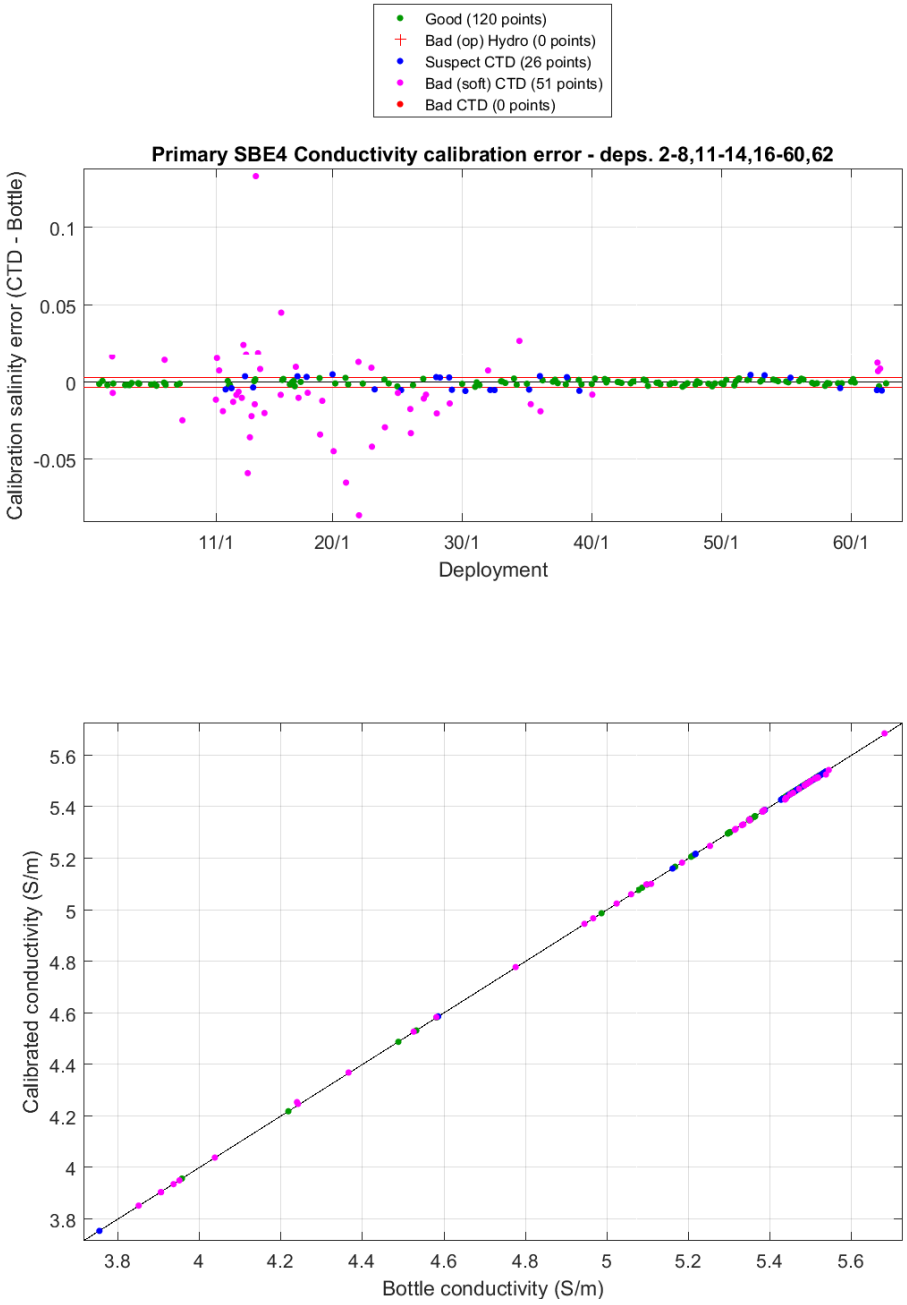


Figure 4 CTD - bottle salinity plot for casts 2-8, 11-14, 16-60 and 62

The final result for the primary conductivity sensor for casts 2-8, 11-14, 16-60 and 62 was

Scale Factor (a1)	0.99957	wrt. Manufacturer's calibration
Offset (a0)	0.00045185	ditto
Calibration S.D. (Sal)	0.0014061 PSU	

The calibration using the secondary conductivity sensor for casts 2-8, 11-14, 16-60 and 62 was –

Scale Factor (a1)	0.99945	wrt. Manufacturer's calibration
Offset (a0)	0.000048983	ditto
Calibration S.D. (Sal)	0.0015425 PSU	

Calibration standard deviation is the difference between the calibrated values and the bottle values. This is well within the range we consider to be 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.

Data from the primary conductivity and temperature sensors were used to produce the averaged salinities.

3.4 Dissolved Oxygen Sensor Calibration

3.4.1 SBE calibration procedure

Sea-Bird (2010a) 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 Sea-Bird (2010b) 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 by Sea-Bird (2010c).

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 casts 2-62 only one dissolved oxygen sensor was connected to the CTD as the secondary was replaced with a fluorometer. Calibration was conducted in two groups; one for CTD 21 and one for CTD 20. Below are plots of these calibration groups with a cutoff of 2 µM difference between sensor dissolved oxygen and bottle values for good values. The outliers marked in Figure 6 with blue dots are used in the calibration but are weighted based on their distance from the mean while those marked with magenta dots have been excluded. Further plots of residuals can be found in Appendix II: Dissolved Oxygen Residuals

