DY008 CTD processing report

March 2014
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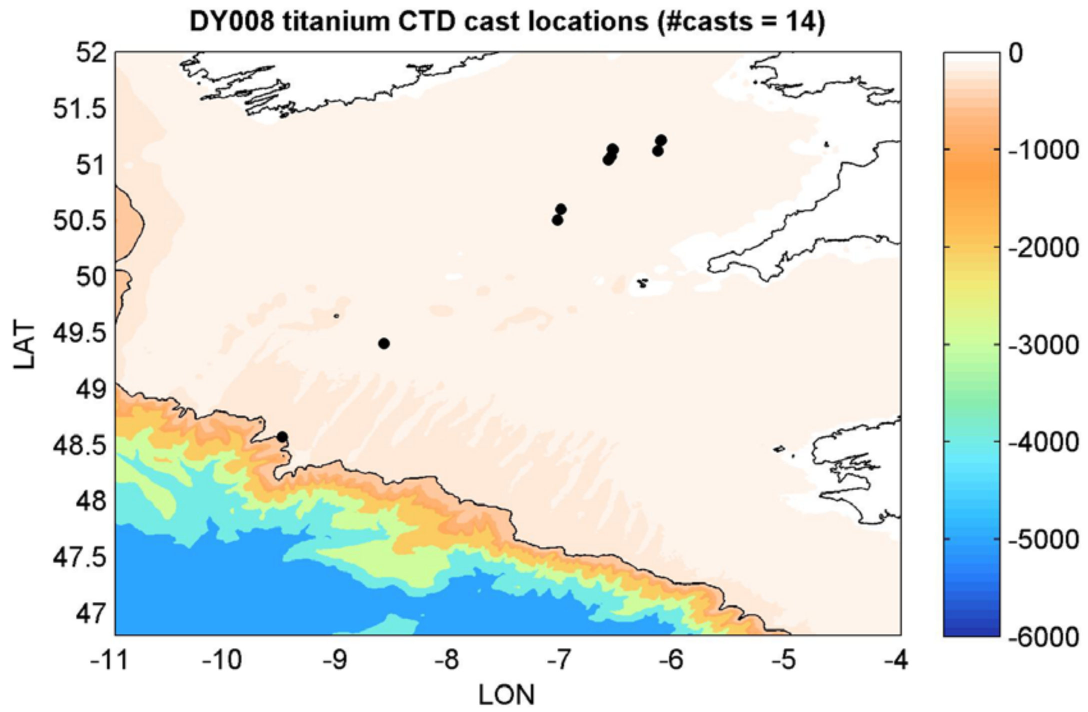
See technical reports from Jeff Benson for sensor serial numbers and channels.
A total of 14 casts with the titanium CTD frame were conducted.

Map of CTD cast locations



Raw data files:

The following raw data files were generated:

DY008_001.bl (a record of bottle firing locations)
DY008_001.hdr (header file)
DY008_001.hex (raw data file)
DY008_001.con (configuration file)

Where _001 is the 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 though 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: -1 seconds (bottles were fired on the fly)
Scan range duration: 1 seconds (bottles were fired on the fly)
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 4: Light scattering Wetlabs BBRTD **
- Voltage channel 5: Altimeter
- Voltage channel 6: Fluorometer
- Voltage channel 7: Transmissometer

* The first cast (DY008_001) configuration file had the PAR sensor in an incorrect voltage channel (V3 instead of V2)
** The light scattering sensor Wetlabs BBRTD was changed after cast 3 because it was giving suspect readings on the up and downcasts. Note the different wavelengths.
BBRTD SN 1055 for casts 001-003 (wavelength 650 nm)
BBRTD SN 182 for casts 004-014 (wavelength 660 nm)

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.

   Output saved to DY008_001.btl

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 4 different casts (1, 2, 7 and 14), a 2 second advance was chosen for the oxygen sensor.

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), but further testing of -1, -2, +1 and +2 scans (on both sensors) showed that an adjustment of -1 scan (= -0.0417 seconds) resulted in the greatest reduction in noise in the salinity channel.

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 DY008_001.cnv (24 Hz resolution)

7. **Derive:** Variables selected are
   Salinity and Salinty 2 [PSU, PSS-78]
   Oxygen SBE43 [µmol/l]
   Oxygen Tau correction: yes (2 second window)

   Output saved to DY008_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 DY008_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. DY008
STNNBR (as per BODC data management guidance for the Shelf Sea Biogeochemistry programme)
DATE and TIME of the cast at the bottom 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: DY008_metadata.mat

