DY029 CTD processing report

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This report documents the sequential processing carried out on CTD profiles from cruise DY029 on RRS Discovery, including bin averaging, despiking and calibrations. A total of 140 CTD casts (leg 1: 1-52, leg 2: 53-140) with the stainless steel (94) and titanium (46) CTDs were completed. See technical reports for sensor serial numbers and channels. The cruise was split into two halves, 1 and 2. Casts 1-52 were conducted on leg 1. Casts 53-140 on leg 2.

The secondary stainless steel salinity sensor displayed problems from CTD017SS and was changed before CTD020SS and used onwards.

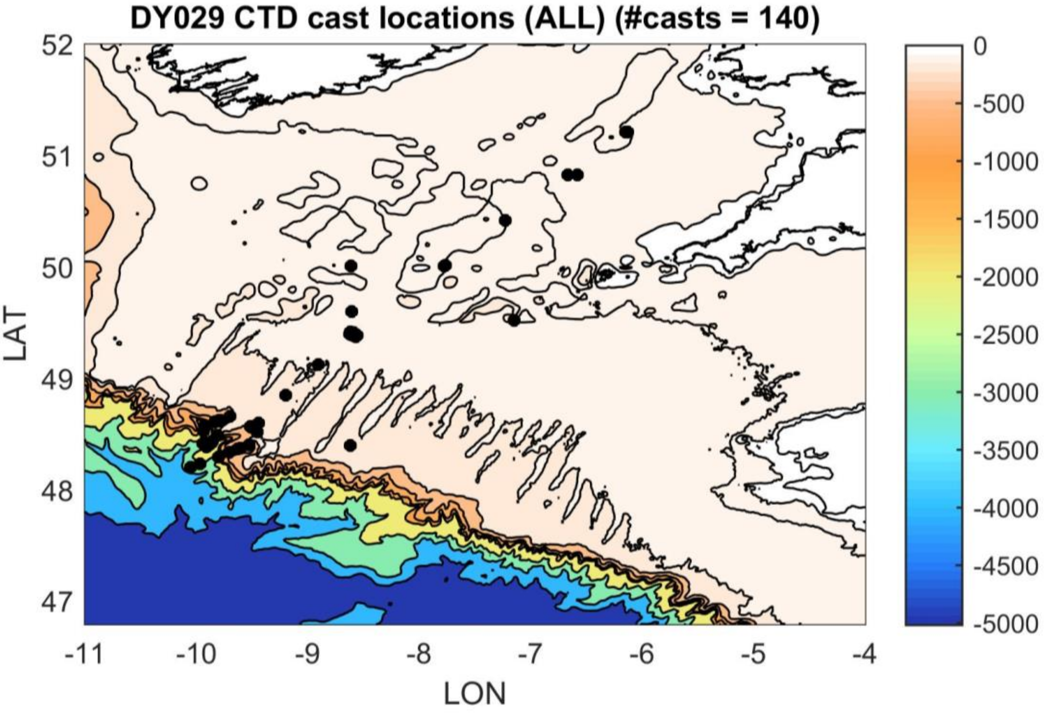
CTD076SS suffered communication failure halfway through and thus was split into to two raw files:
CTD076SS – Niskins 1 -7 fired
CTD076SSA – Niskin bottles 8 – 19, 23 – 24 fired, but are labelled as Niskins 1-14 in the raw data files provided by NMF. In the processed data files these have been corrected (.ROS, .BTL. CNV).
*Note that data for Niskins 20, 21, 22 are missing from the raw data file as they were not recorded for unknown reason.

A number of CTD casts had technical issues, these are listed here:
CTD015T (aborted)

- The cable was replaced after this CTD.

CTD019SS (aborted)
CTD055SS (bottomed)
CTD095SS (aborted)

Map of CTD cast locations



Raw data files:

The following raw data files were generated for both stainless steel and titanium:

DY029_001.bl (a record of bottle firing locations)
DY029_001.hdr (header file)
DY029_001.hex (raw data file)
DY029_001.con (configuration file)

Where _001 is the CTD cast number (not STNNBR)

SBEDataProcessing steps

The following processing routines were run in the SBEDataProcessing software (Seasave Version 7.23.2):

1. **DatCnv:** A conversion routine to read in the raw CTD data file (.hex) containing data in engineering units output by the CTD hardware. Calibrations as appropriate through the instrument configuration file (.CON) are applied.

   Data Setup options were set to the following:

   Process scans to end of file: yes
   Scans to skip: 0
   Output format: ascii
   Convert data from: upcast & downcast
   Create file types: both bottle and data
   Source of scan range data: bottle log .BL file
   Scan range offset: -2.5 seconds
   Scan range duration: 5 seconds for
   Merge separate header file: No
   Apply oxygen hysteresis correction: yes (2 second window)
   Apply oxygen Tau correction: yes

   Selected output variables:

   - Time [seconds]
   - Pressure [db]
   - Temperature [ITS-90, °C] and Temperature 2 [ITS-90, °C], referring to primary and secondary sensors)
   - Conductivity and Conductivity 2 [S/m]
   - Salinity and salinity 2 [PSU, PSS-78]
   - Oxygen raw, SBE 43 [V]
   - Oxygen, SBE 43 [µmol/l]
   - Beam attenuation [1/m]
   - Fluorescence [µg/l]
   - PAR/irradiance, downwelling [W m^2]
   - Turbidity [m^{-1} sr^{-1}]
   - Altimeter [m]
   - Voltage channel 2: Downwelling Irradiance sensor (DWIRR)
   - Voltage channel 3: Upwelling Irradiance sensor (UWIRR)
   - Voltage channel 4: Altimeter
   - Voltage channel 5: Light scattering Wetlabs BBRTD
   - Voltage channel 6: Transmissometer
   - Voltage channel 7: Fluorometer

2. **Bottle Summary** was run to create a .BTL file containing the average, standard deviation, min and max values at bottle firings. .ROS files were placed in the same directory as the .bl files during this routine to ensure that bottle rosette position was captured in the .btl file.

   The output was saved to DY029_XXX.btl for each CTD cast, and a summary excel spreadsheet of the bottle data was created as the cruise progressed as an uncalibrated reference.

3. **Wild Edit:** Removal of pressure spikes
   Standard deviations for pass 1: 2
   Standard deviations for pass 2: 20
   Scans per black: 100
   Keep data within this distance of the mean: 0
   Exclude scans marked as bad: yes

4. **Filter:** Run on the pressure channel to smooth out high frequency data
   Low pass filter time B: 0.15 seconds

5. **AlignCTD:** Based on examination of different casts **a 2.5 second** advance was chosen for alignment of the oxygen sensor on the stainless steel frame and **1 second** for the titanium. This alignment is a function of the temperature and the state of the oxygen sensor membrane. The colder (deeper) the water the greater the advance needed. The above alignments were chosen as a compromise between results in deep (cold) and shallow (warmer) waters.

   The deck unit was set to advance both the primary and secondary conductivity channels by + 1.75 scans (equivalent to 0.073 seconds at 24 Hz), no further adjustment was applied.

6. **CellTM:** Removes the effect of thermal inertia on the conductivity cells. Alpha = 0.03 (thermal anomaly amplitude) and 1/beta = 7 (thermal anomaly time constant) for both cells.

   Output of steps 1-6 above saved in DY029_001.cnv (24 Hz resolution)

7. **Derive:** Variables selected are
   Oxygen SBE43 [µmol/l]
   Oxygen Tau correction: yes (2 second window)

   Output saved to DY029_001_derive.cnv (24 Hz resolution)

8. **BinAverage:** Average into 2Hz (0.5 seconds),
   Exclude bad scans: yes
   Scans to skip over: 0
   Casts to process: Up and down

9. **Strip:** Remove salinity and oxygen channels from the 2 Hz file that were originally created by DatCnv, but then later regenerated by Derive.