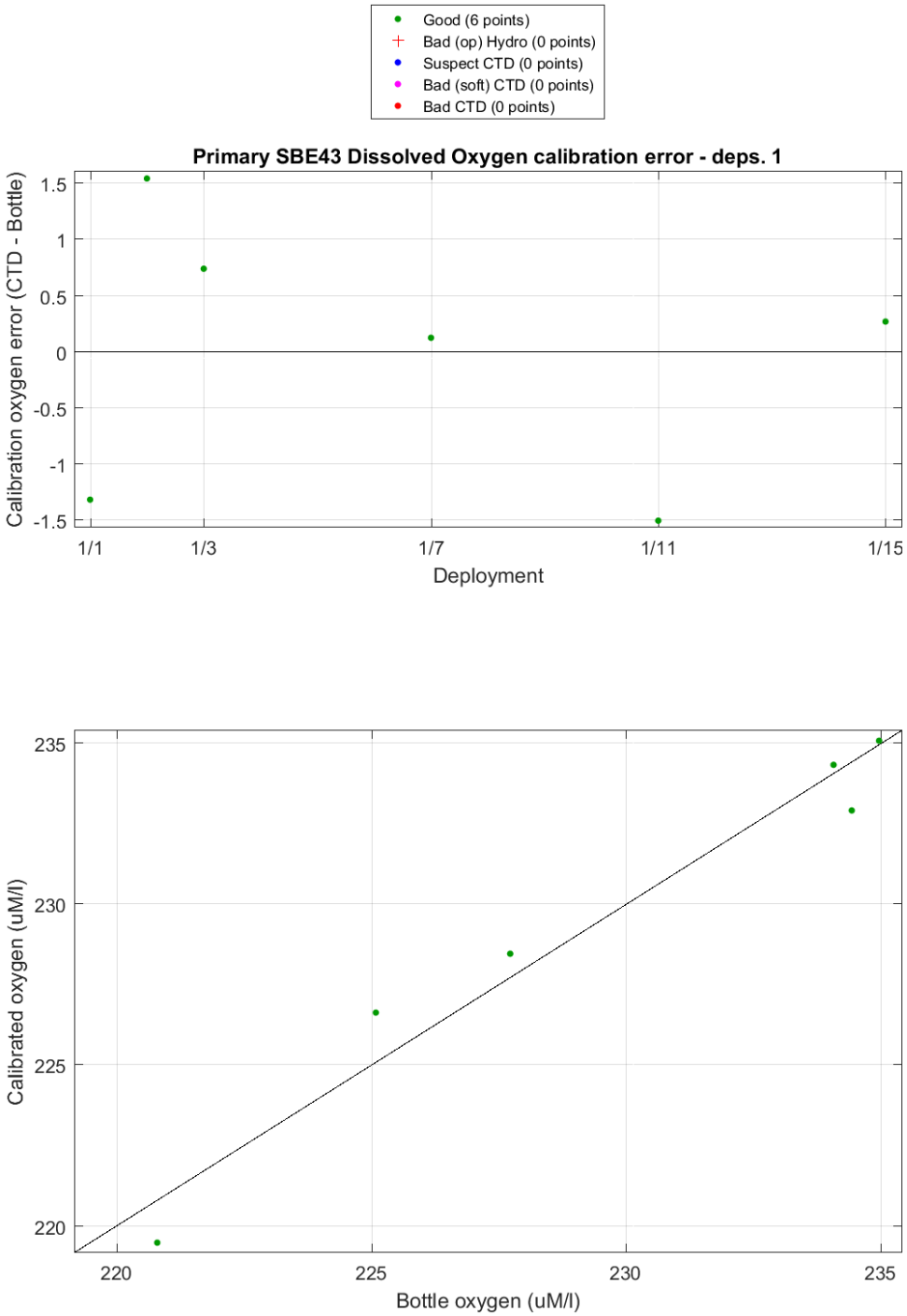


Figure 5 (SBE43 - Bottle) Oxygen Difference with upcast CTD data for deployment 1