(2) Extract data from 2Hz averaged files (e.g. DY008_001_derive_2Hz.cnv), merge with metadata and save into a matlab structure for each cast. Each file (DY008_001_derive_2Hz.mat) contains the following <u>un-calibrated</u> channels.

```
CTD001 =

           CRUISE: 'DY008'
             CAST: 1
           STNNBR: 3
             DATE: '21/03/2014'
             TIME: '15:10'
              LAT: 51.1210
```

```
              LON: -6.1662
            DEPTH: 103              [m]
          CTDtime: [1973x1 double] [seconds]
          CTDpres: [1973x1 double] [db]
         CTDtemp1: [1973x1 double] [°C]
         CTDtemp2: [1973x1 double] [°C]
         CTDcond1: [1973x1 double] [S/m]
         CTDcond2: [1973x1 double] [S/m]
       CTDoxy_raw: [1973x1 double] [V]
           CTDatt: [1973x1 double] [1/m]
         CTDfluor: [1973x1 double] [µg/l]
           CTDpar: [1973x1 double] [Wm2]
          CTDturb: [1973x1 double] [m-1 sr-1]
           CTDalt: [1973x1 double] [m]
    CTDpar_dn_raw: [1973x1 double] [V]
      CTDturb_raw: [1973x1 double] [V]
       CTDalt_raw: [1973x1 double] [V]
     CTDfluor_raw: [1973x1 double] [V]
       CTDatt_raw: [1973x1 double] [V]
          CTDsal1: [1973x1 double] [PSU]
          CTDsal2: [1973x1 double] [PSU]
     CTDoxy_umoll: [1973x1 double] [µmol/l]
          CTDflag: [1973x1 double]
```

(3) Extract data from 24Hz files (e.g. DY008_001_derive.cnv), merge with metadata and save into a matlab structure for each cast. Each file (DY008_001_derive.mat) contains the following <u>un-calibrated</u> channels.

```
CTD001 =

             CRUISE: 'DY008'
               CAST: 1
             STNNBR: 3
               DATE: '21/03/2014'
               TIME: '15:18'
                LAT: 51.1210
                LON: -6.1662
              DEPTH: 103               [m]
            CTDtime: [23672x1 double] [seconds]
            CTDpres: [23672x1 double] [db]
           CTDtemp1: [23672x1 double] [°C]
           CTDtemp2: [23672x1 double] [°C]
           CTDcond1: [23672x1 double] [S/m]
           CTDcond2: [23672x1 double] [S/m]
          CTDsal1_1: [23672x1 double] [PSU]
          CTDsal2_1: [23672x1 double] [PSU]
         CTDoxy_raw: [23672x1 double] [V]
    CTD_oxy_umoll_1: [23672x1 double] [µmol/l]
             CTDatt: [23672x1 double] [1/m]
           CTDfluor: [23672x1 double] [µg/l]
             CTDpar: [23672x1 double] [Wm2]
            CTDturb: [23672x1 double] [m-1 sr-1]
             CTDalt: [23672x1 double] [m]
      CTDpar_dn_raw: [23672x1 double] [V]
```

```
   CTDturb_raw: [23672x1 double] [V]
    CTDalt_raw: [23672x1 double] [V]
  CTDfluor_raw: [23672x1 double] [V]
    CTDatt_raw: [23672x1 double] [V]
       CTDsal1: [23672x1 double] [PSU]
       CTDsal2: [23672x1 double] [PSU]
  CTDoxy_umoll: [23672x1 double] [µmol/l]
       CTDflag: [23672x1 double]
```

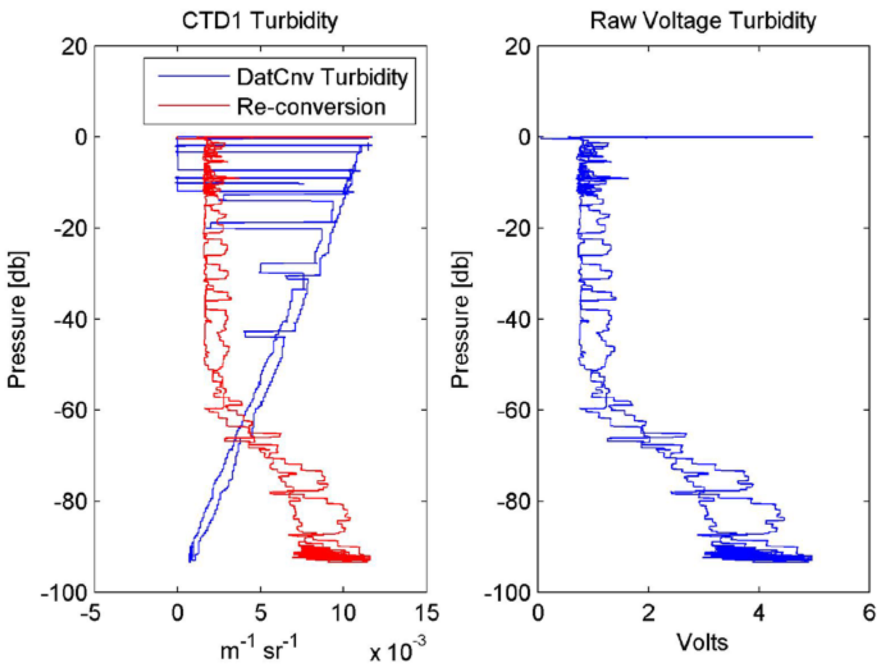
Note that '_1' for the first instances of salinity and oxygen in this file are variables before re-derivation in the SeaBird Processing routines.

