

Continuous thermosalinograph oceanography along RV POLARSTERN cruise track PS128

Data Processing Report

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1 Introduction

This report describes the processing of raw data acquired by the thermosalinographs on board RV Polarstern during expedition PS128 to receive cleaned up and corrected salinity data. Detailed description of the processing of the data and the workflow is given in “General processing report of continuous thermosalinograph oceanography from RV POLARSTERN expeditions: PS127, PS128, PS129, PS130_1 and PS130_2”.

Cruise details

Vessel name:	RV Polarstern
Expedition number:	PS128
Expedition leader:	Tiedemann, Ralf
Expedition start:	2022-01-06 , Cape Town
Expedition end:	2022-02-28 , Cape Town
Duration:	53 days
BSH ID:	20210061
Expedition report:	https://www.pangaea.de/expeditions/bybasis/Polarstern
Expedition map:	https://www.awi.de/fileadmin/user_upload/MET/PolarsternExpeditionMaps/PS128.png
Event list:	https://www.pangaea.de/expeditions/events/PS128

2 Sensor Details

Following sensors were installed during cruise PS128. Only data from **TSG1** are uploaded to PAN-GAEA for cruise PS128 and are furthermore considered in this report (for reasoning see General Processing Report). Find calibration sheets for **TSG1** in the appendix of this document.

Table 1: Sensor details during PS128

	TSG1	TSG2
Serial number	SBE21-3189	SBE21-3354
Installation	2021-12-04	2021-12-04
Deinstallation	2022-05-31	2022-05-31
Days installed	178	178
External temperature sensor	SBE38-0137	SBE38-0154

3 Processing Report

Database Extraction

Table 2 shows the number of data and other details from the DShip database extraction.

Table 2: Details of database extraction

Data source	DSHIP database (dship.awi.de)
Start of raw file	2022-01-06T04:00:00
End of raw file	2022-02-28T03:59:59
Number of lines in hexadecimal raw file	1307226
First dataset	2022-01-07T08:31:01
Last dataset	2022-02-28T03:26:30
TSG1 valid data	1090242

Calculation of 1 minutes means

The calculation of 1 minutes means included the removal of outliers outside a 2-times standard deviation for each data interval. The number of outliers for each parameter are given Table 3.

Table 3: Number of outliers removed from calculation of 1 minutes means

Number of outliers >2*std	
Internal temperature	28612
Conductivity	27231
External temperature	30592
Salinity	31604
Result after outlier removal	
Number of 1 minute means	72223

Manual flagging

After processing the data were visually inspected. The whole data from a specific timestamp were deleted if there was only one parameter to be manually flagged. 4 data points were manually removed from the TSG1 dataset of PS128.

Assigning navigational data

Data from the corrected mastertrack of PS128 were assigned to the 1 minute means of the TSG dataset. Only TSG data with available coordinates were kept. Thus, gaps in the navigation file result in gaps in the TSG dataset. See Figure 1 and Figure 2 for the processed and corrected data of TSG1. **Number of TSG data without navigational data: 1**