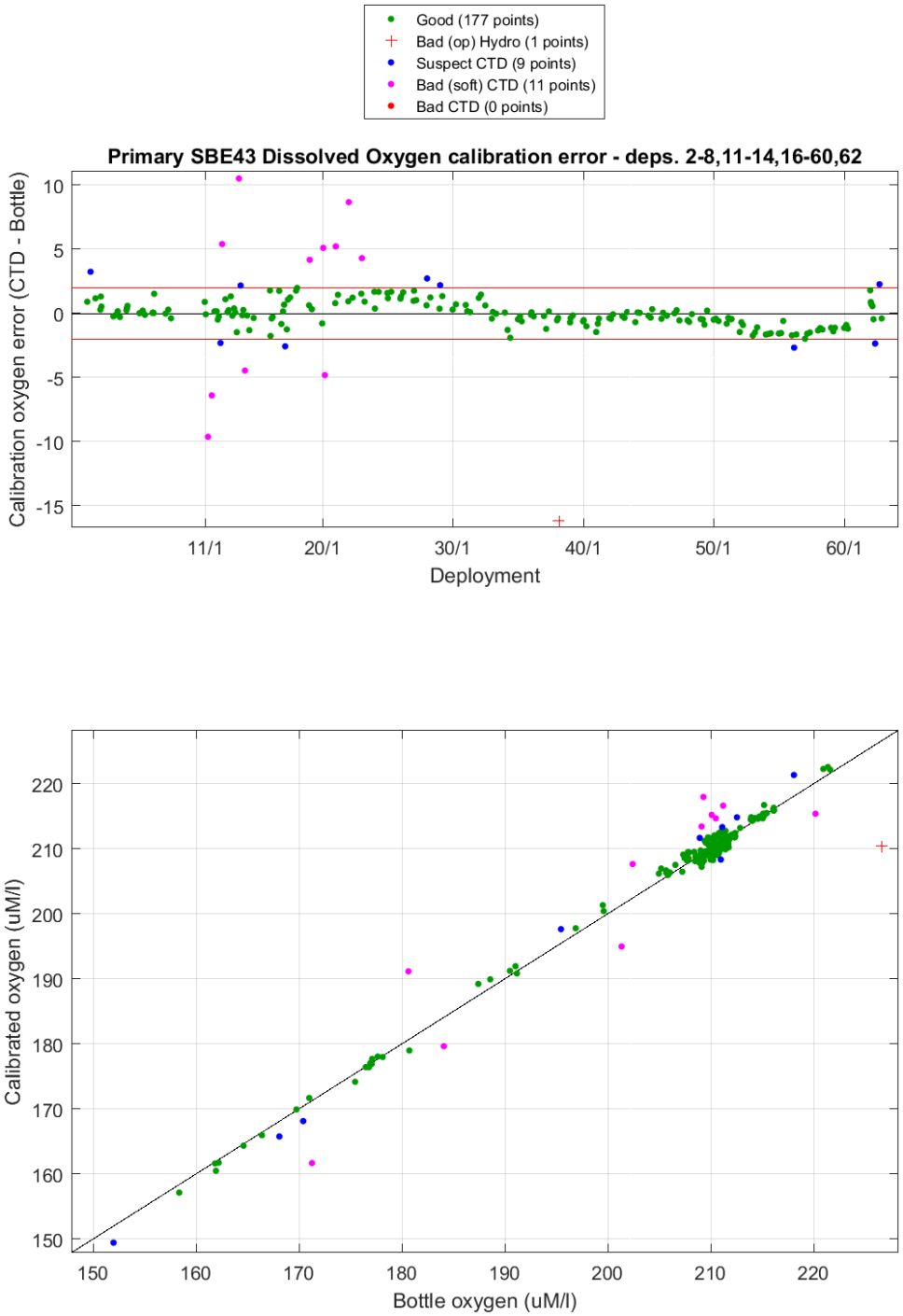


Figure 6 (SBE43 - Bottle) Oxygen Difference with upcast CTD data for deployments 2-8, 11-14, 16-60, 62

The old and new Soc and Voffset values for DO sensors are listed in Table 5 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.

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

Casts		**Calibration Lab primary sensor calibration values**	**Deployment primary sensor calibration values**
1	Voffset	-0.50133997	-0.60363
	Soc	0.47520554	0.52449
	Fit SD (uM)		0.62853
2-8, 11-14, 16-60 and 62	Voffset	-0.50133997	-0.48167
	Soc	0.47520554	0.49794
	Fit SD (uM)		0.67142

Table 5 Dissolved oxygen calibrations

3.5 Other sensors

The Chelsea fluorometer was used from deployment 2 onwards, replacing the secondary oxygen sensor. The ECO FL CDOM and altimeter were used for all deployments. The transmissometer was used for deployments 1-12 at which point it was replaced with the nephelometer. This was due to the transmissometer exhibiting strange 'loops' in the profiles. The fluorometer, CDOM, transmissometer and nephelometer had been calibrated to give nominal outputs of 0-100 full scale deflection (FSD) while the altimeter gave outputs of 0-50.

The Biospherical PAR sensor was also used for all deployments. The output is a nominal 0-5 volts. 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.

The Satlantic ISUS V3 Nitrate sensor was used for all deployments. The analogue output is a nominal 0-4.096 volts and had been calibrated to give values in µM for Nitrate and the Nitrate Uncertainty (also known as Nitrate Fitting) used default minimum and maximum values of -5 and 50 µM respectively.

The LADCP was used on all casts. This data is treaded separately to CTD data and will be processed by the end-user.

3.6 Bad data detection

The limits for each sensor are configured in the CAP the CTD acquisition software and are written to the netCDF scan file. Typical limits used for the sensor range and maximum second difference are in Table 3 below. The rejection rate is recorded in the CapPro processing log file.

Sensor	Range min	Range max	Max Second Diff
temperature	-2	40	0.05
conductivity	-0.01	7	0.01
oxygen	-1	500	0.5
fluorometer	0	100	0.5
altimeter	0	50	5.0
CDOM	-	-	-
PAR	-5	5000	50.0
transmissometer	-1	100	5.0
nephelometer	-	-	-
nitrate	-10	100	-
nirate uncertainty	-5	50	-

Table 6 Sensor limits for bad data detection

3.7 Averaging

The calibrated data were 'filtered' to remove pressure reversals and binned into the standard product of 1 dBar 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.

Due to the slow decent require for the safe deployment of the CTD in shallow waters around the reef, heave filtering to flag data quality was altered to reduce the flagging of data as suspect or bad.

Each binned parameter is assigned a QC flag. Our quality control flagging scheme is described in 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

Ristovski, Z., 2016: The RV Investigator. Voyage Plan IN2016_V05 - http://mnf.csiro.au/~/media/Files/Voyage-plans-and-summaries/Investigator/Voyage%20Plans%20summaries/2016/IN2016_V05%20voyage%20plan-FINAL.ashx

Pender, L., 2000: Data Quality Control Flags. http://www.cmar.csiro.au/datacentre/ext_docs/DataQualityControlFlags.pdf

Sea-Bird Electronics Inc., 2010a: Application Note No 64: SBE 43 Dissolved Oxygen Sensor -- Background Information, Deployment Recommendations, and Cleaning and Storage. http://www.seabird.com/pdf_documents/ApplicationNotes/appnote64Feb10.pdf

Sea-Bird Electronics Inc., 2010b: Application Note No 64-2: SBE 43 Dissolved Oxygen Sensor Calibration and data Corrections using Winkler Titrations. http://www.seabird.com/pdf_documents/ApplicationNotes/Appnote64-2Feb10.pdf

Sea-Bird Electronics Inc., 2010c: Application Note No 64-3: SBE 43 Dissolved Oxygen (DO) Sensor - Hysteresis Corrections. http://www.seabird.com/pdf_documents/ApplicationNotes/Appnote64-3Feb10.pdf