Inspection of the turbidity channel (CTDturb) and comparison to the raw voltage (CTDturb_raw) revealed a potential bug in the SeaBird DatCnv conversion module whereby precision in the final converted value was lost. This was noticed on DY018 (Nov-Dec 2014) and Seabird was contacted by Dougal Mountifield (details of the communications are appended at the end of this report for reference). The original turbidity channel is therefore re-derived (for all casts) using the following conversion and taking the scale factor (SF) and dark counts (DC) from the manufacturer's calibration (note that the sensors were swapped after cast 3 so the calibration coefficients are different).

CTDturb = CTDturb_raw .* SF – (SF * DC)

This resolves the issue and is in agreement with the advice provided by SeaBird (see emails attached).

Additionally, for casts 1-4 the raw turbidity voltage channel was not even converted into the correct profile shape (see example below). The reason for this is unknown but has been rectified by the re-derivation.



(right) Raw turbidity voltage channel. (left) DatCnv conversion into m^{-1} sr^{-1} vs. own conversion in Matlab using manufacturer calibration sheet. This was the case for casts 1-4 (despite a sensor change after cast 3).

(4) Manual identification of the surface soak (while waiting for pumps to turn on) and out of water readings using the 2Hz files. Times to crop were saved to DY008_castcrop_times.mat.

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

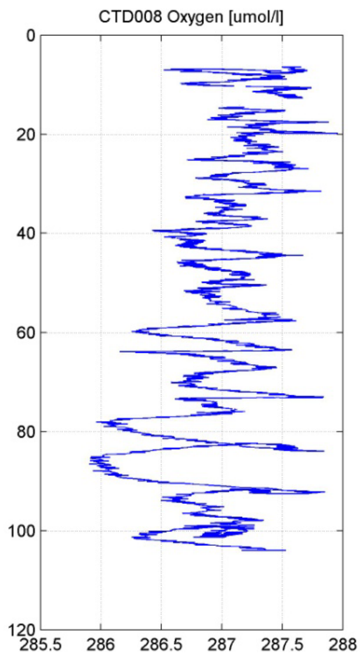
This was then used to crop both the 2Hz and 24Hz files and output saved to DY008_001_derive_2Hz_cropped.mat and DY008_001_derive_cropped.mat respectively.

(5) De-spiking of 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, attenuation	100	2	200	3

Auto-despiking saved to DY008_001_derived_cropped_autospike.mat



Example of downcast oxygen impacted by pitch and roll of ship.

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

Large 'spikes' were often 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 D352, D376); 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 (as was the case on CD173).

The largest and most significant warm anomalies identified in the primary and secondary CT sensors were removed. This was at times up to 5 m of the profile. 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.

Although 'old' water would also have been flushed back past the auxiliary sensors (turbidity, oxygen, chlorophyll, attenuation) the coincident measurements in these channels were (a) not always anomalous and/or (b) the associated anomaly did not always exactly coincide (or could even be confidently identified, especially for oxygen – see plot). As such removal of data from auxiliary channels using scans flagged as bad in the primary/secondary CT channels was not always appropriate or did not improve data quality. The worst individual spikes within these channels however were manually identified and removed (NaN'd).

Output saved to DY008_001_derived_cropped_autospike_manualspike.mat

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 archiving purposes only.

```
Pindex: [18900x3 double]
Sindex: [18900x3 double]
Aindex: [18900x4 double]
```

(6) Average 24Hz (cropped and de-spiked data) into 1 db bins. Linear interpolation is performed here to fill gaps in the profile.

File output: DY008_001_1db_dn.mat

All the 1 db profiles (except PAR) are then further smoothed with a 10 m running median window.

File output: DY008_001_1db_dn_smth.mat

(7) Application of calibrations to salinity and chlorophyll 1db smoothed downcasts. Calibrated files saved to DY008_001_1db_dn_smth_calib.

No calibration was applied for oxygen– see notes below.