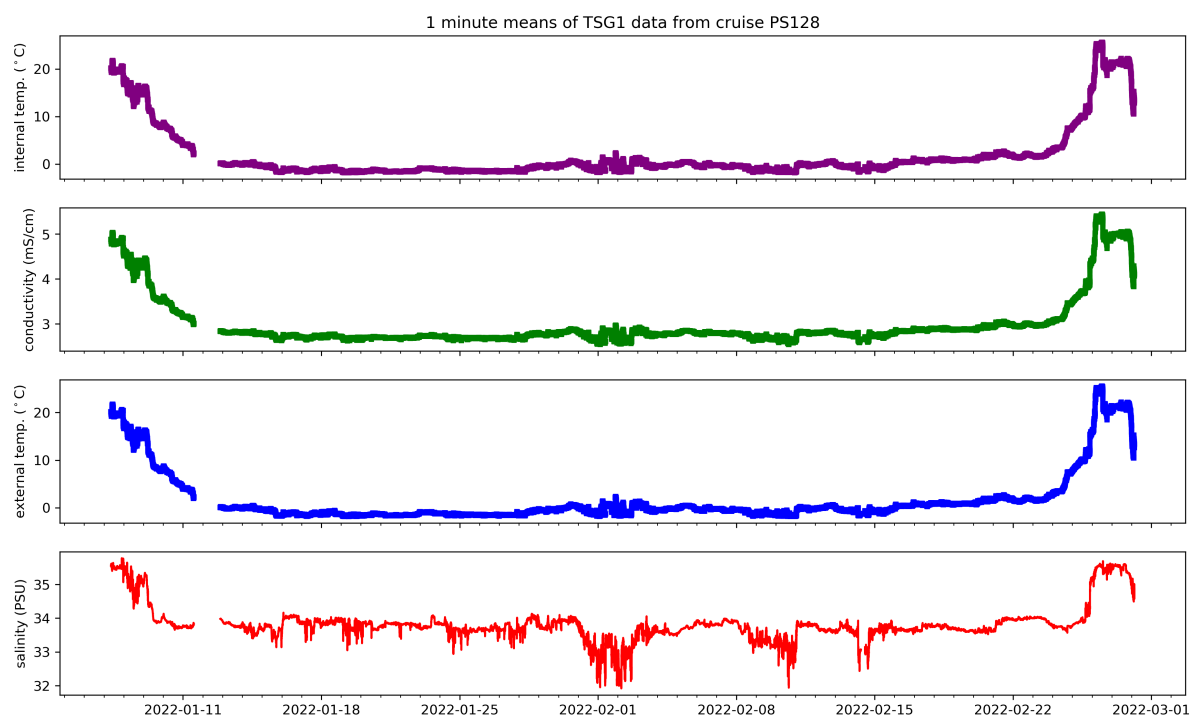


Figure 1: 1 minutes means of data from TSG1

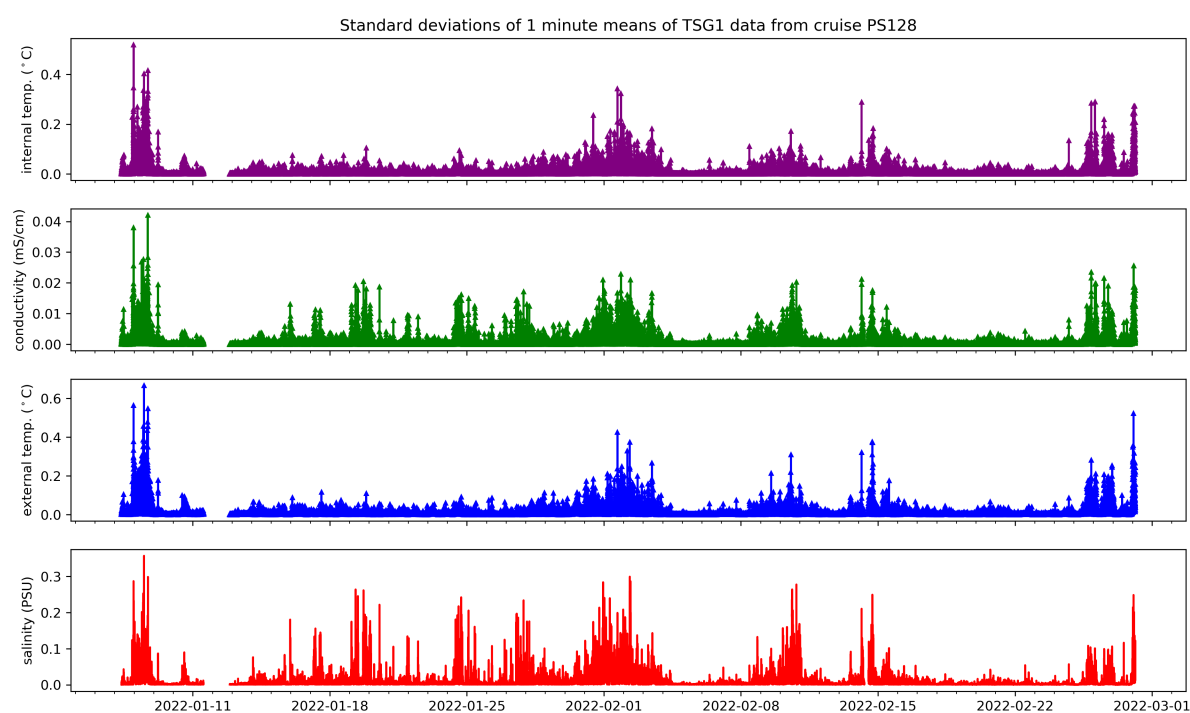


Figure 2: Standard deviations of 1 minutes means of data from TSG1

Differences between internal and external temperature of TSG1 temperature sensors

Temperature differences between the internal and the external temperature sensors have to be small under normal circulation conditions. Means and standard deviations for the temperature differences as well as the number of data with a difference larger than 1 °C are given in Table 4 and are shown in Figure 3.