Appendix I: Conductivity Residuals

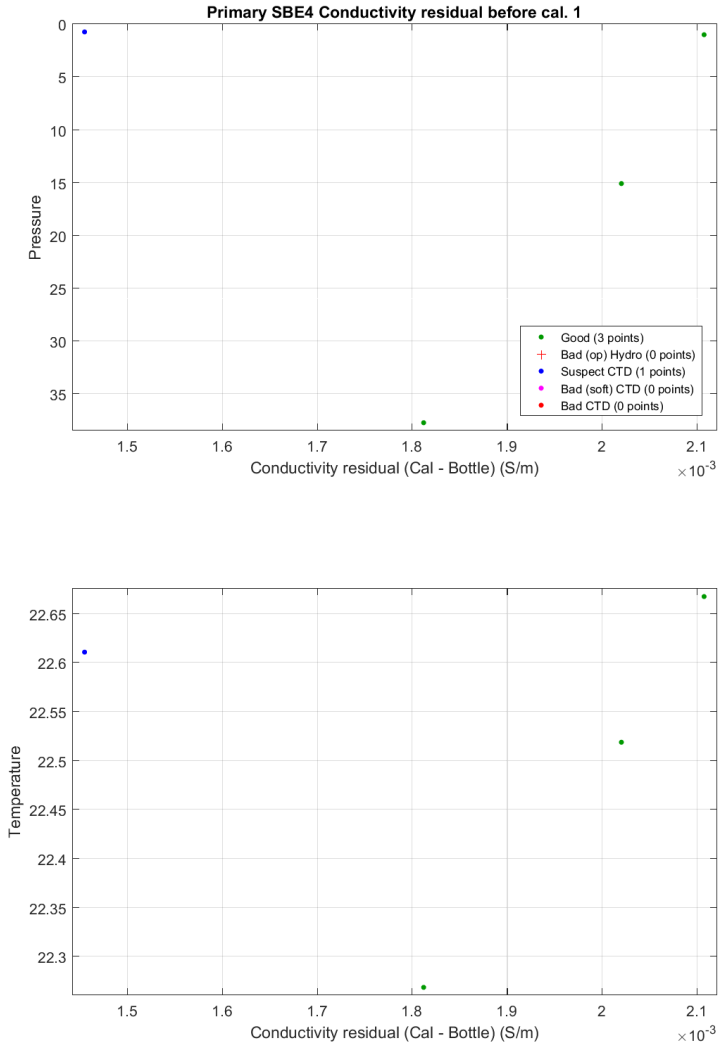


Figure 7 Primary conductivity residuals for cast 1 before calibration

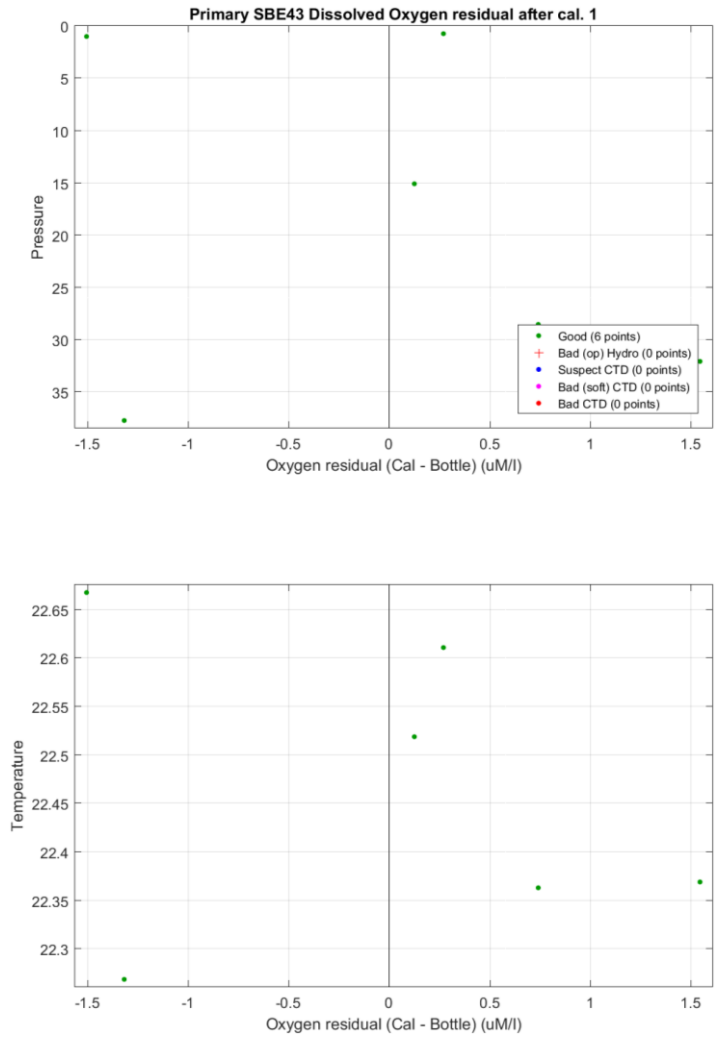


Figure 8 Primary conductivity residuals for cast 1 after calibration

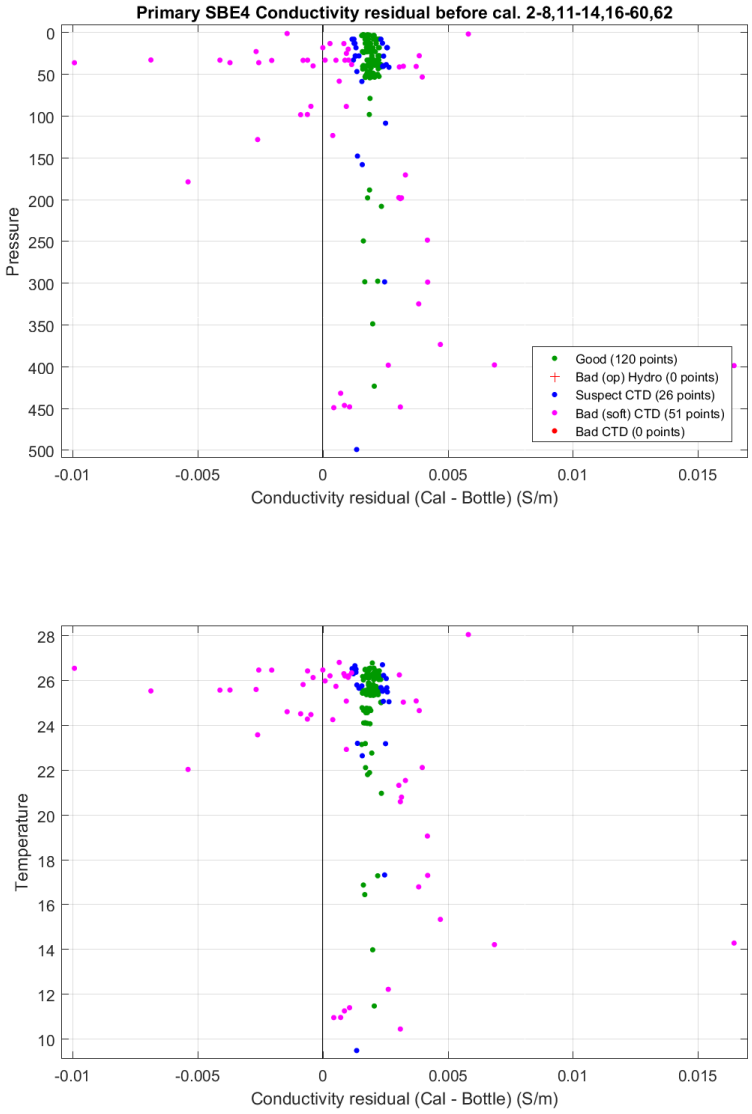


Figure 9 Primary conductivity residuals for casts 2-8, 11-14, 16-60 and 62 before calibration

