Processing report for CTD data obtained on RV Meteor, cruise M157

Jens Faber, Toralf Heene, Volker Mohrholz

Contents

Principal investigator

Volker Mohrholz
Email: volker.mohrholz@io-warnemuende.de
ORCID: 0000-0003-0778-9182

Data curator

Jens Faber
Email: jens.faber@io-warnemuende.de
ORCID: 0000-0001-6869-545X

1 Overview and sensor layout

The data were gathered with a CTD-system *SBE 911plus* by Sea-Bird Scientific (USA). The following physical parameters were measured by the particular sensors noted in brackets.

- Pressure (Paroscientific Digiquartz)
- Temperature (2x SBE 3)
- Conductivity (2x SBE 4)
- Oxygen concentration (2x SBE 43)
- Fluorescence (WET Labs ECO-AFL/FL)
- Turbudity (WET Labs ECO)
- Photosynthetically active radiation (Seabird PAR and SPAR sensors)

For detailed information and a technical description of the CTD, please refer to the manual that can be accessed at Sea-Bird Scientific (2016).
The temperature, conductivity and oxygen concentration sensors of the CTD unit are arranged in a tube system, where water is pumped through the sensors at a constant flow rate. This ensures that these measurements are always taken in the same water mass, thereby avoiding artificial spikes on salinity data. The system consists of two equal sets of temperature, conductivity and oxygen concentration sensors to provide redundancy in case of failure and for permanent check of sensor performance (Figure 1).
Data gathered during the casts were stored on hard disk using a *SBE 11 deck unit* and Seabird's data acquisition software *SeaSave*, Version 7 (Sea-Bird Scientific, 2017b). For each cast, a configuration file (DEPLOYMENTNAME.xmlcon) containing the sensor calibration information and the specific program settings used for data acquisition has been written. Temperatures are retrieved according to the ITS-90 temperature scale, practical salinities are calculated according the 1978 Practical Salinity equations (Sea-Bird Scientific, 2015, 1989).

Sensor	Type	Serial №	Lab Calibration date	Sensor Uncertainty	Measurement uncertainty	Unit
Pressure	Digiquartz	1072	10.10.2011	± 0.3	± 0.3	dbar
Temperature 0	SBE 3	4451	06.05.2019	± 0.005	± 0.1	°C
Temperature 1	SBE 3	5261	06.05.2019	± 0.005	± 0.1	°C
Conductivity 0	SBE 4	3722	06.05.2019	± 0.005	± 0.1	$\mathrm{ms\,cm^{-1}}$
Conductivity 1	SBE 4	2936	06.05.2019	± 0.005	± 0.1	$\mathrm{ms\,cm^{-1}}$
Oxygen 0	SBE 43	0644	15.06.2018	± 5	± 15	$\mu\mathrm{mol\,kg^{-1}}$
Oxygen 1	SBE 43	1732	15.11.2018	± 5	± 15	$\mu\mathrm{mol\,kg^{-1}}$
PAR/Irradiance		4381	06.09.1994	Uncertainty n.a.		-
SPAR		6321	Uncalibrated data			-
Fluorometer	ECO-AFL/FL	3274	27.09.2013	Uncertainty n.a.		$\mathrm{mg\,m^{-3}}$
Turbudity	ECO-NTU	3274	27.09.2013	Uncertainty n.a.		NTU

Table 1: Uncertainty and calibration information regarding the individual sensors used on the CTD.

2 Quality monitoring during data acquisition

During the cruise, the CTD sensors were checked by comparison measurements for oxygen concentration. Temperature and conductivity data were monitored by comparing both sensor groups. The differences between primary and secondary sensors were continuously monitored to discover sensor failures.
Furthermore, the pressure sensor has been compared on deck against air pressure measurements from the weather station of the ship. The differences where found to be below the uncertainty of 0.3 dbar.
Thus, we rely on the calibrations of our temperature, conductivity and pressure sensors by the accredited calibration lab of the Institute for Baltic Sear Research in Warnemünde, Germany. The calibration dates are shown in Table 1. Accordingly, no correction of the recorded temperature and conductivity data has been applied during post processing. Furthermore, the stability of the internal frequency generator of the CTD has been checked by an external frequency source at the start of each profile. During the entire cruise no drift was observed.
A first visual check of the recorded data showed a better quality on the first data channel. Accordingly, Temperature 0, Conductivity 0 and Oxygen 0 are used for the final dataset.