Table 4: Means and standard deviations of the difference between internal and external temperature for the spot values and the 1 minutes means of TSG1 .

	TSG1 temperature difference	
	mean \pm standard dev.	no. > 1 °C
Spot values	0.0347 \pm 0.0274 °C	15
1 min means after manual flagging	0.0347 \pm 0.0175 °C	0

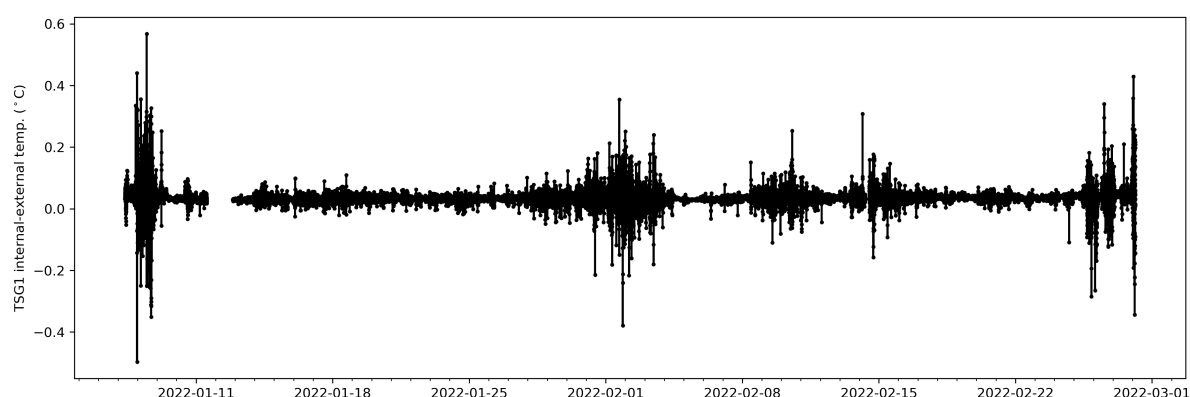


Figure 3: Differences between internal and external temperature sensors of TSG1

Result file

The result file is a plain tab-delimited text file named **PS128_surf_oce.tab** in which each row represents a 1 minute mean. This file does not include any timestamps in which no TSG data are available, resulting in a number of gaps in the time vector. After manual despiking and clipping to the mastertrack, **2358** minutes distributed over **10** gaps are missing between the start and the end of the valid dataset. Salinity values are calculated from the 1 minute means of conductivity and internal temperature data, assuming a constant pressure of 11 dbar for the calculations. The pressure refers to the 11 m water depth of the water inlet of the TSG system on RV Polarstern. Water temperature taken from the TSG1 external temperature sensor is given for reference. Table 5 shows a summary of the data during processing.

Table 5: Number of records in result file

Summary data	
Number of 1 minute mean values	72223
Number of manually removed data	4
Number of missing 1 minute values because of gaps in mastertrack	1
Result after processing	
Number of 1 min means in result file PS128_surf_oce.tab	72218

Table 6: Structure of PS128_surf_oce.tab result file

Column separator	Tabulator "\t"
Column 1	Date and time expressed according to ISO 8601
Column 2	Latitude in decimal format, unit degree
Column 3	Longitude in decimal format, unit degree
Column 4	Water Temperature, unit degree celsius
Column 5	TSG Internal Temperature, unit degree celsius
Column 6	Conductivity, unit mS/cm
Column 7	Salinity, PSU
Column 8	Quality flag of water temperature
Column 9	Quality flag of salinity