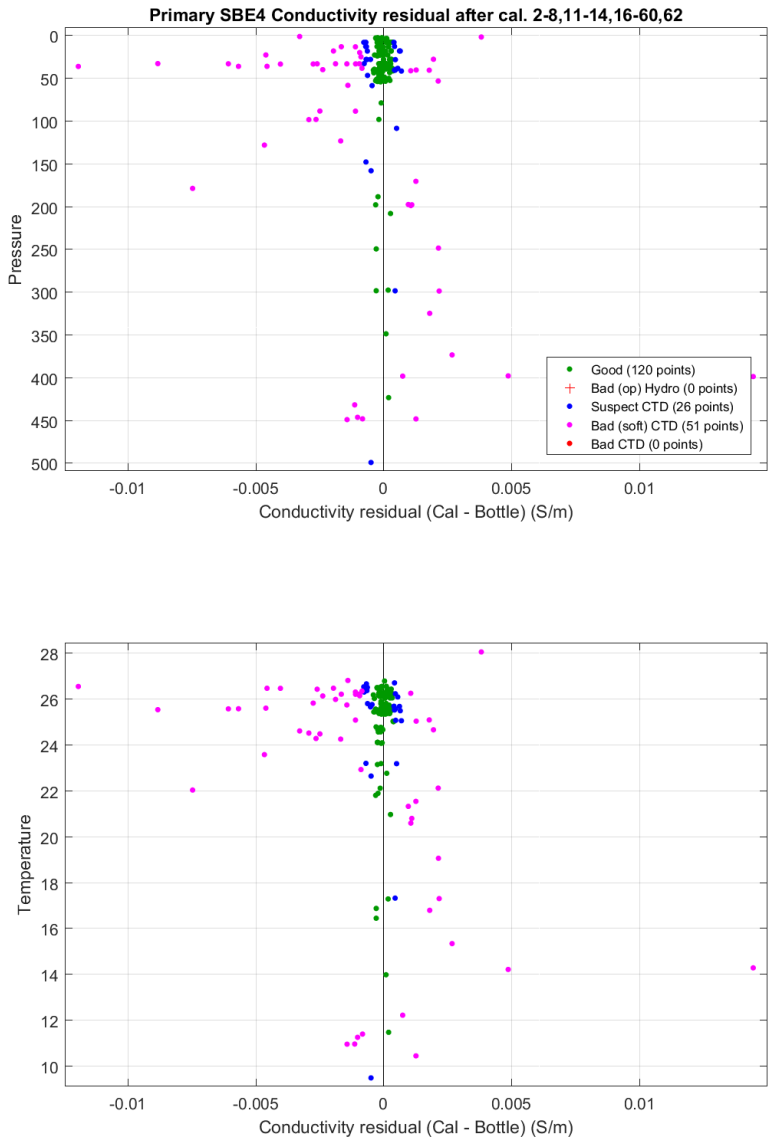


Figure 10 Primary conductivity residuals for casts 2-8, 11-14, 16-60 and 62 after calibration