   Output saved to DY029_001_derive_2Hz.cnv

Matlab processing steps
The following processing steps were performed in MATLAB:

(1) Create a .mat file of meta data extracted from the cruise Event Log with the following variables:

CRUISECODE e.g. DY029
STNNBR (as per BODC data management guidance for the Shelf Sea Biogeochemistry programme)
DATE and TIME of the cast at the START of the profile
LAT and LON when the CTD was at the bottom of the profile
DEPTH (nominal water depth in metres from echo sounder)
CAST (CTD cast number, e.g. 001)

File created: DY029_metadata.mat

(2) Extract data from 2Hz averaged files (e.g. DY029_001_derive_2Hz.cnv), merge with metadata and save into a matlab structure for each cast. Each file (DY029_001_derive_2Hz.mat) contains the following <u>un-calibrated</u> channels.

```
CTD001 =

           CRUISE: 'DY029'
             CAST: 1
           STNNBR: 1
             DATE: '02/04/2015'
             TIME: '17:13'
              LAT: 49.5268
              LON: -7.149
            DEPTH: 127                  [m]
          CTDtime: [3658x1 double]     [seconds]
          CTDpres: [3658x1 double]     [db]
         CTDtemp1: [3658x1 double]     [°C]
         CTDtemp2: [3658x1 double]     [°C]
         CTDcond1: [3658x1 double]     [S/m]
         CTDcond2: [3658x1 double]     [S/m]
       CTDoxy_raw: [3658x1 double]     [V]
           CTDatt: [3658x1 double]     [1/m]
         CTDfluor: [3658x1 double]     [µg/l]
           CTDpar: [3658x1 double]     [Wm²]
          CTDturb: [3658x1 double]     [m⁻¹ Sr⁻¹]
           CTDalt: [3658x1 double]     [m]
    CTDpar_dn_raw: [3658x1 double]     [V]
    CTDpar_up_raw: [3658x1 double]     [V]
       CTDalt_raw: [3658x1 double]     [V]
      CTDturb_raw: [3658x1 double]     [V]
       CTDatt_raw: [3658x1 double]     [V]
     CTDfluor_raw: [3658x1 double]     [V]
          CTDsal1: [3658x1 double]     [PSU]
          CTDsal2: [3658x1 double]     [PSU]
     CTDoxy_umoll: [3658x1 double]     [µmol/l]
          CTDflag: [3658x1 double]
```

(3) Extract data from 24Hz files (e.g. DY029_CTD001_derive.cnv), merge with metadata and save into a matlab structure for each cast. Each file (DY029_001_derive.mat) contains the following <u>un-calibrated</u> channels.

```
CTD001 =

           CRUISE: 'DY029'
             CAST: 1
           STNNBR: 1
             DATE: '02/04/2015'
             TIME: '17:13'
              LAT: 49.5268
              LON: -7.149
            DEPTH: 127                [m]
            CTDtime: [43896x1 double] [seconds]
            CTDpres: [43896x1 double] [db]
           CTDtemp1: [43896x1 double] [°C]
           CTDtemp2: [43896x1 double] [°C]
           CTDcond1: [43896x1 double] [S/m]
           CTDcond2: [43896x1 double] [S/m]
          CTDsal1_1: [43896x1 double] [PSU]
          CTDsal2_1: [43896x1 double] [PSU]
         CTDoxy_raw: [43896x1 double] [V]
    CTD_oxy_umoll_1: [43896x1 double] [µmol/l]
             CTDatt: [43896x1 double] [1/m]
           CTDfluor: [43896x1 double] [µg/l]
             CTDpar: [43896x1 double] [Wm^2]
            CTDturb: [43896x1 double] [m^-1 Sr^-1]
             CTDalt: [43896x1 double] [m]
      CTDpar_dn_raw: [43896x1 double] [V]
      CTDpar_up_raw: [43896x1 double] [V]
         CTDalt_raw: [43896x1 double] [V]
        CTDturb_raw: [43896x1 double] [V]
         CTDatt_raw: [43896x1 double] [V]
       CTDfluor_raw: [43896x1 double] [V]
          CTDsal1: [43896x1 double] [PSU]
          CTDsal2: [43896x1 double] [PSU]
       CTDoxy_umoll: [43896x1 double] [µmol/l]

            CTDflag: [43896x1 double]
```

Note that ‘_1’ for the first instances of oxygen in this file are variables before re-derivation in the SeaBird Processing routines.

As observed in an earlier cruise (DY018, DY026), inspection of the turbidity channel (CTDturb) and comparison to the original raw voltage (CTDturb_raw) revealed a potential bug in the SeaBird DatCnv conversion module for both the titanium and stainless steel frames. As previously discussed with SeaBird, the converted ECO-BB output was being reported to a fixed precision. Direct conversion using the scale factor (SF) and dark counts (DC) supplied in the manufacturer’s calibration appears to rectify this problem. We therefore replace the original turbidity channel in the .cnv files with a corrected version using:

> STAINLESS FRAME
> CTDturb = CTDturb_raw .* SF - (SF x DC);
> Where the scale factor (SF) for this sensor = 0.002365
> and the dark count (DC) = 0.061000

TITANIUM FRAME
CTDturb = CTDturb_raw .* SF - (SF x DC);
Where the scale factor (SF) for this sensor = 0.002903
and the dark count (DC) = 0.043100

By applying this correcting to the raw turbidity sensor output we appear to retrieve the original resolution.

(4) Manual identification of the surface soak (the time taken while waiting for pumps to turn on) and the end of the downcast using the 2Hz files. Times to crop were saved to DY029_stainless_castcrop_times.mat and DY029_titanium_castcrop_times.mat

```
       CAST: [14x6 char]
     STNNBR: [14x1 double]
   CTDstart: [14x1 double] [seconds]
    CTDstop: [14x1 double] [seconds]
```

This was then used to crop both the 2Hz and 24Hz files and output (i.e. just the downcast recordings) saved to DY029_CTD001_derive_2Hz_cropped.mat and DY029_CTD001_derive_cropped.mat respectively.

(5) De-spiking of downcast 24 Hz data. The salinity, conductivity, temperature, oxygen, attenuation, turbidity and fluorescence channels were all de-spiked. The worst spikes were identified using an automated routine (similar to WildEdit) where the data was scanned twice and points falling outside a threshold of *nstd* x standard deviations from the mean within a set window size were removed (turned into NaNs).

Window size (#scans) and number of standard deviations from the mean (nstd) used for each channel.

Channel	*Pass 1 window*	*Pass 1 nstd*	*Pass 2 window*	*Pass 2 nstd*
Temperature, conductivity, fluorescence	100	3	200	3
Salinity, turbidity	200	2	200	3
Oxygen	100	2	200	3

Auto-despiking saved to DY029_CTD001_derived_cropped_autospike.mat

Manual de-spiking was then performed to remove larger sections of bad data or any remaining isolated spikes in each channel.

Large ‘spikes’ were regularly observed in the CT sensors lasting a few seconds, predominantly in the thermocline. This is a persistent problem in shallow water with strong property gradients (e.g. see for example DY018, D352, D376, DY026); particularly where a large CTD package carrying large volume bottles is used. The spikes coincide with a decrease in the decent rate of the CTD package and are therefore likely associated with inefficient flushing of water around the sensors. It is caused by the pitch and roll of the boat, so is accentuated in rough weather. As the decent rate of the CTD package slows on the downcast ‘old’ water (from above and therefore typically warmer) is pushed back passed the sensors.

As the decent rate increases again ‘new’ water is flushed past the sensors. A similar problem can occur if the veer rate on the CTD winch varies.