Quality control: Global range, spike and gradient test

The time series of external temperature and salinity were checked and flagged after passing several quality control (QC) tests. These tests follow the "SeaDataNet Data Quality Control Procedures (version from May 2010)" (<https://www.seadatanet.org/Standards/Data-Quality-Control>) and include a global range test, a spike and a gradient test. The flagging scheme is also taken from SeaDataNet (see Table 7 and Table 8). Initially, all 1 minute records receive the flag "0". After passing the global range test, records get the flag "2". To the values which did not pass this test, the flag "4" is assigned. Values, which did not pass the spike or the gradient test, obtain the flag "3". During these tests, all values are compared with their adjacent records. Values, which do not have adjacent records (e.g. gaps in the time series), the flag "2" is assigned. Because two TSG are running on RV Polarstern simultaneously, TSG data are validated by comparison with the second TSG. If the comparison shows good accordance between both TSG the quality flag "1 - good" is assigned to the data of the uploaded TSG.

Spike test: Test value = $|V_2 - (V_3 + V_1)/2| - |(V_3 - V_1)/2|$

Gradient test: Test value = $|V_2 - (V_3 + V_1)/2|$

$V2 \triangleq$ value tested as a spike/gradient

$V1, V3 \triangleq$ previous and next value

Table 7: Meaning of quality control flags

Key	Term	Definition
0	no QC	no QC has been applied
1	good	good quality data which has been verified
2	probably good	good quality data which has not been verified
3	probably bad	data value which is obviously inconsistent to the phenomenon
4	bad	obviously erroneous
5	not used	
6	not used	
7	not used	
8	interpolated	value derived by interpolation
9	missing	value is missing

Table 8: Quality control test criteria

Test	Limiting criteria for temperature	Limiting criteria for salinity
Globale range check	$-2.5^{\circ}\text{C} \leq T \leq 45^{\circ}\text{C}$	$0 \leq S \leq 60$
Spike test	test value must not exceed 6°C	test value must not exceed 0.9
Gradient test	test value must not exceed 9°C	test value must not exceed 1.5

Table 9: Results of quality control tests

Parameter	Global range	Spike test	Gradient test
Water temperature	0	0	0
Salinity	0	0	0

Comments

Data gaps are caused by system maintenance, system shutdown during harbour time, gaps in the navigation file, outlier removal or manual flagging.

Data gaps longer than 5 minutes are found in following time intervals:

- 11/01/2022 13:14 to 12/01/2022 21:18
- 19/01/2022 02:57 to 19/01/2022 04:15
- 01/02/2022 08:44 to 01/02/2022 09:19

- 14/02/2022 07:23 to 14/02/2022 12:16
- 27/02/2022 11:03 to 27/02/2022 11:09
- 27/02/2022 11:10 to 27/02/2022 11:32

4 Appendix

Salinity data from Polarstern cruise PS128
SBE21-3189 (TSG1)