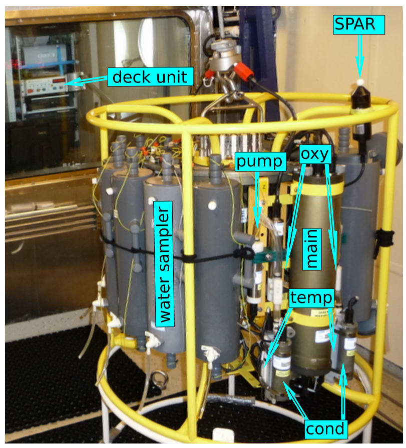


Figure 1: Picture of the CTD 911plus system aboard RV Elisabeth Mann Borgese. The second train of sensors is partly hidden by the main housing. Image courtesy of Johann Ruickoldt, IOW.

3 Sensor field calibration

Usually, sensors for oxygen concentration depict a significant drift on large time scales. Thus, they have to be calibrated by reference measurements.
Slope and offset of the oxygen sensors SBE 43 were determined using water samples taken at each cast. The oxygen content of the samples was retrieved with a titration set (Winkler method, accuracy of $0.9\mu\mathrm{mol\,kg^{-1}}$). The ratio between the oxygen sensors and all valid Winkler values were calculated in order to correct the slope. This ratio was constant over the entire cruise, so a

Quantity	Derived from	Method	Uncertainty
Depth	Pressure, latitude	Seabird	$\pm 0.3\,\mathrm{m}$
Practical salinity	Conductivity, temperature, pressure	Seabird	$\pm 0.006\,\mathrm{PSU}$

Table 2: Information on derived quantities including error estimates.

constant factor was used to correct the slope of the oxygen sensor. As we use the primary sensor channel only, we will limit the discussion to the data of *Oxygen 0*.
The coefficient of determination of the regression $r^2 = 0.9996$ and the correction factor for the oxygen values is 1.0378 (Figure 2). Oxygen concentrations are calculated using Seabird's *Seasoft*, oxygen formula *Sea-Bird* as described in Sea-Bird Scientific (2017a, p. 64).
A summary of the applied calibration coefficients and remaining uncertainties is given in Table 1. For our error estimation, we separate uncertainties of the sensors and uncertainties of the whole measurement system. The former are given in Column 5 of Table 1. Under unfavourable circumstances, the latter can be 20 times as high as the sensor uncertainties. This is the case, because there is a wake of water masses behind the sonde. This wake drags water from lower depths to higher dethps. Due to ship heave, the descent rate of the sonde typically varied by $\pm 0.5\,\mathrm{m}s^{-1}$, while the typical average descent rate was between $0.3\,\mathrm{m}s^{-1}$ and $1\,\mathrm{m}s^{-1}$ during M157. Due to the inertia of the wake behind the sonde the sensors become immersed in the trailing wake when the descent speed reduces as part of the ship heave cycle. This is counteracted by the *loopRem* post processing software module. It removes part of the descent, where wake effects are to be expected (please the enumeration of post processing routines in Section 4 for details).

4 Data post processing

The data post processing has been done using the software package *SBE Data Processing*, Version 7.26.7. In the course of this procedure, the corrections described in Section 3 have been applied. The details of the data processing software are described in Sea-Bird Scientific (2017a).
The first CTD cast of M157 (M157_6) hat to be removed from the dataset due to unidentified differences between both temperature sensors in the order of 1 K. During post processing water depth and practical salinity were calculated from the measured quantities (Table 2). Unfortunately, Seabird does not disclose the formula they use for depth retrieval. Therefore, the uncertainty does not include possible systematic errors inherent to the derivation scheme.
In addition to the derivation of variables that cannot be measured directly, corrections and filter functions have been applied to the measured data in order to suppress typical error sources of CTD measurements. Below, these subsequently applied post processing modules of the *SBE Data Processing* software are listed with a short description. If not noted otherwise, each module has been applied to every variable.
These routines have been applied twice: in the first run, no bin averaging was done. Afterwards, the IOW routine *magicEye* was used to find outliers in the data as described below. These outliers have then been removed during the second run before applying the other routines.

datcnv: Conversion of CTD raw data to physical units.