The largest and most significant warm anomalies identified in the primary CT sensors were removed from all variables (incl. turbidity, oxygen, chlorophyll and attenuation since these sensors would also be sampling ‘old’ water during these periods). This was at times up to 5 m of the profile. However, in many cases oxygen, chlorophyll, turbidity and attenuation profiles that had valued nulled from selected spikes were revisited and identified manually. This is because misalignment of sensors to the CT sensors on the CTD package can be up to 1m and therefore automatically omitting data based on CT spikes can potentially be incorrect. Anomalies identified in the secondary sensors were only removed from the secondary temperature, salinity and conductivity channels. The impact of smaller scale anomalies that were not removed is mostly minimised during the averaging processes, but care should be taken when interpreting smaller scale features, particularly through the thermocline. The casts are more than good enough for looking at large scale trends and anomalies but should probably not be used for Thorpe scale analysis and interpretation of fine scale structures. To achieve this in a shelf sea environment free fall profiling techniques are more suitable.

Individual, isolated spikes within each channel were only removed (NaN’d) from that particular variable.

Output saved to DY029_CTD001_derived_cropped_autospike_manualspike.mat

Additional channels added into this file:

Vectors of 0’s and 1’s indicating data that has been NaN’d (=1). Outputs depend on channels loaded and viewed so each column may have variable meaning and is saved for processing archive purposes only.

(6) Average 24Hz (cropped and de-spiked data) into 1 db. Linear interpolation used when no data available for averaging.

Files for each cast were created: DY029_001_1db_dn.mat

(7) Smoothing of the 1db casts using zsmth.m, this helps clean up a lot of the noise that may have been missed in the auto and manual de-spiking process. A smoothing filter of #?# was used to clean up noise but preserve natural variability in profiles.

Files for each cast were created: DY029_001_1db_dn_smth.mat

(8) Application of calibrations to salinity, chlorophyll and oxygen in 1db downcasts. Calibrated files saved to DY029_001_1db_dn_calib.mat.

Sigma theta (σ_θ) (relative to 0 pressure) is also calculated at this stage using the matlab function `sw_pden-1000` from the `SEAWATER` toolkit.

The calibrations were also applied to the 24 Hz data (cropped and de-spiked) and output to .mat files DY029_001_derive_cropped_autospike_manualspike_calib.mat containing the same variables as above.

(9) Application of salinity, chlorophyll and oxygen calibrations to bottle firing data. A new file, DY029_stainless_btl_calib.mat/ DY029_titanium_btl_calib.mat, with variables CTDsal1_cal, CTDsal2_cal, CTDoxy_umoll_cal and CTDfluor_cal was created.

CALIBRATIONS

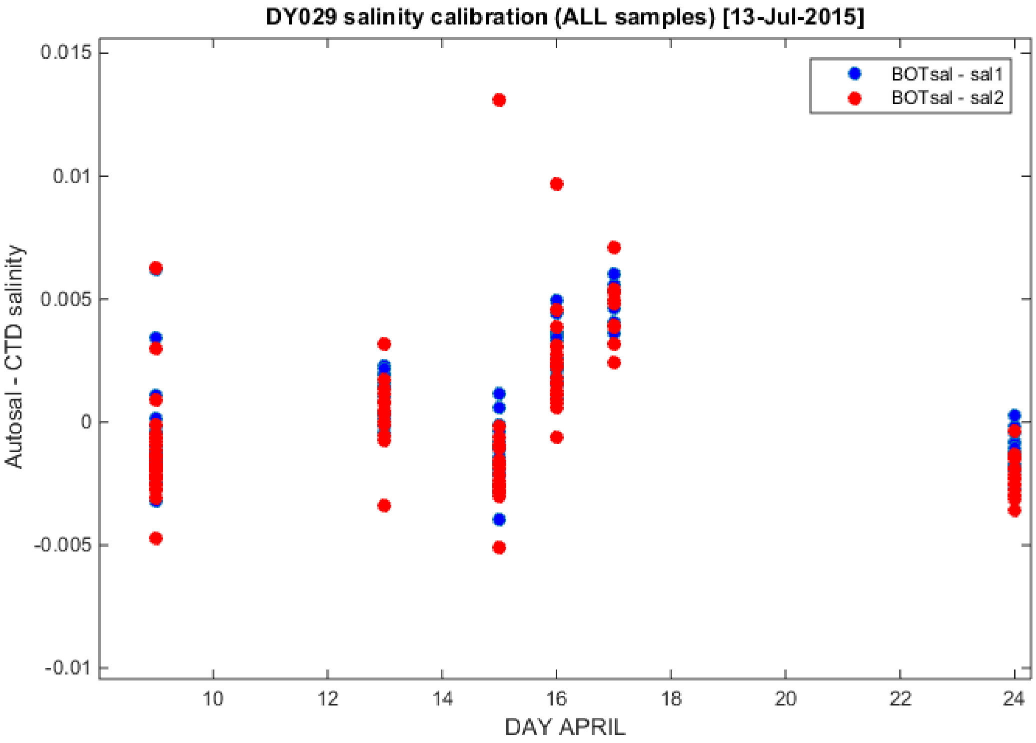
Salinity

A total of 263 salinity samples from the stainless and titanium CTDs were taken and used for calibration.
There was a primary and secondary sensor on both the stainless and titanium CTD. The secondary sensor (Sal2) on the stainless steel CTD frame showed problems on CTD018SS, after investigation the sensor was changed ready for CTD020SS. The Sal2 readings from CTD017SS and CTD018SS were clear outliers (see below) when performing calibration and thus have been removed when calculating the calibration for Sal2. There are two separate calibrations applied to Sal2, pre CTD020ss and post CTD020SS to account for the changing of the sensor.

A second calibration was applied to both the stainless and titanium sensors to allow for an unexplained autosal related drift in the middle days of analysis (15th, 16th, 17th – see below figure). This drift is thought to be due to the autosal analysis and not sample related as the measurements of the autosal standards at the beginning and end of each autosal run on the 15th, 16th and 17th showed a drift.
This offset was applied to the salinity data analysed during this time and did not improve the calibration.

12th October 2015:
Therefore instead of applying a second calibration for the autosal drift, the autosal samples from dates 15th – 17th April were omitted in the calibration. This improved the calibration.

Samples including autosal drift:



STAINLESS

143 stainless bottle salinities were taken.
Using all samples the mean and standard deviation of residuals from the stainless primary and secondary sensors were:

Mean difference between BOTsal and SAL1 = 0.0026811 (std = 0.0050375)

Mean difference between BOTsal and SAL2 (up to CTD019SS)= -2.7486 (std = 7.3602)

Mean difference between BOTsal and SAL2(after CTD019SS) = -0.92063 (std = 4.4306)

After removal of outliers where the difference between Autosal and CTD values was greater than 1standard deviations the mean ± standard deviations for the stainless primary and secondary sensors was reduced to:

(After removal of outliers (+/- 2 stds))

Mean difference between BOTsal and SAL1 = 0.0022377 (std = 0.0023854)

Mean difference between BOTsal and SAL2(up to CTD019SS) = 0.0029619 (std = 0.0076094)

Mean difference between BOTsal and SAL2(after CTD019SS) = 0.0029635 (std = 0.0049118)