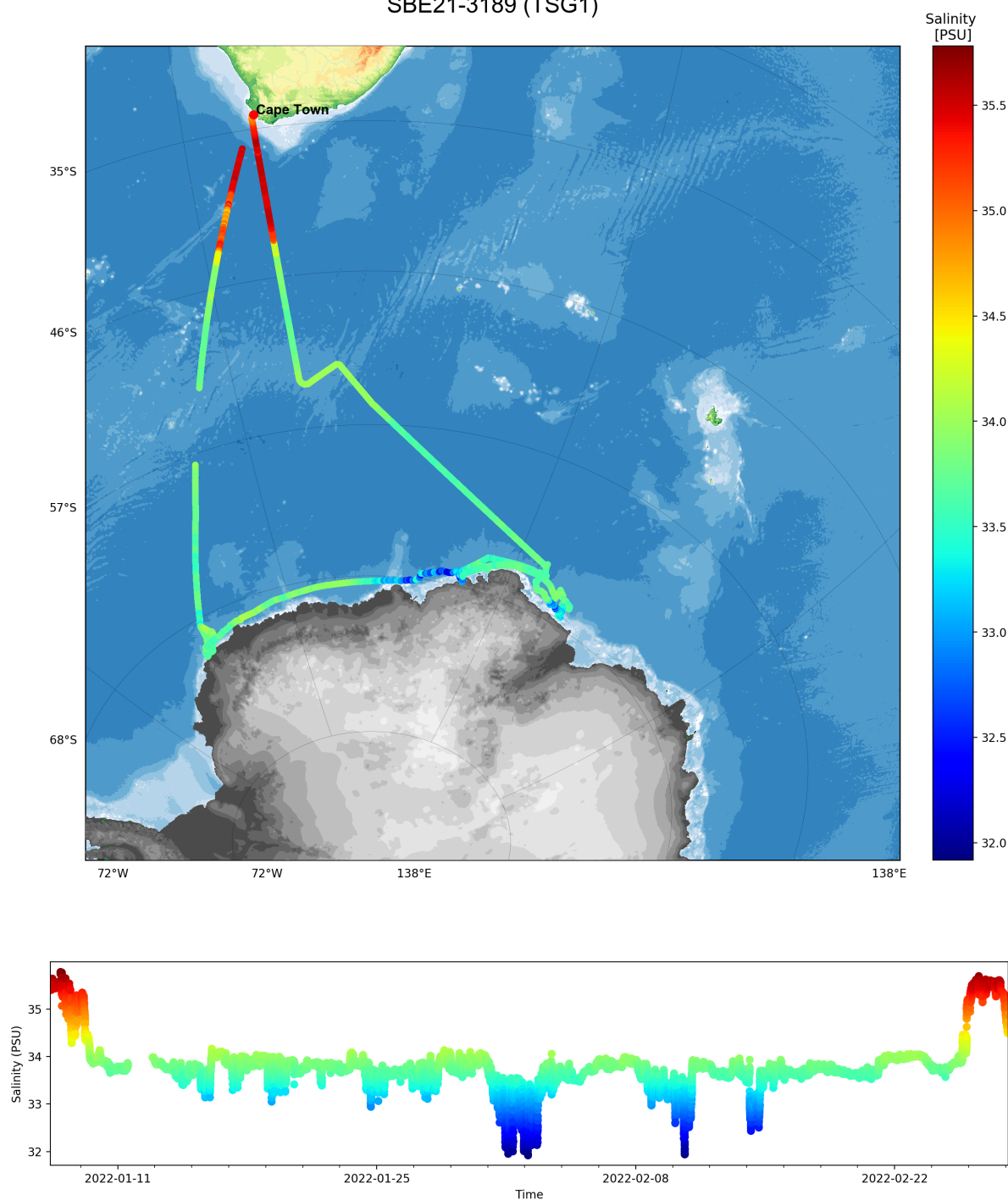


Figure 4: Salinity data from TSG1

Water temperature from Polarstern cruise PS128
SBE38-0137 (TSG1)