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.

```
CRUISE: 'DY008'
      CAST: 8
    STNNBR: 54
      DATE: '25/03/2014'
      TIME: '07:23'
       LAT: 50.5037
       LON: -7.0581
     DEPTH: 110
      pres: [99x1 double] [db]
      time: [99x1 double] [seconds]
     temp1: [99x1 double] [°C]
```

```
      temp2: [99x1 double] [°C]
       sal1: [99x1 double] [PSU] - calibrated
       sal2: [99x1 double] [PSU] - calibrated
      cond1: [99x1 double] [S/m] – not calibrated
      cond2: [99x1 double] [S/m] – not calibrated
  oxy_umoll: [99x1 double] [μmol/l] – not calibrated
      fluor: [99x1 double] [μg/l] – calibrated
        par: [99x1 double] [Wm2]
       turb: [99x1 double] [m-1 sr-1]
        att: [99x1 double] [1/m]
sigma_theta: [99x1 double]
```

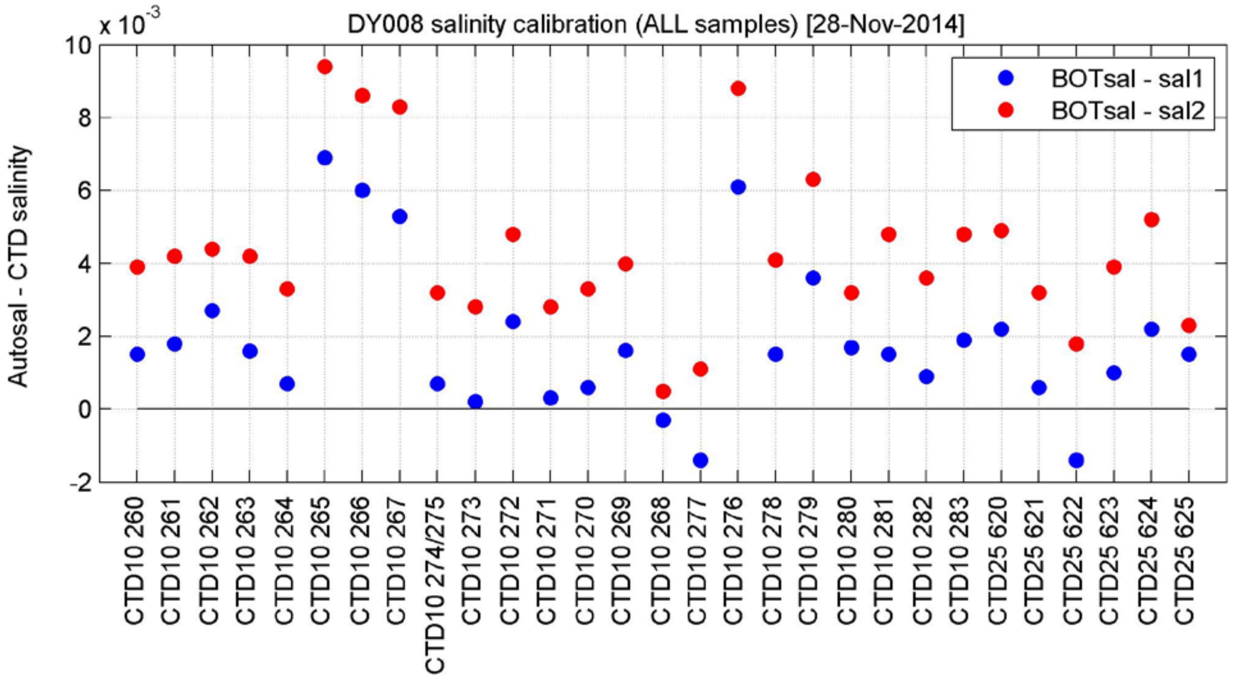
The calibrations were also applied to the 24 Hz data (cropped and de-spiked) and output to .mat files DY008_001_derive_cropped_autospike_manualspike_calib.mat containing the same variables as above.

(8) Application of salinity and chlorophyll calibrations to bottle firing data. The primary and secondary salinity records from the .btl files were calibrated using the offsets shown below. A new file, DY008_btl_calib.mat, with variables CTDsal1_cal, CTDsal2_cal and CTDfluor_cal was created. Oxygen has not been calibrated (see below).