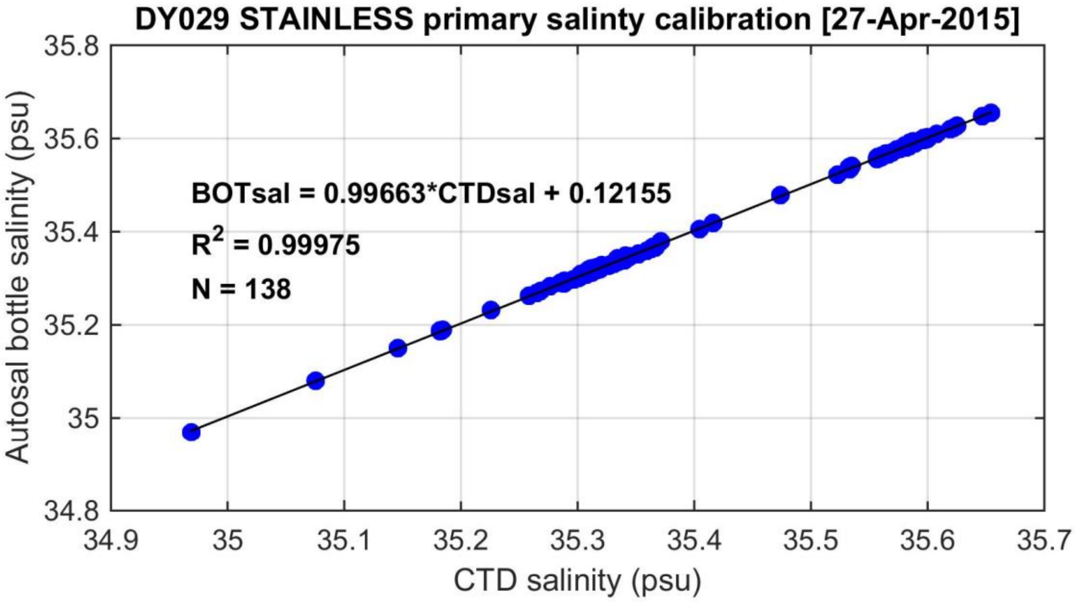
After calibrations applied to both stainless sensors:

Mean difference between BOTsal and SAL1 = -6.848e-15 (std = 0.0023332)

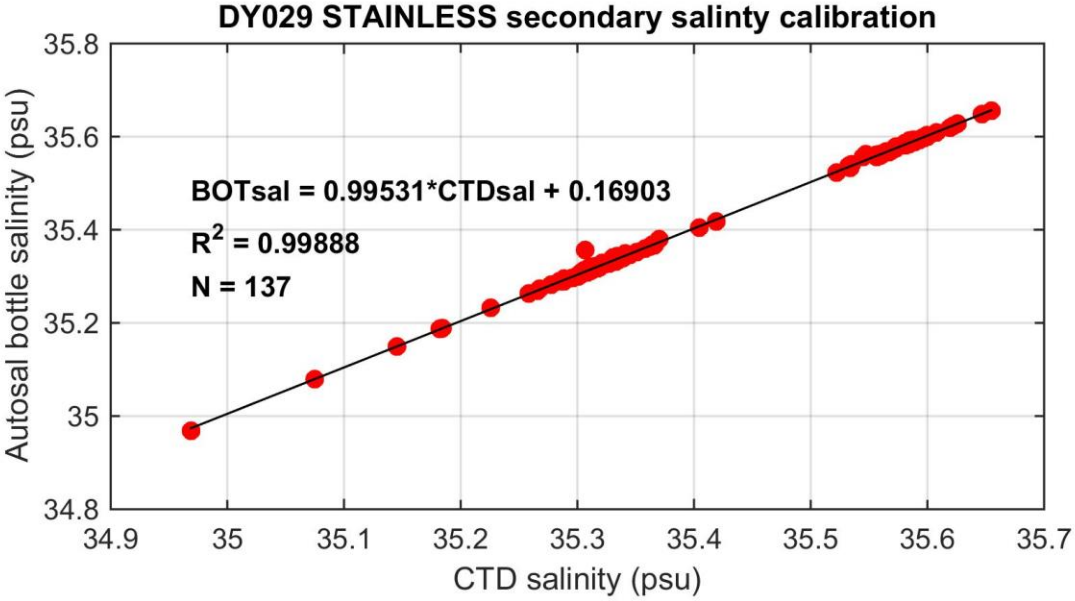
Mean difference between BOTsal and SAL2(up to CTD019SS) = 4.737e-15 (std = 0.0075398)

Mean difference between BOTsal and SAL2 (after CTD019SS) = 1.0269e-14 (std = 0.0048638)

Orignal calibration including autosal samples with drift:

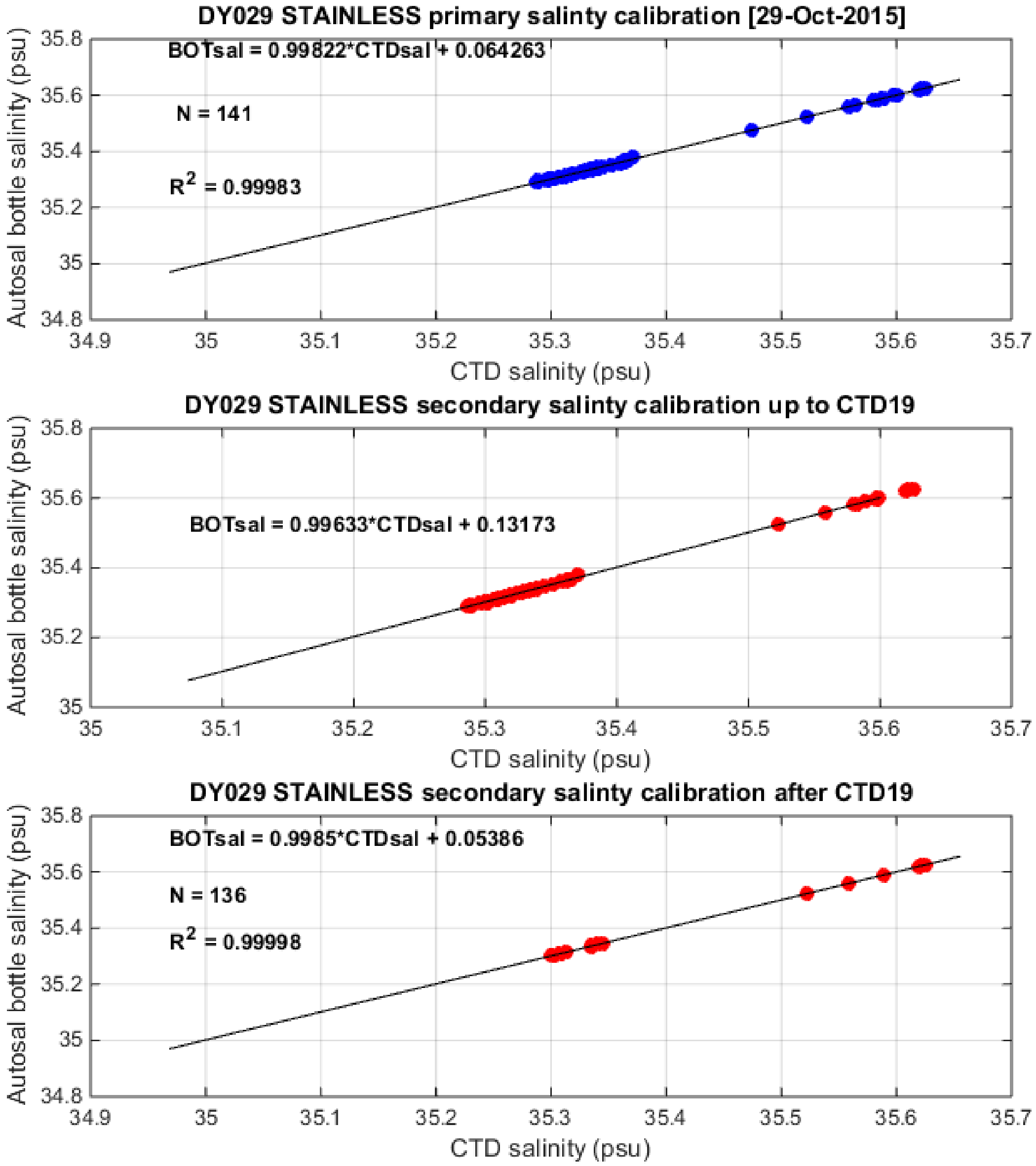


DY029 STAINLESS primary salinty calibration [27-Apr-2015]