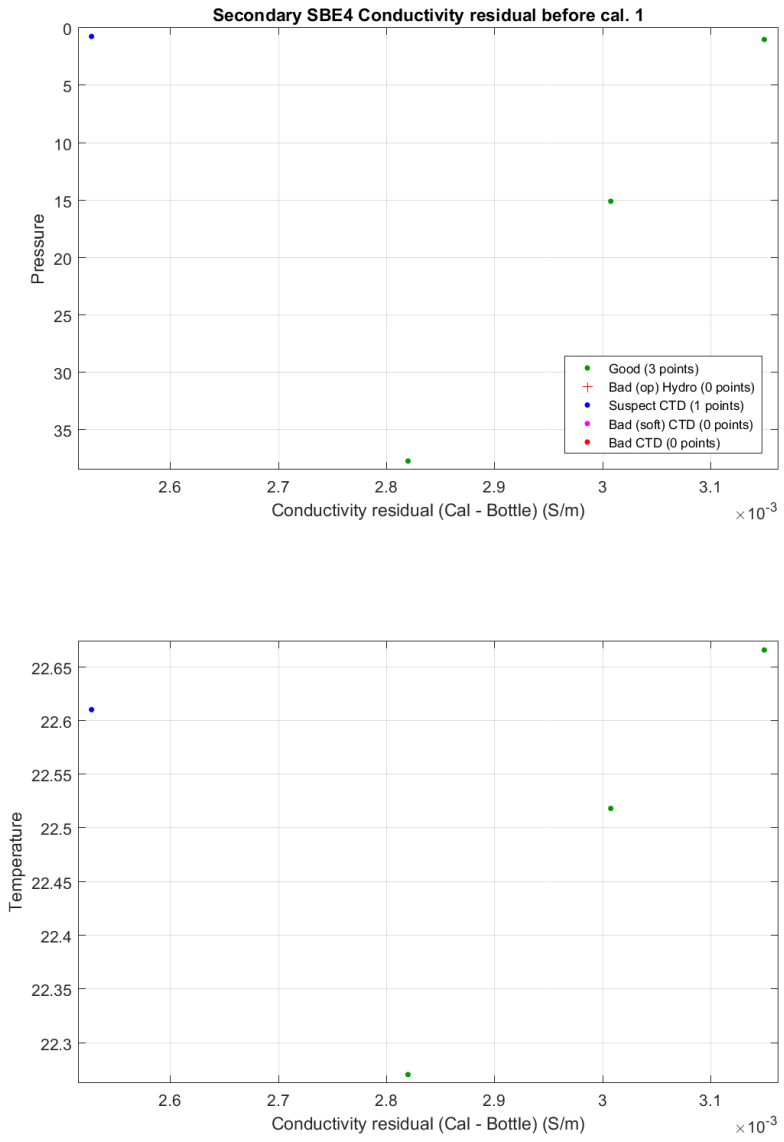


Figure 11 Secondary conductivity residuals for cast 1 before calibration

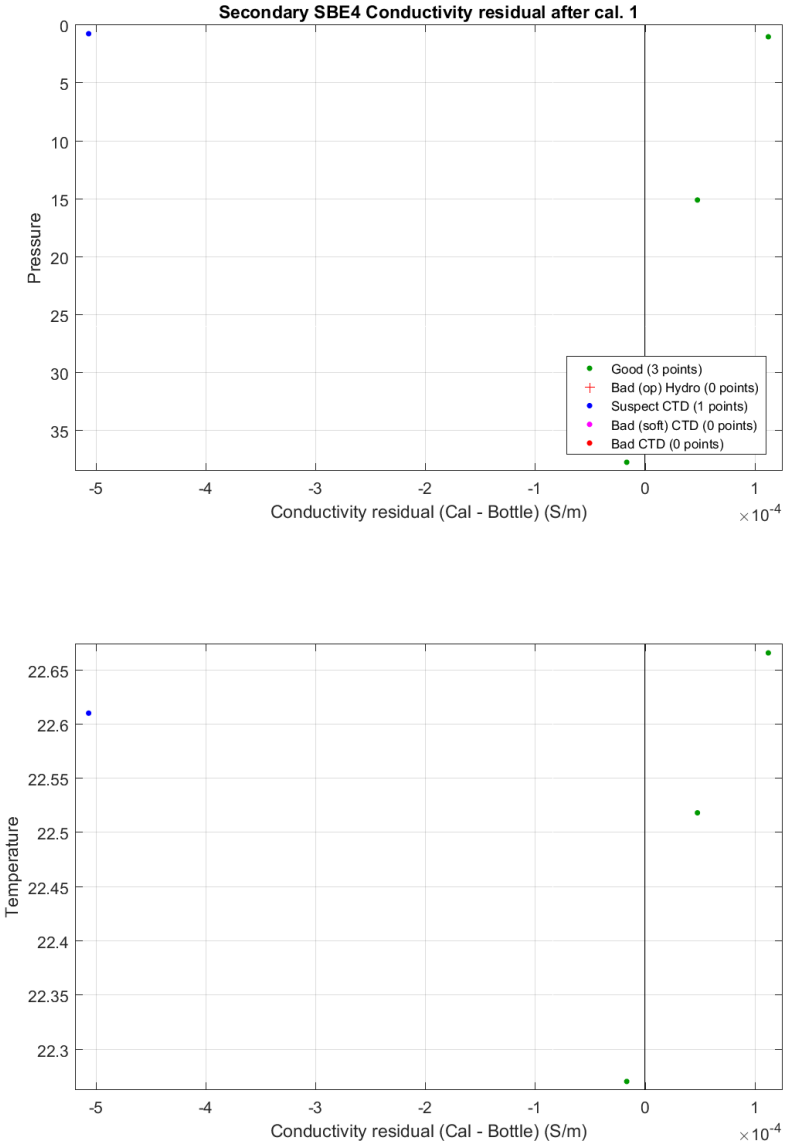


Figure 12 Secondary conductivity residuals for cast 1 after calibration

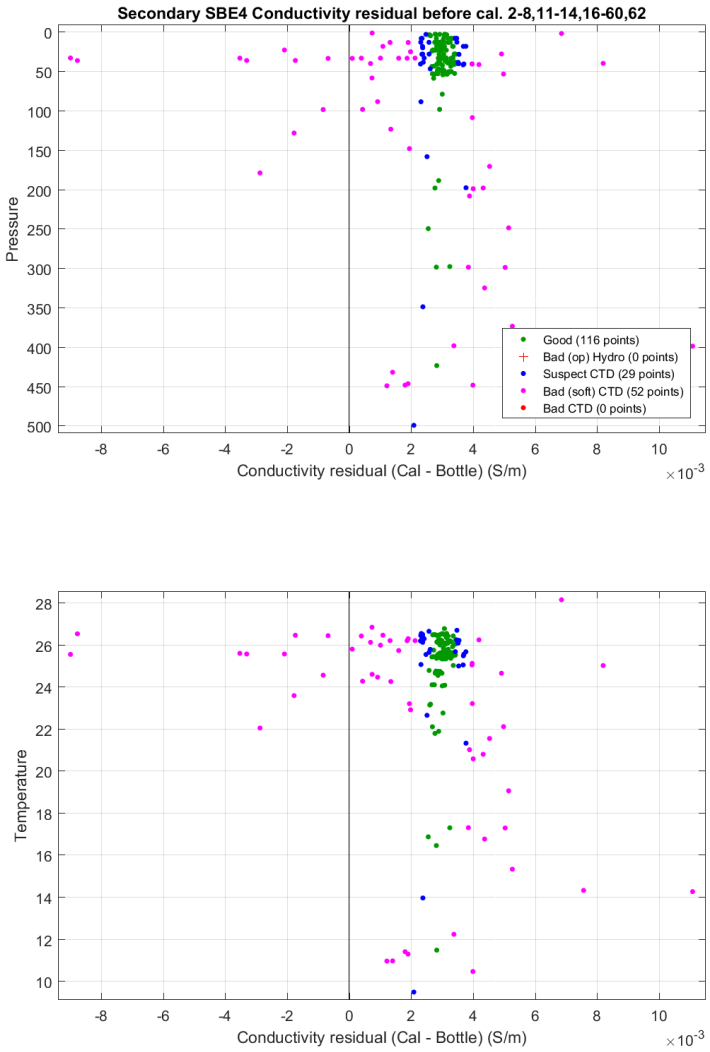


Figure 13 Secondary conductivity residuals for casts 2-8, 11-14, 16-60 and 62 before calibration