Calibrations

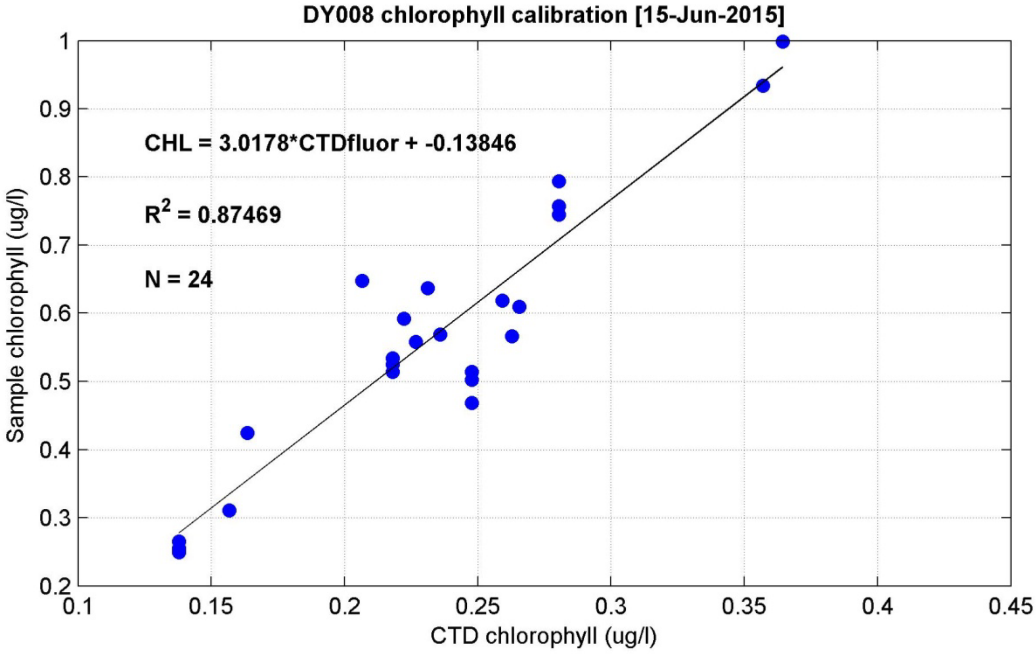
Salinity

29 useable salinity samples were taken and analysed on a Guildline Autosal salinometer (SN 71126). Using all samples the mean and standard deviation of residuals from the primary and secondary sensors were 0.0018586 ± 0.0020348 and 0.0043345 ± 0.0021767 respectively. After removal of outliers where the difference between Autosal and CTD values was greater than 2 standard deviations the mean ± standard deviations for the primary and secondary sensors was reduced to 0.0013423 ± 0.001392 and 0.0039815 ±0.0017942 respectively. These mean values were then used to correct the CTD salinity channels. Following calibration the mean difference between the primary and secondary salinity channels (from all bottle file data) was -3.69e-05 (std = 3.98e-04).



Chlorophyll

24 samples were collected for the CTD chlorophyll calibration. The figure below shows the regression.



This calibration however should be treated with caution for the following reasons:

- Of the 24 samples taken only 12 were from different bottle firings – there were 4 sets of triplicates taken from the same bottles:
  - Cast 8 – 3 samples from 13 m
  - Cast 9 – 3 samples from 11 m
  - Cast 10 – 3 samples from 11 m
  - Cast 11 - 3 samples from 12 m

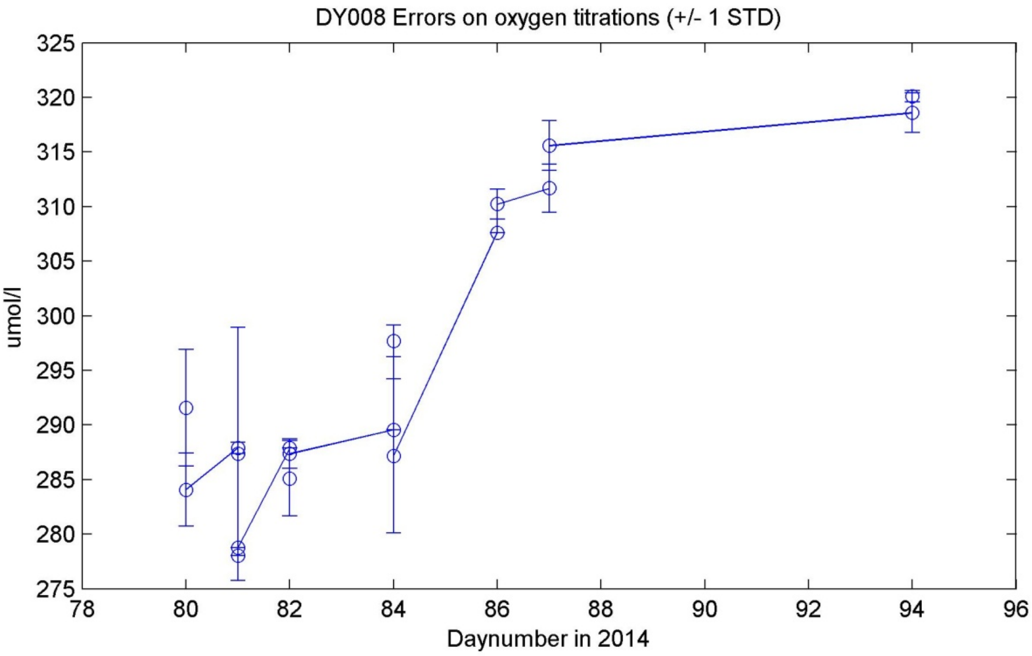
This is therefore a very small sample size for a statistically significant correlation.

- Removing samples taken above 30 m during daylight hours to avoid contamination by quenching, only 11 samples remain (3 of which being from the same bottle). Using only these 11 points the calibration does not improve.