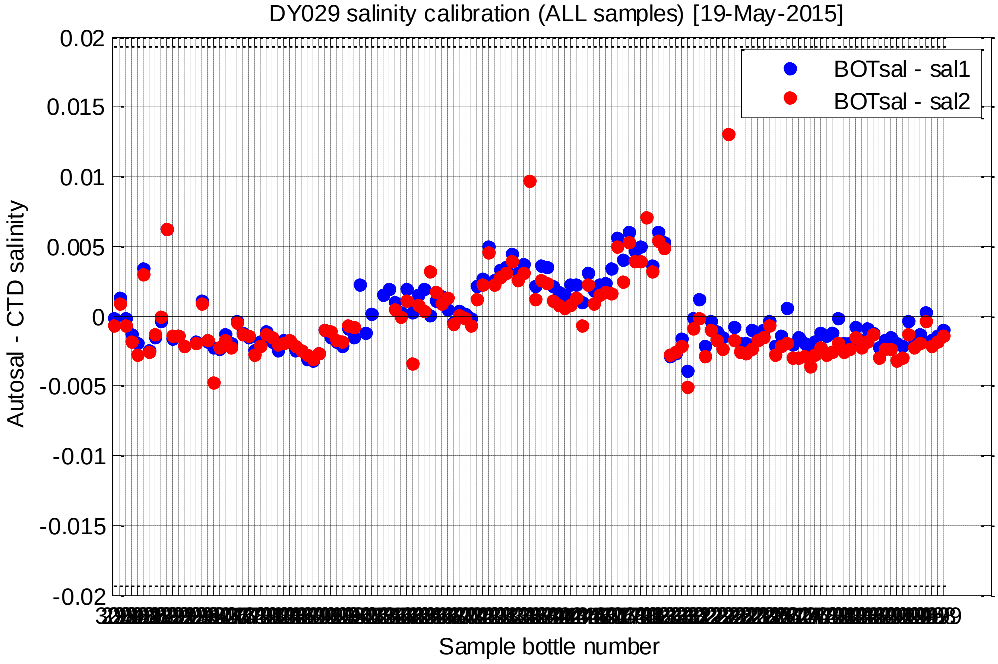


DY029 STAINLESS secondary salinty calibration

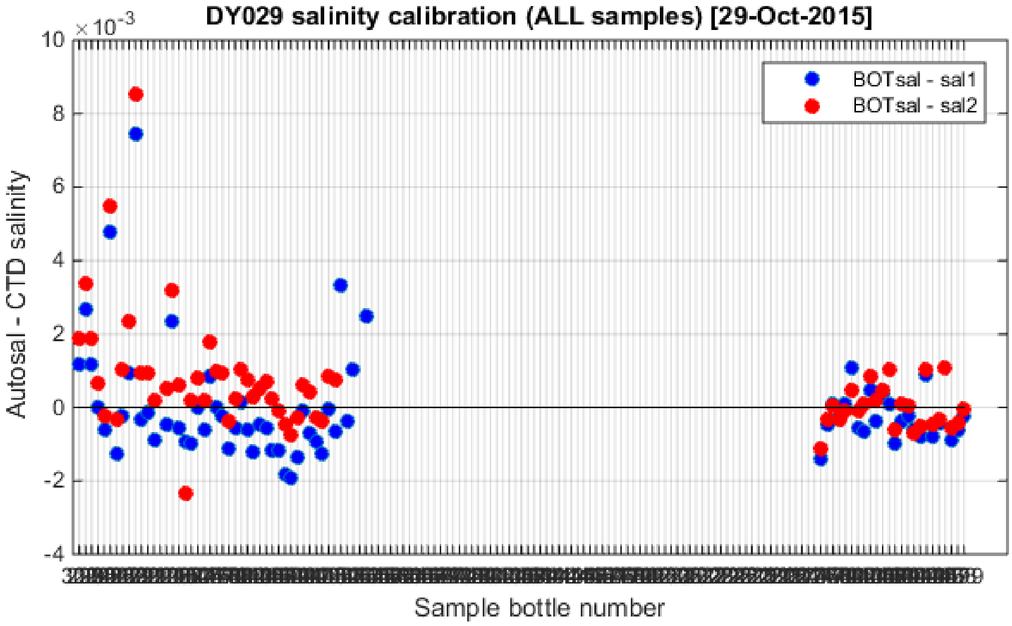
Updated calibration omitting samples with autosal drift:



Difference between bottle salinity and CTD salinity measurement pre calibration and pre correction:



Difference between bottle salinity and CTD salinity measurement post calibration when autosal drift samples omitted:



TITANIUM

120 titanium bottle salinities were taken.
Using all samples the mean and standard deviation of residuals from the titanium primary and secondary sensors were:

Mean difference between BOTsal and SAL1 = 0.0027692 (std = 0.012453)

Mean difference between BOTsal and SAL2 = 0.0030375 (std = 0.012359)

After removal of outliers (+/- 2 stds):

Mean difference between BOTsal and SAL1 = 0.0039915 (std = 0.0043402)

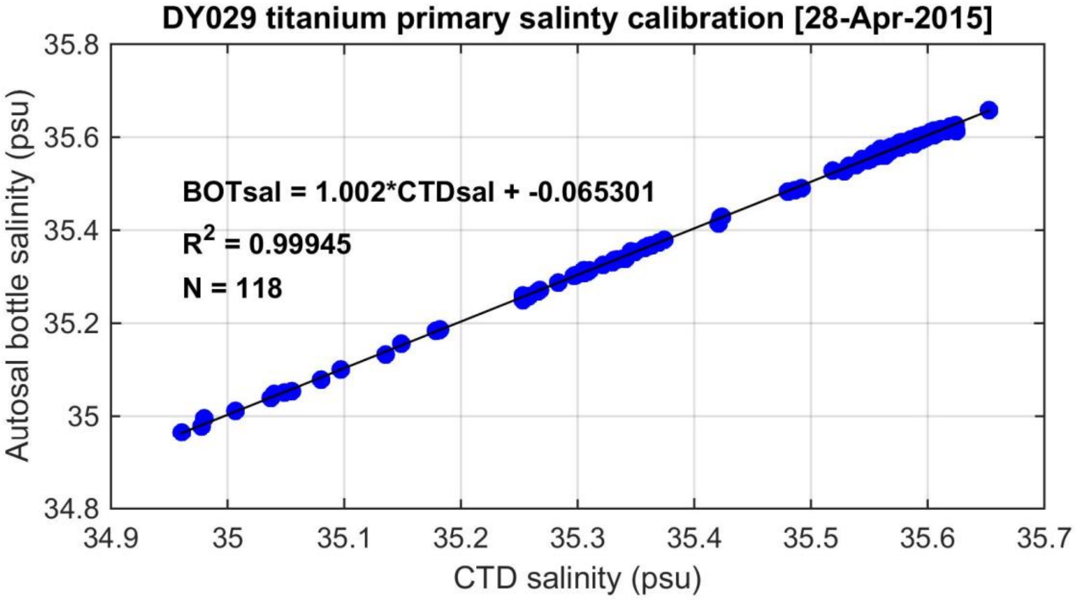
Mean difference between BOTsal and SAL2 = 0.0042542 (std = 0.0042027)