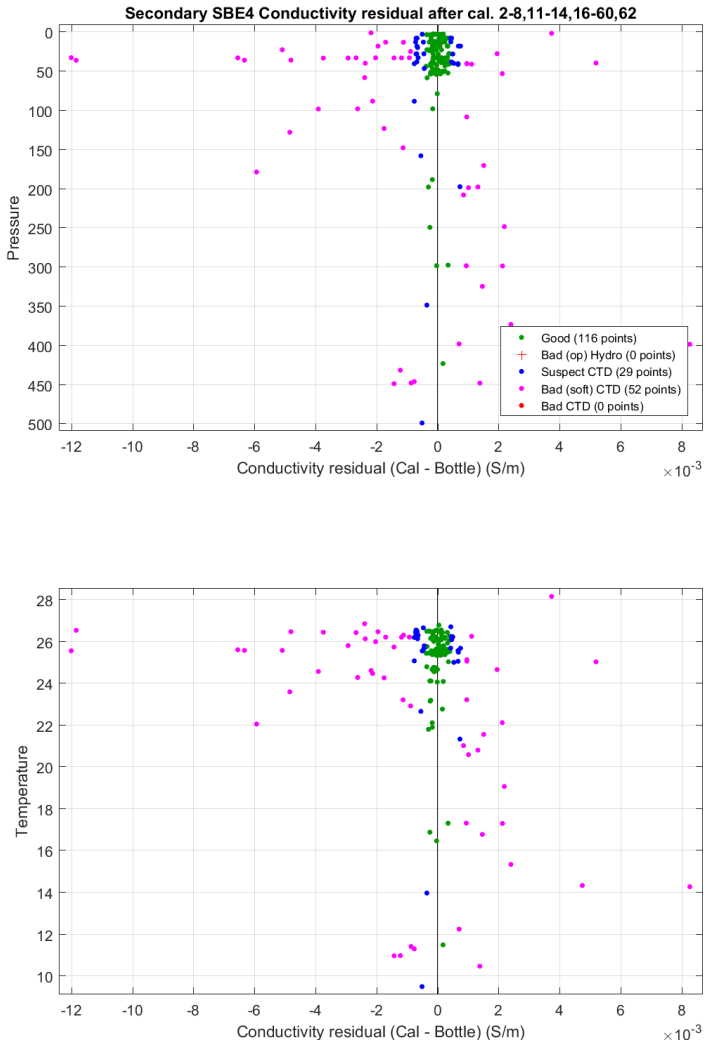


Figure 14 Secondary conductivity residuals for casts 2-8, 11-14, 16-60 and 62 after calibration