Oxygen

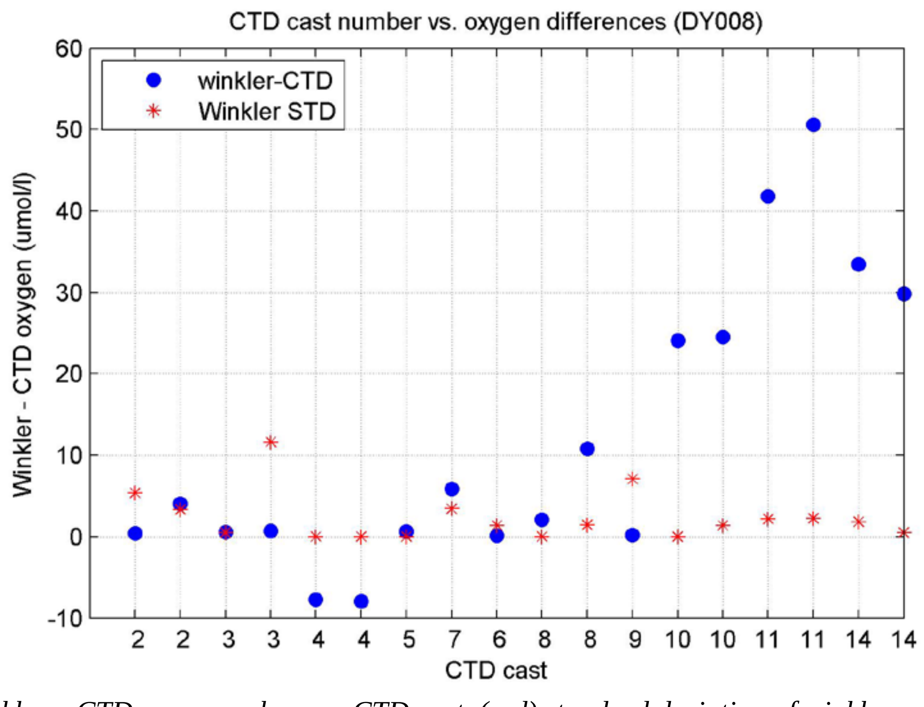
A total of 19 samples were taken for oxygen titration. A confident calibration however could not be determined so nothing has been applied (oxygen values in files left un-calibrated). The pre- and post cruise calibration of the CTD oxygen sensor does not show any problems. There is no indication in the NMF cruise reports that there was a problem with the CTD oxygen sensor and it was not changed during the cruise.

Bottle oxygen values were typically taken as the mean of 2-3 replicas. Even after removal of values where the standard deviation about this mean was > 20 umol/l, some very large standard deviations remain.



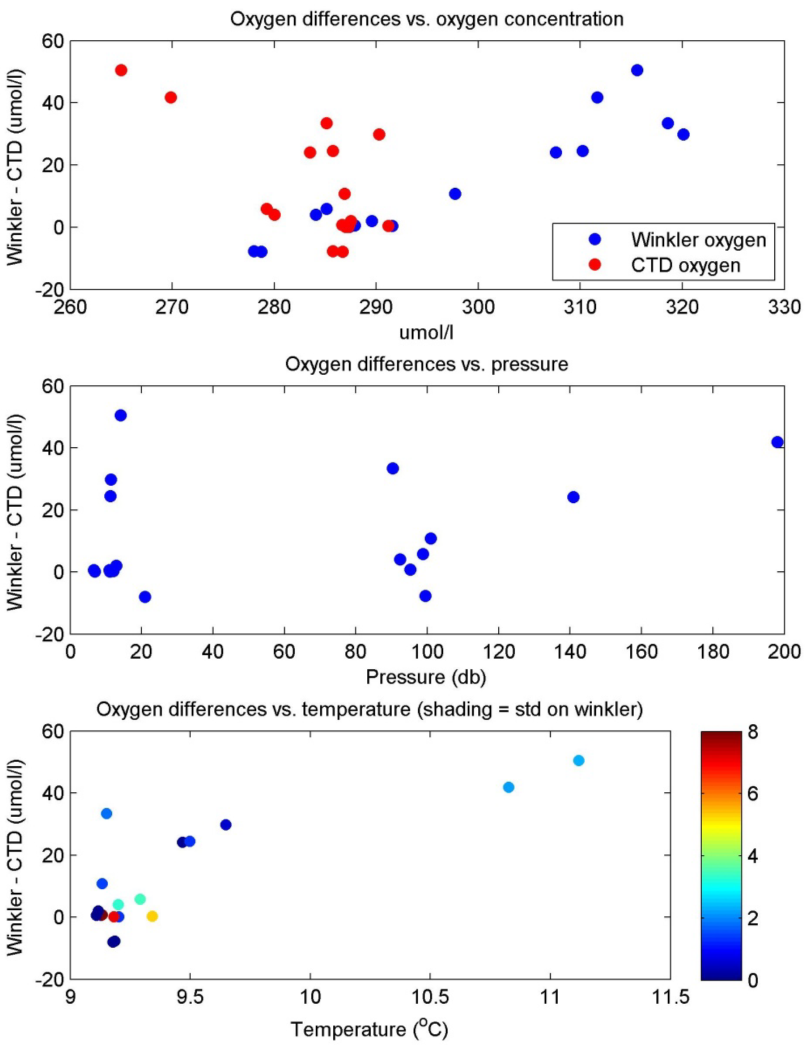
Error bars on winkler titrations (after removal of STD > 20 umol/l)

There is a suggestion that casts 2-9 and 10-14 require different calibrations, although sampling and Winkler analysis error cannot be ruled out.