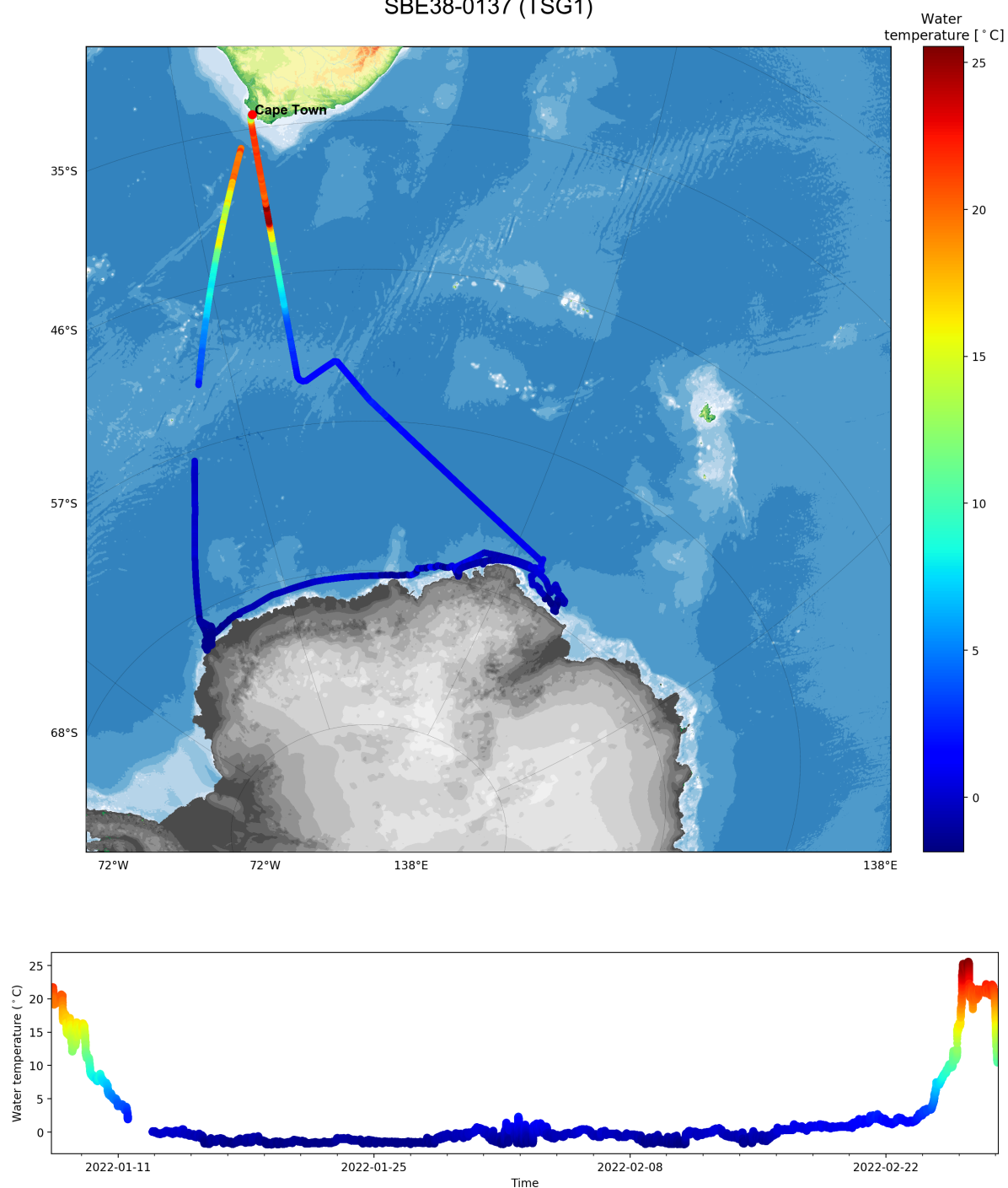


Figure 5: Temperature data from TSG1



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SENSOR SERIAL NUMBER: 3189
CALIBRATION DATE: 09-Feb-21