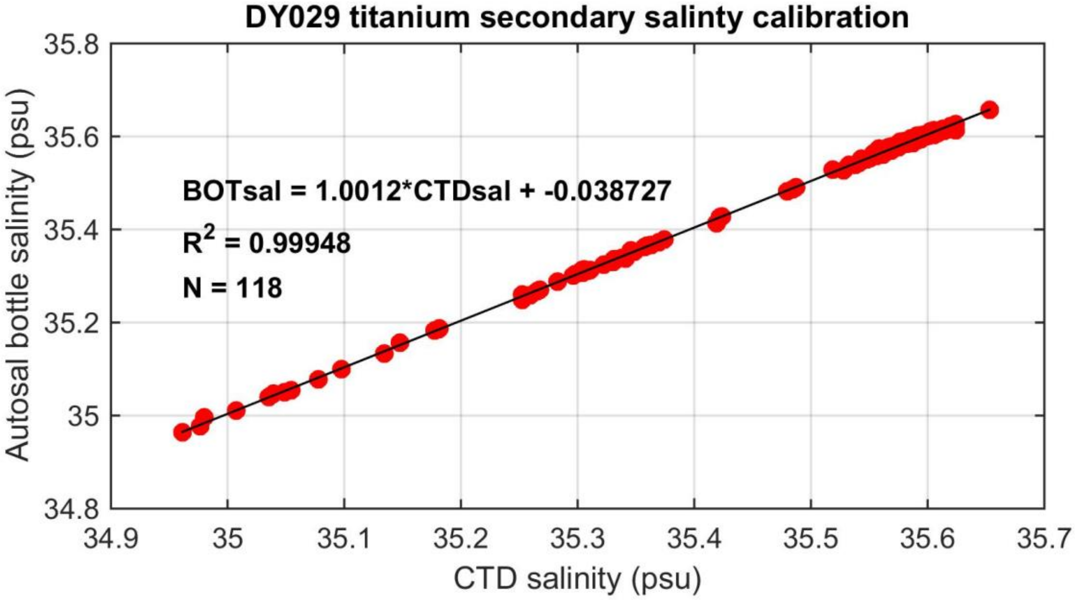
After calibrations:

Mean difference between BOTsal and SAL1 = 5.6603e-15 (std = 0.0043254)

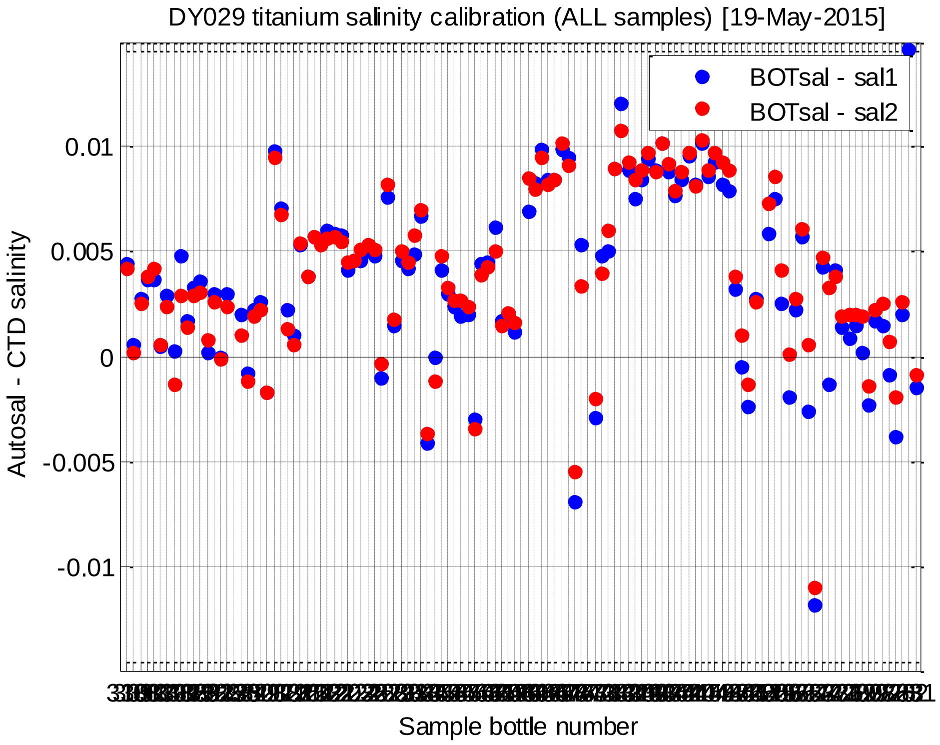
Mean difference between BOTsal and SAL2 = -1.8245e-14 (std = 0.0041968)

Orignal calibration including autosal samples with drift:

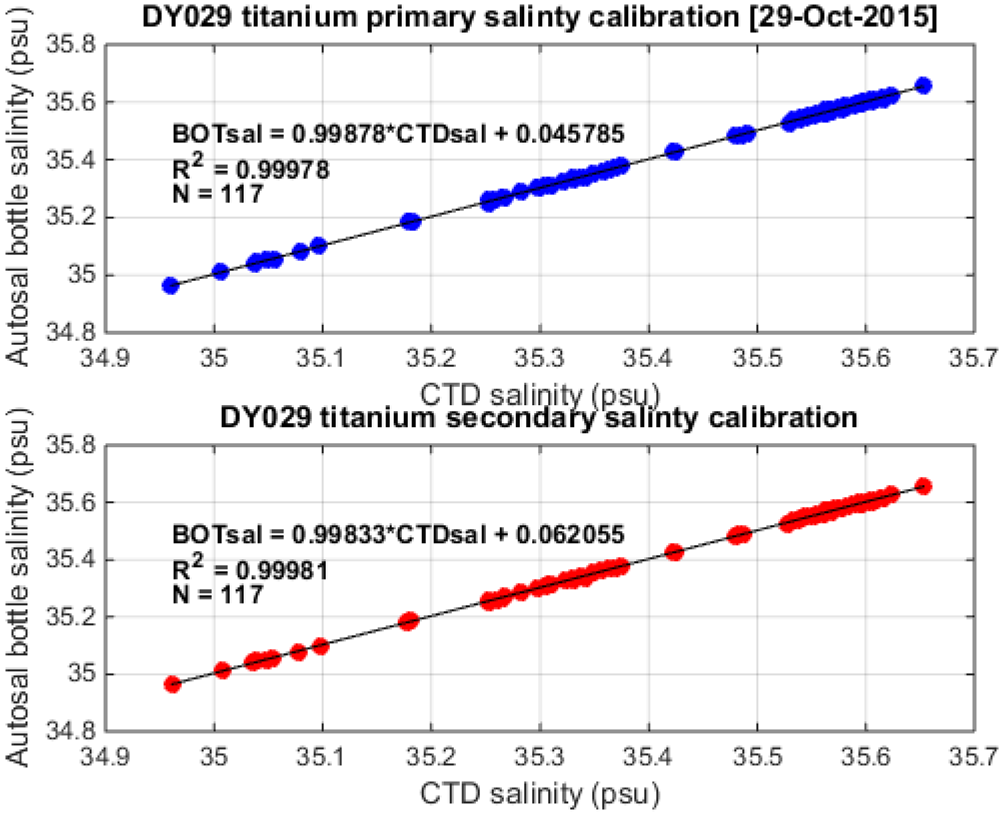




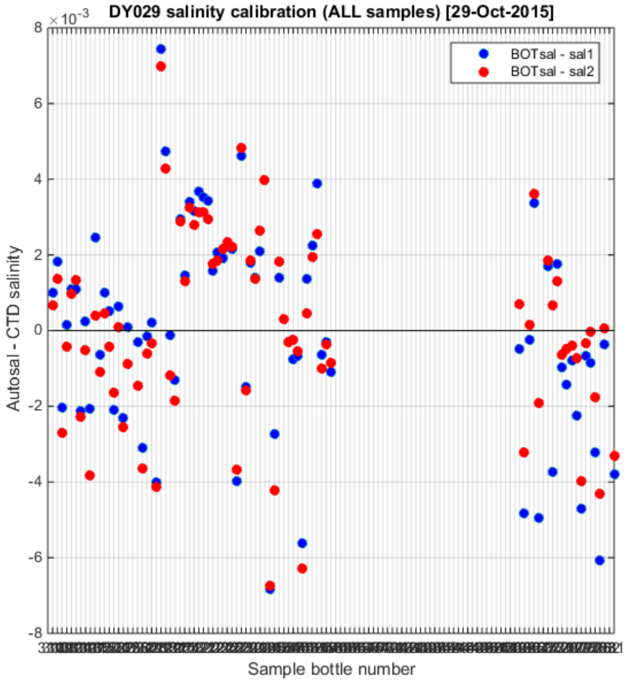
Difference between bottle salinity and CTD salinity measurement pre calibration and pre correction for autosal drift:



Updated calibration omitting samples with autosal drift:

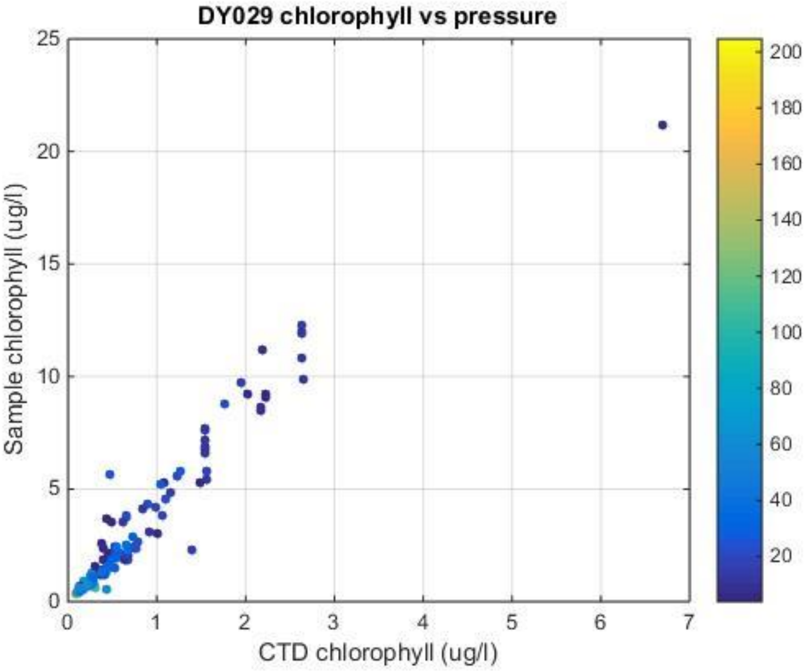


Difference between bottle salinity and CTD salinity measurement post calibration when autosal drift samples omitted:

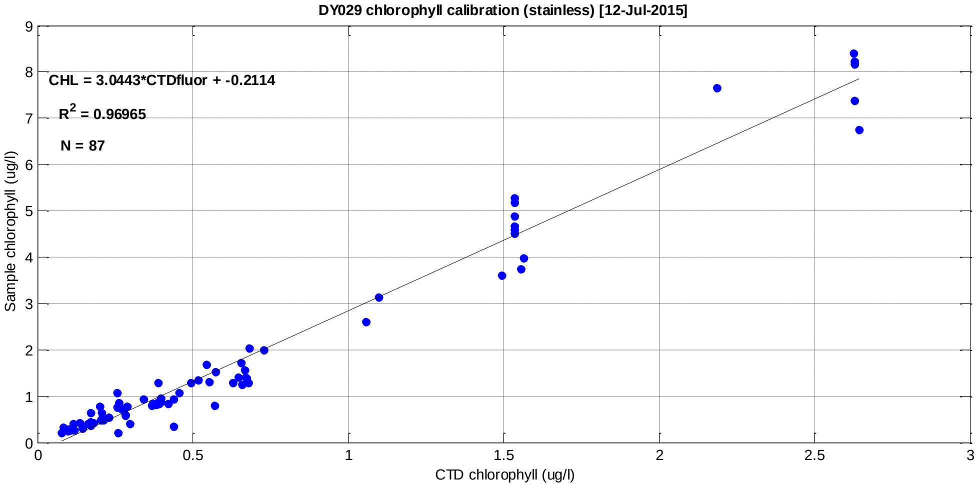


Chlorophyll

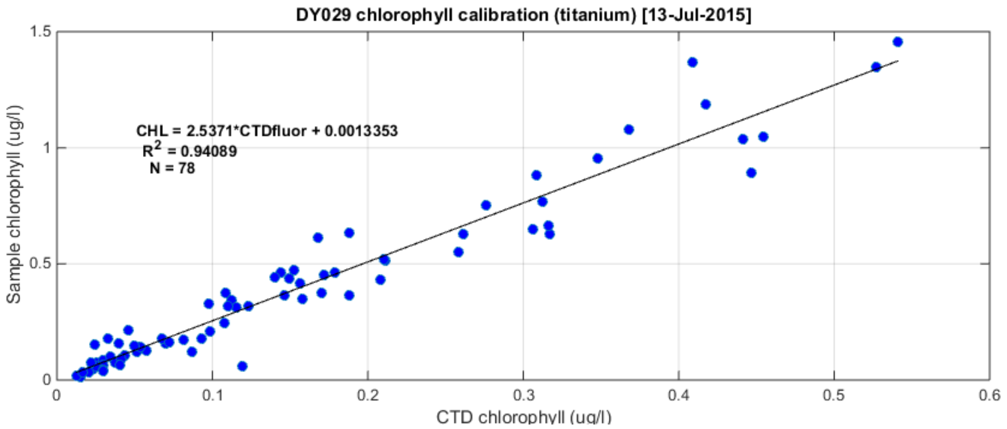
There were 223 discrete chlorphyll samples taken from the stainless and the titanium CTD.