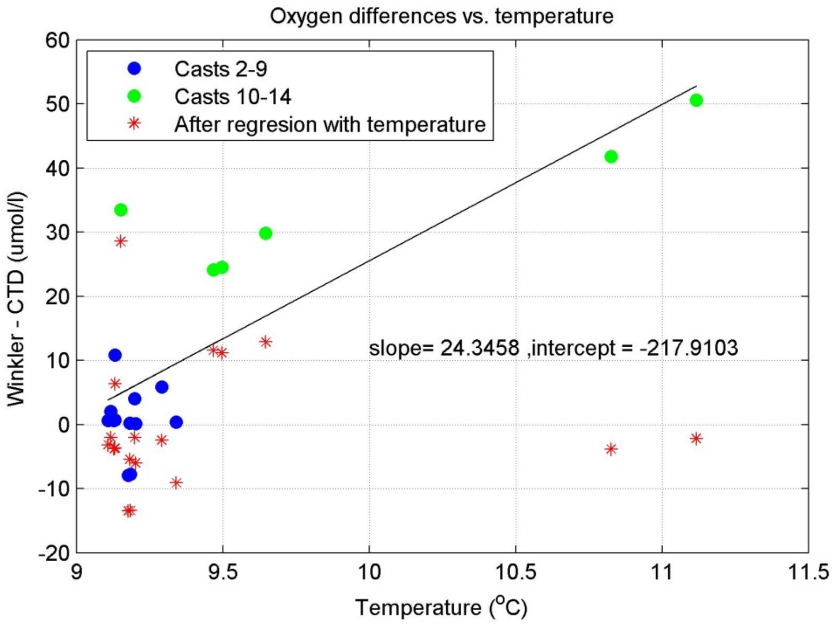


(blue) Winkler – CTD oxygen values vs. CTD cast. (red) standard deviation of winkler oxygen value

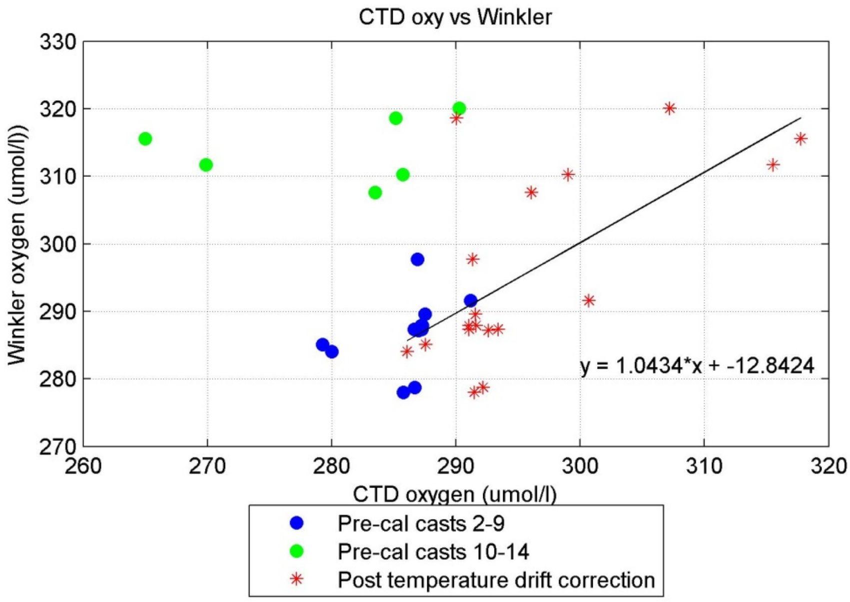
Plotting the winkler-CTD offset against pressure, temperature and oxygen concentration from both the winkler and CTD sensor suggests that there may be a trend in the offset with temperature. There are not enough samples to be confident of this though and too many other uncertainties. Any attempt at calibration could potentially degrade rather than improve the CTD oxygen values.