SBE 21 TEMPERATURE CALIBRATION DATA ITS-90 TEMPERATURE SCALE

COEFFICIENTS:

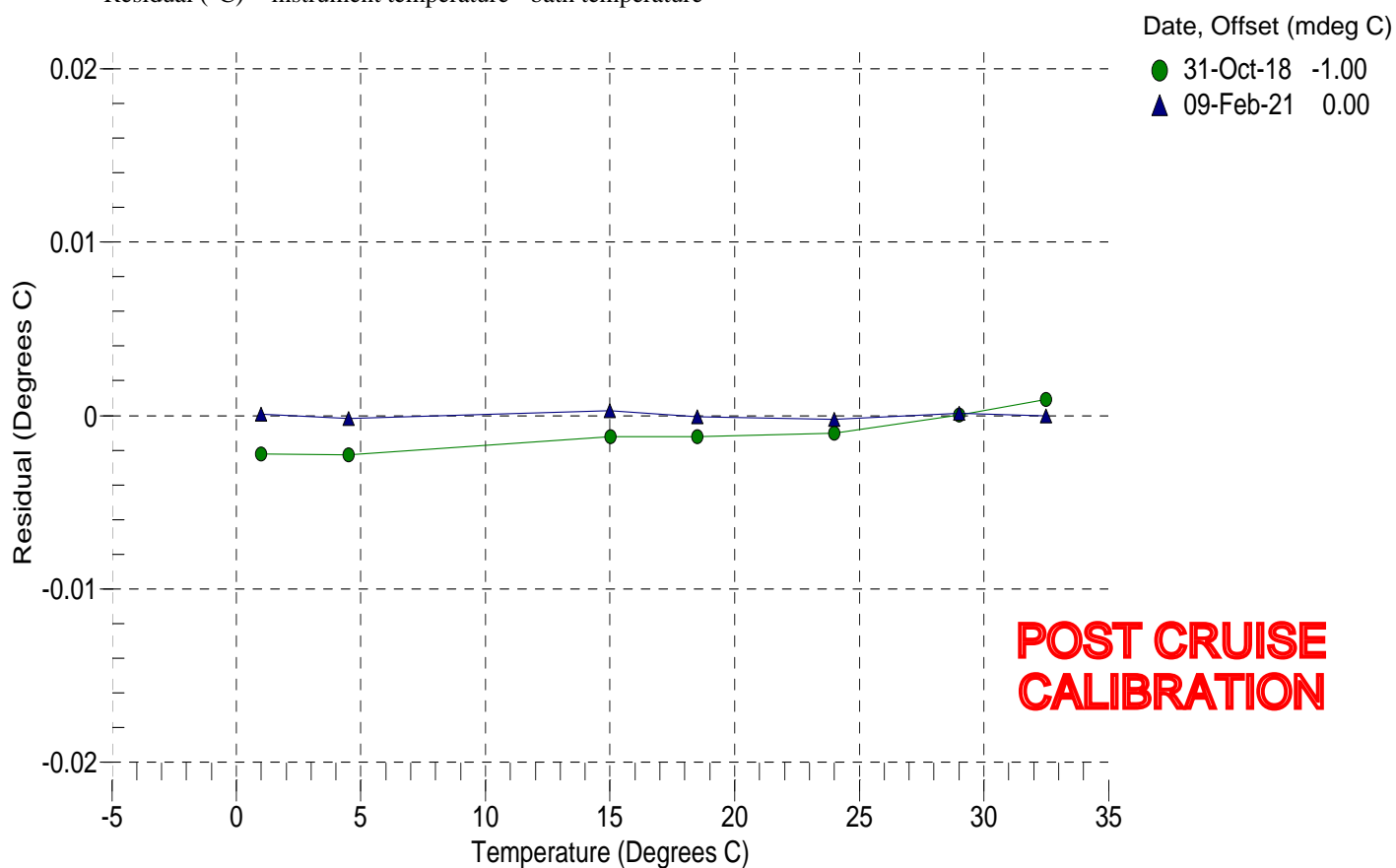
$g = 4.19418916e-003$
 $h = 6.20233385e-004$
 $i = 1.86827067e-005$
 $j = 1.31098627e-006$
 $f0 = 1000.0$