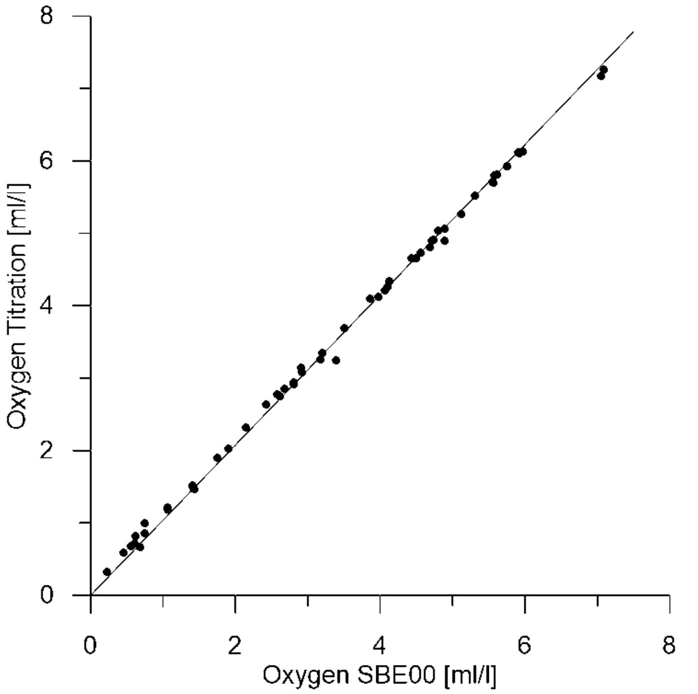
magicEye (2nd): IOW specific software for manual inspected for obvious outliers or sensor failures, which were set to *bad_flag* (-9.990e-29). This includes parts with differences between both sensor chains larger than their uncertainty due to pumping issues and loops in the data due to the missing ship heave compensation. It has been done to ensure the continuing usability of the data according to IOW's data policy given in: Leibniz Institute for Baltic Sea Research Warnemünde (2018).

airpress: IOW specific software to correct the sea pressure data for air pressure deviations from the standard sea-level pressure (1013.25 hPa).

wildedit: Find outliers using a statistical approach. In a first run, acquire the standard deviation of the data in blocks of 50 data points. Flag all data as outliers that exceed three standard deviations from the mean. Then recalculate the standard deviation without the outliers in a

M157

Correlation between the SBE43 oxygen Sensor 0 (Sbeox0ML/L) and water samples



Fit Results

Fit 1: Through origin
Equation Y = 1.037840884 * X
Number of data points used = 57
Average X = 3.27882
Average Y = 3.42886
Residual sum of squares = 0.383939
Coef of determination, R-squared = 0.999552
Residual mean square, sigma-hat-sq'd = 0.00685606

Figure 2: Calibration regression of the primary oxygen sensor. Measured values of the SBE34 are shown against values from the Winkler titration.

second run. Additionally, flag all data as outliers that exceed ten standard deviations from the mean.

wfilter: Filter used for spike removal and data smoothing. For pressure, temperature conductivity, oxygen concentration and salinity a moving Gaussian window with a half width of 24 data points has been used. On all other data channels a running median with a window length of 5 data points has been used. During this process, flagged outliers are not considered.

alignctd: Align several measurements on the CTD with respect to pressure. This module may correct height differences in the CTD frame and/or different time constants of the sensors. Due to the pumping system described above, only an advance of oxygen measurements by one second was needed to correct for the time delay caused by the longer path of the pumped water to this sensor.

loopRem: IOW specific software to remove data that are affected by the sonde's wake. This happens for example when the vertical velocity is reversed due to ship heave ("loops in the data"). Due to strong ship heave on cruise M157 we cut away all data, where the vertical velocity is below the mean velocity. The mean velocity is calculated with a third order butterworth low-pass filter with a cut-off length of 30 s. The removal is subject to a time delay of 1.1 s in order to account for the time it takes for the wake water to reach the sensors.

celltm: Correct conductivity data for the thermal mass of the sensor. This includes an amplitude correction by $\alpha = 0.03$ and a correction for the time constant of $\tau = 9$ for both conductivity sensors. For further information on the formulae used for the correction please see Sea-Bird Scientific (2017a).

binavg (2nd): Reduce data resolution by binning. In the case of M157, bins are formed according to pressure and time with a bin size of 0.1 dbar, 0.25 dbar, 1 dbar, and 1 s, respectively. The surface bin has not been included in the data.

References

Leibniz Institute for Baltic Sea Research Warnemünde: IOW Data Policy, URL `https://www.io-warnemuende.de/data-policy.html`, accessed: 08-02-2022, 2018.

Sea-Bird Scientific: Application note No14: 1978 Practical Salinity Scale, URL `https://www.seabird.com/asset-get.download.jsa?id=54627861526`, accessed: 09-02-2022, 1989.

Sea-Bird Scientific: Manual: SBE 9plus CTD, URL `https://www.seabird.com/asset-get.download.jsa?id=54627861544`, accessed: 09-02-2022, 2015.

Sea-Bird Scientific: Application note No 42: ITS-90 Temperature Scale., URL `https://www.seabird.com/asset-get.download.jsa?id=54663149001`, accessed: 09-02-2022, 2016.

Sea-Bird Scientific: Seasoft V2: SBE Data Processing, URL `https://www.seabird.com/asset-get.download.jsa?code=251446`, accessed: 09-02-2022, 2017a.

Sea-Bird Scientific: Seasoft V2: Seasave V7, CTD Real-Time Data Acquisition Software for Windows, URL `https://www.seabird.com/asset-get.download.jsa?code=251445`, accessed: 07-02-2022, 2017b.