Appendix II: Dissolved Oxygen Residuals

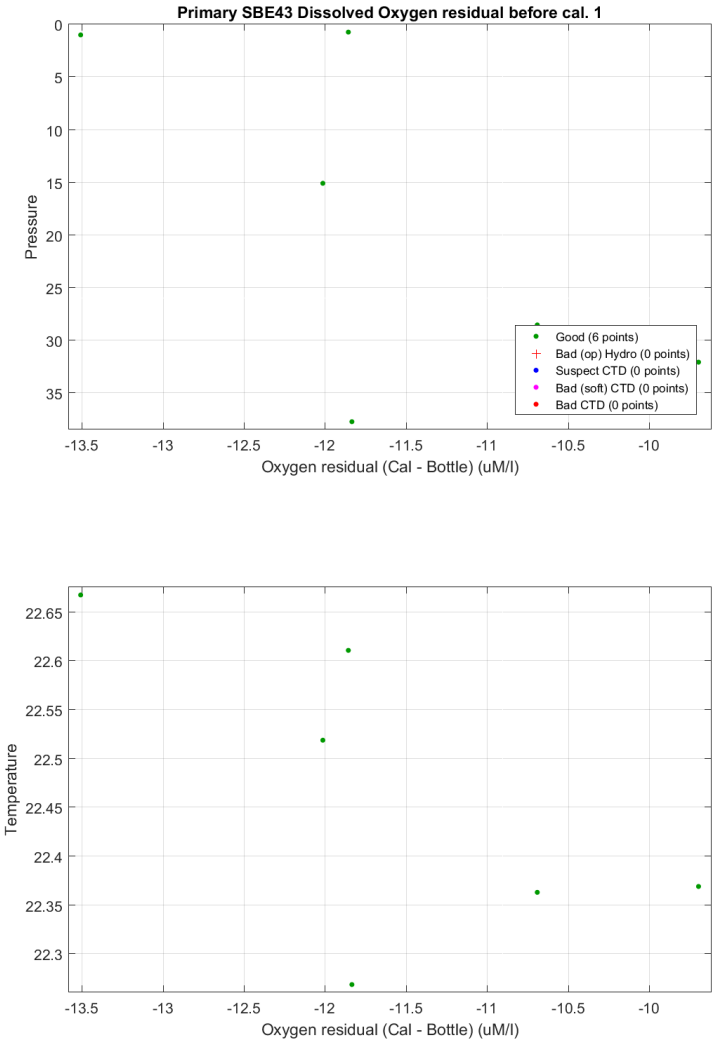


Figure 15 Primary oxygen residuals for cast 1 before calibration

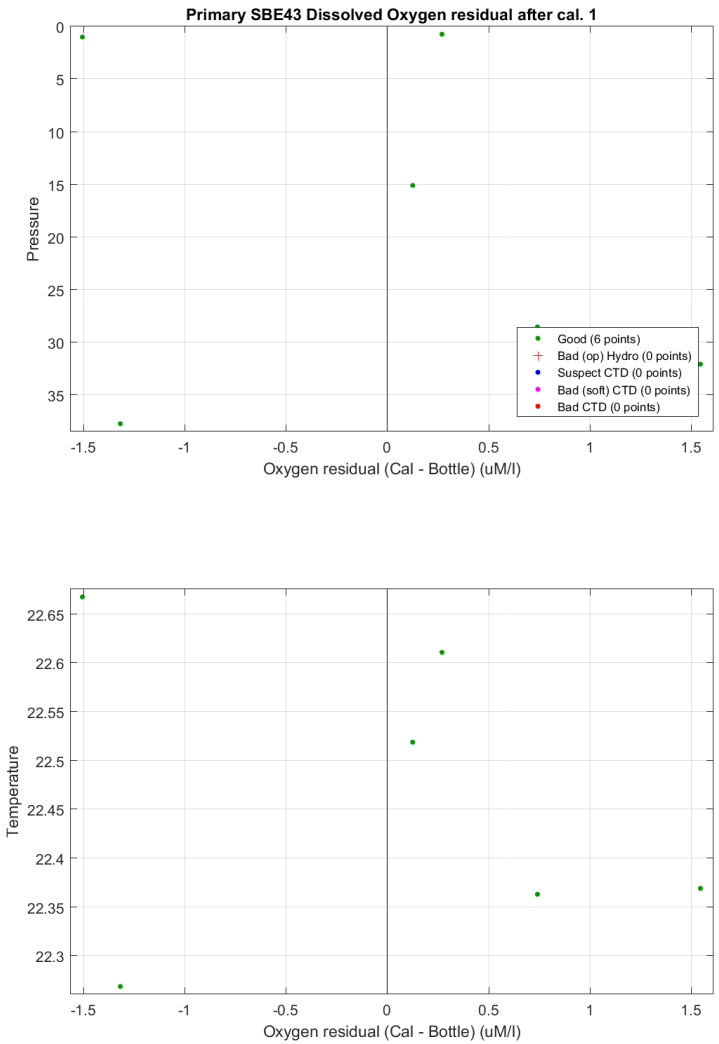


Figure 16 Primary oxygen residuals for cast 1 after calibration

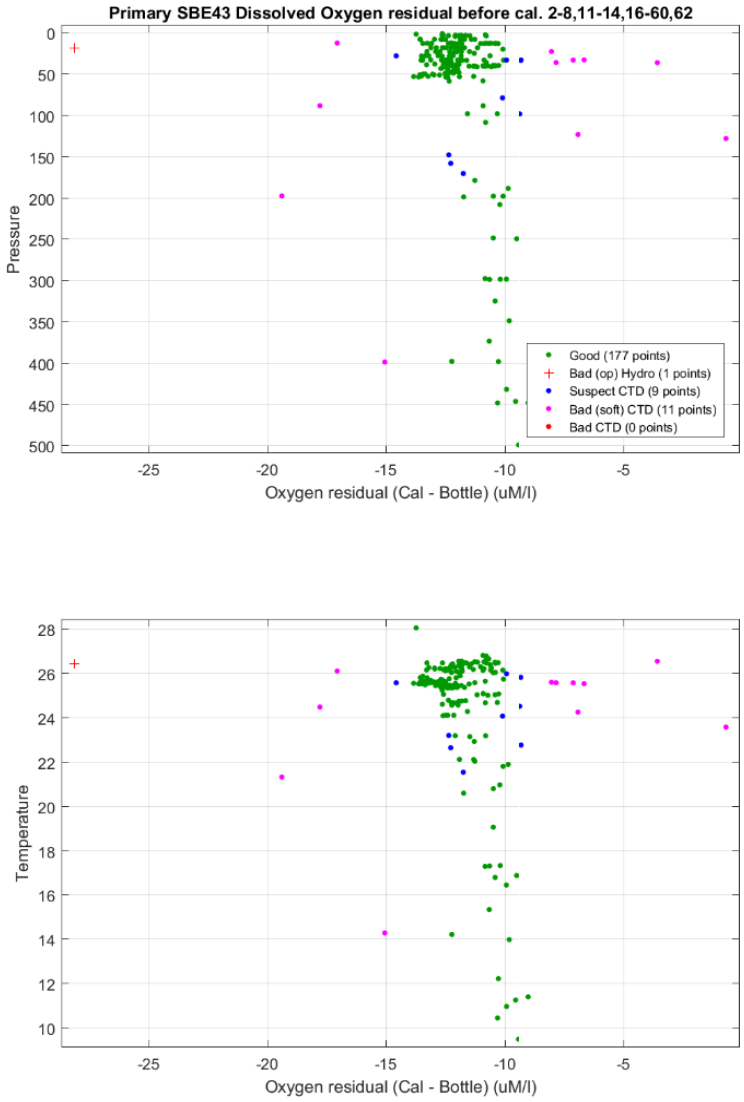


Figure 17 Primary oxygen residuals for cast 2-8, 11-14, 16-60 and 62 before calibration

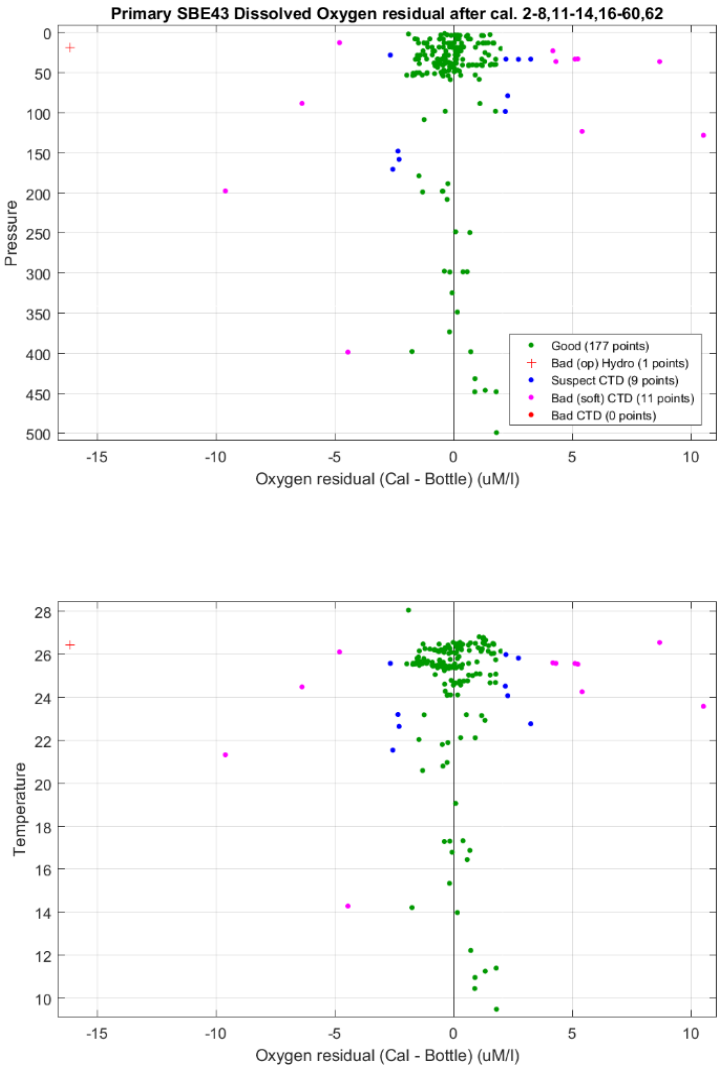


Figure 18 Primary oxygen residuals for cast 2-8, 11-14, 16-60 and 62 after calibration