(top) Winkler – CTD vs. winkler [blue] and CTD [red] oxygen values. (middle) Winkler – CTD vs. pressure. (bottom) Winkler – CTD vs. temperature (shading = winkler std)



(green and blue) Winkler – CTD oxygen. (red) Winkler – CTD oxygen after trend with temperature removed



(green and blue) Winkler vs CTD oxygen. (red) Winkler vs CTD oxygen after trend with temperature removed. The regression is similar to those applied on other cruises (e.g. DY018 and DY021)

Emails between Seabird and Dougal Mountifield regarding ECO-BB module conversion

Urgent: Wetlabs BB con file module SBE Data Processing problem
Date: Wed, 19 Nov 2014 08:28:13 +0000
From: Dougal Mountifield
To: SeaBird

Hi,

I am currently at sea on RRS Discovery. We are deploying 2 CTD packages which both have Wetlabs BBrtd instruments installed as a 0-5V analog channel on a SBE 9+ underwater unit. We are using the Wetlabs BB module in the con file. 9+ When acquiring the data in Seasave the data from the instrument looks fine, however after data conversion in SBE data processing, and plotting in Seaplot, the profile from the BB is quantised resulting in very poor resolution. The voltage channel is fine (V5). If the BB module in the con file is replaced with a user poly (as used prior to the introduction of the Wetlabs con file module) the result is fine. Have you seen this problem before? Is it possible that the RS-232 digital version of the Wetlabs BB module is applied in error with a 9+ instead of the 0-5V analog version?

Please see the attached graphs, one with V5 and Wetlabs BB module and one with V5 and user poly. Also attached is the cast specific con file with the BB module selected and the associated instrument calibration sheet from Wetlabs. We don't have sufficient network bandwidth to send the data file. We are using v.7.23.2, but have also tried some older versions with the same result.

Urgent assistance would be appreciated.

Dougal Mountifield
National Marine Facilities - Sea Systems Sensors & Moorings Group National Oceanography Centre, Southampton UK.
Aboard RRS Discovery.

****

From: Stephanie Jaeger [mailto:sjaeger@seabird.com]
Sent: 19 November 2014 21:54
To: dm1@noc.ac.uk
Cc: techsupport@seabird.com; Benson, Jeffrey Ray; Hopkins, Joanne
Subject: RE: Urgent: Wetlabs BB con file module SBE Data Processing problem

Hi Dougal,

Thanks for bringing this to our attention. We haven't noted this issue before, and I will check with the software engineer to clarify the conversion formula that is currently used for the parameter "Turbidity Meter, WET Labs, ECO-BB" in the .xmlcon file. Has the data in the plot that you sent been processed at all beyond the data conversion step?

In the meantime, it sounds like you have found a workaround while on the cruise, using the user polynomial function. It should be a simple conversion step:

Turbidity = ?(?c) = (Output – Dark Output) * Scale Factor

When possible, it will be helpful to have the raw data, if you could send a copy of a HEX file? It could also work if you would like to send a short section of the cast (such as 100 m), as an example.

Let us know if you have any further questions on this.

Regards,

Stephanie

Stephanie Jaeger, M.Sc.
Technical Support
Sea-Bird Electronics

****

From: Stephanie Jaeger [sjaeger@seabird.com]
Sent: 12/10/2014 9:25 AM
To: dougal.mountifield@noc.ac.uk;
dm1@noc.ac.uk
Cc: daves@wetlabs.com; jeh200@noc.ac.uk; jrbn@noc.ac.uk
Subject: RE: Urgent: Wetlabs BB con file module SBE Data Processing problem [ref:_00D7096pT._50070vbxjt:ref]

Hi Dougal,

Thanks for the update. We were able to reproduce the issue that you mentioned. The software engineer found that the converted ECO-BB output is reported to a fixed precision. The user polynomial function reports a fixed number of significant figures, rather than a fixed precision, so it will provide the same resolution as raw data, regardless of the mean data level.

I'm checking in with Wetlabs directly about your question, in order to get further feedback about the best output to use, given the limits on data resolution for the ECO-BB.

Regards,
Stephanie

****

From: Stephanie Jaeger [sjaeger@seabird.com]
Sent: 18/12/2014 19:54
To: dougal.mountifield@noc.ac.uk;
dm1@noc.ac.uk
Cc: daves@wetlabs.com; jeh200@noc.ac.uk; jrbn@noc.ac.uk
Subject: RE: Urgent: Wetlabs BB con file module SBE Data Processing problem [ref:_00D7096pT._50070vbxjt:ref]

Hi Dougal,

I'm following up regarding your question on this processing the ECO-BB data. I did check in with Wetlabs, and they confirmed that the raw resolution (given in voltage on the A/D channel) should match the resolution of the converted engineering output. So, the output should show up as it does with the User Polynomial function, as you mentioned.

Also, we noted that the units of the output variable should be in "scattering" rather than "turbidity." So, the variable will be fixed to be named "OBS Meter, WET Labs, ECO-BB" rather than turbidity.

We have reported this to the software engineer, and he'll work to resolve this in a future version of SBE Data Processing.

Thank you for letting us know about this, and let me know if you have further questions.
Regards,
Stephanie