Chlorophyll: Stainless steel

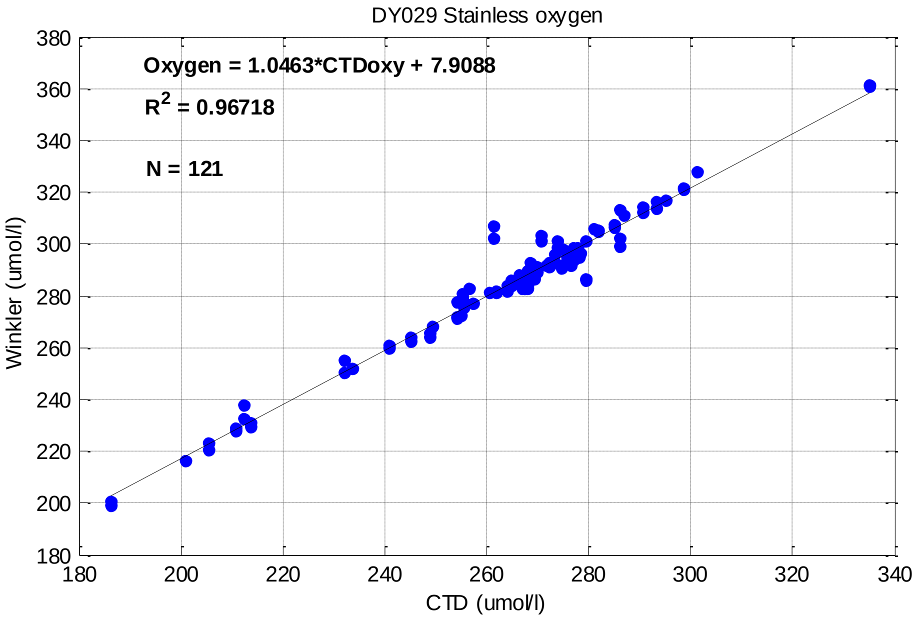


Chlorophyll: Titanium

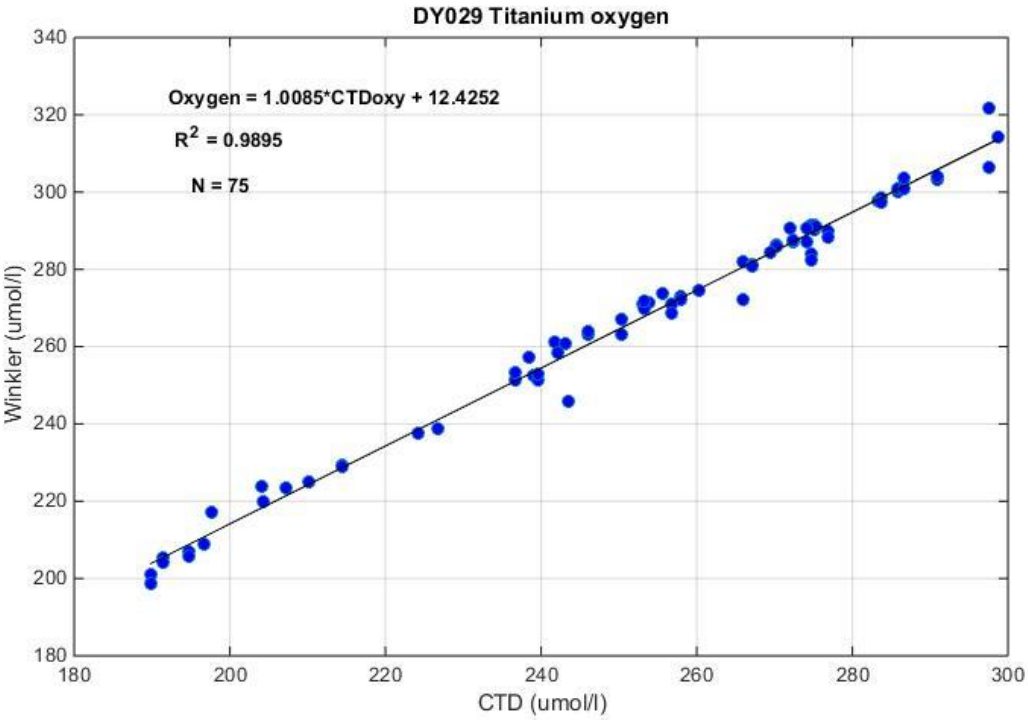


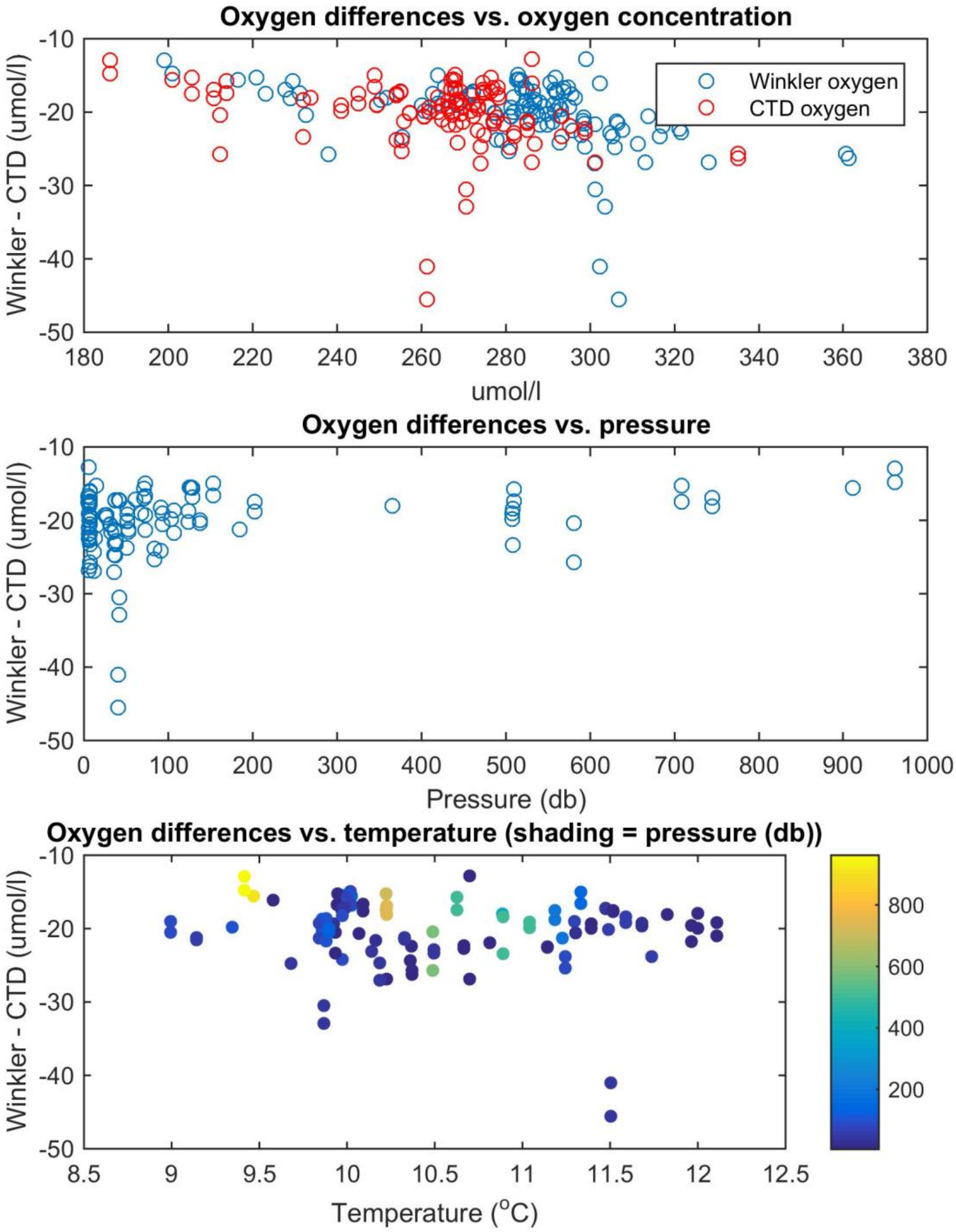
Oxygen: Stainless steel

There were 186 discrete samples taken from the stainless and the titanium CTD for oxygen analysis using the Winkler method. The calibrations that have been applied to the data are as follows:



Oxygen: Titanium


DY029 Titanium oxygen
Oxygen = 1.0085*CTDoxy + 12.4252
R^2 = 0.9895
N = 75
Winkler (umol/l)
340
320
300
280
260
240
220
200
180
CTD (umol/l)
180
200
220
240
260
280
300


Oxygen differences vs. oxygen concentration
Winkler - CTD (umol/l)
-10
-20
-30
-40
-50
180
200
220
240
260
280
300
320
340
360
380
umol/l
Winkler oxygen
CTD oxygen
Oxygen differences vs. pressure
Winkler - CTD (umol/l)
-10
-20
-30
-40
-50
0
100
200
300
400
500
600
700
800
900
1000
Pressure (db)
Oxygen differences vs. temperature (shading = pressure (db))
Winkler - CTD (umol/l)
-10
-20
-30
-40
-50
8.5
9
9.5
10
10.5
11
11.5
12
12.5
Temperature (°C)
800
600
400
200

Turbidity: Stainless Steel and titanium

Decision made to not calibrate turbidity sensor with SPM samples.