BATH TEMP (° C)	INSTRUMENT OUTPUT (Hz)	INST TEMP (° C)	RESIDUAL (° C)
1.0000	2470.134	1.0001	0.00010
4.5000	2670.861	4.4998	-0.00019
14.9999	3343.828	15.0002	0.00028
18.5000	3592.804	18.4999	-0.00010
24.0000	4010.215	23.9998	-0.00021
29.0000	4418.325	29.0001	0.00015
32.5000	4720.662	32.5000	-0.00003

f = Instrument Output (Hz)

Temperature ITS-90 (°C) = $1 / \{g + h[\ln(f0 / f)] + i[\ln^2(f0 / f)] + j[\ln^3(f0 / f)]\} - 273.15$

Residual (°C) = instrument temperature - bath temperature





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SENSOR SERIAL NUMBER: 3189
CALIBRATION DATE: 09-Feb-21

SBE 21 CONDUCTIVITY CALIBRATION DATA
PSS 1978: C(35,15,0) = 4.2914 Siemens/meter

COEFFICIENTS:

g = -4.30704390e+000
h = 5.08195165e-001
i = -2.87506572e-004
j = 4.08729109e-005

CPcor = -9.5700e-008 (nominal)
CTcor = 3.2500e-006 (nominal)

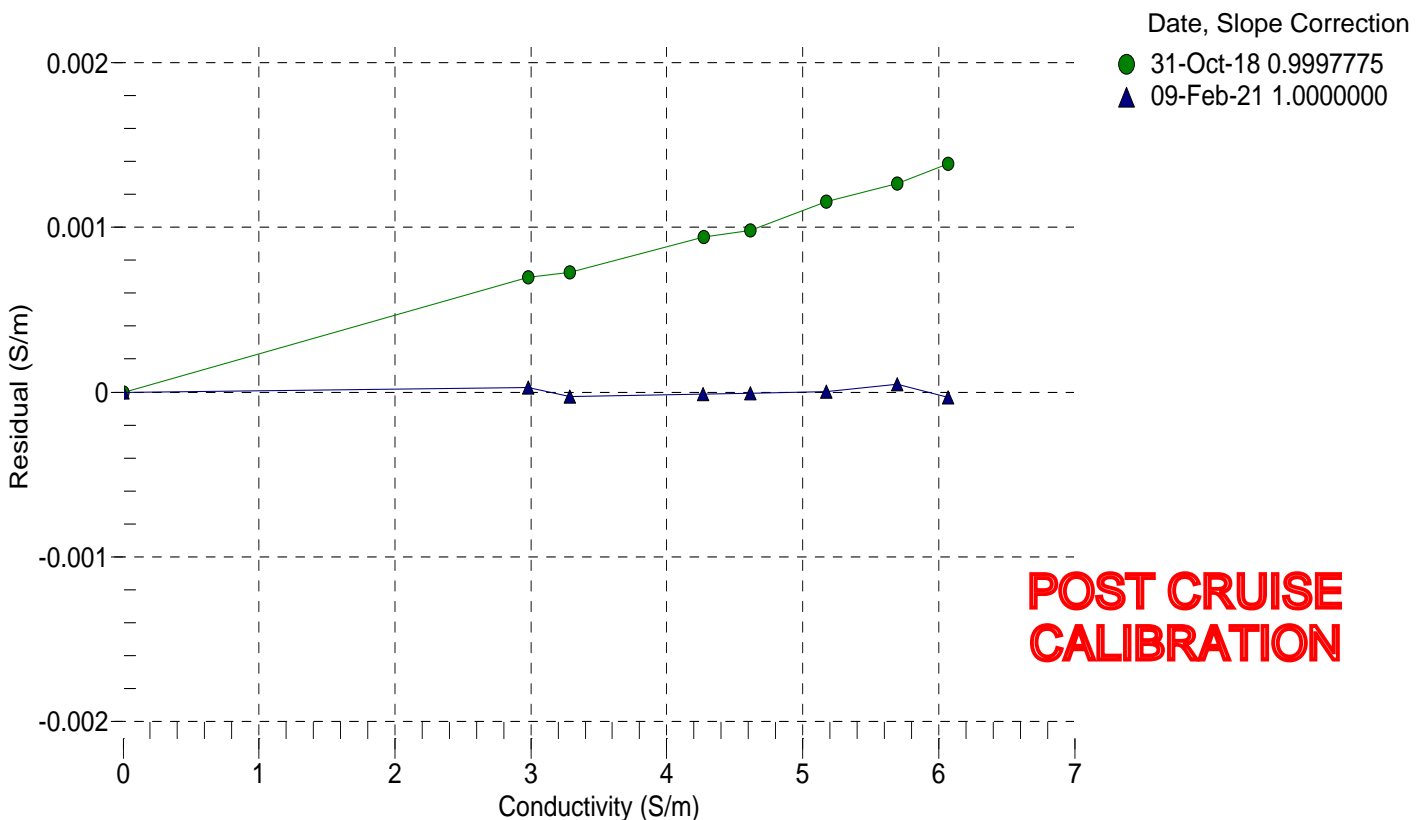
BATH TEMP (° C)	BATH SAL (PSU)	BATH COND (S/m)	INSTRUMENT OUTPUT (kHz)	INSTRUMENT COND (S/m)	RESIDUAL (S/m)
22.0000	0.0000	0.00000	2.91262	0.00000	0.00000
1.0000	34.8561	2.97904	8.18810	2.97907	0.00003
4.5000	34.8361	3.28641	8.54797	3.28638	-0.00003
14.9999	34.7930	4.26905	9.60727	4.26903	-0.00001
18.5000	34.7832	4.61445	9.95238	4.61445	-0.00001
24.0000	34.7720	5.17276	10.48571	5.17277	0.00000
29.0000	34.7645	5.69479	10.96038	5.69483	0.00005
32.5000	34.7592	6.06716	11.28636	6.06713	-0.00003

f = Instrument Output (kHz)

t = temperature (°C); p = pressure (decibars); δ = CTcor; ϵ = CPcor;

Conductivity (S/m) = $(g + h * f^2 + i * f^3 + j * f^4) / 10 (1 + \delta * t + \epsilon * p)$

Residual (Siemens/meter) = instrument conductivity - bath conductivity





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SENSOR SERIAL NUMBER: 3189
CALIBRATION DATE: 05-Jul-22

SBE 21 TEMPERATURE CALIBRATION DATA
ITS-90 TEMPERATURE SCALE

COEFFICIENTS:

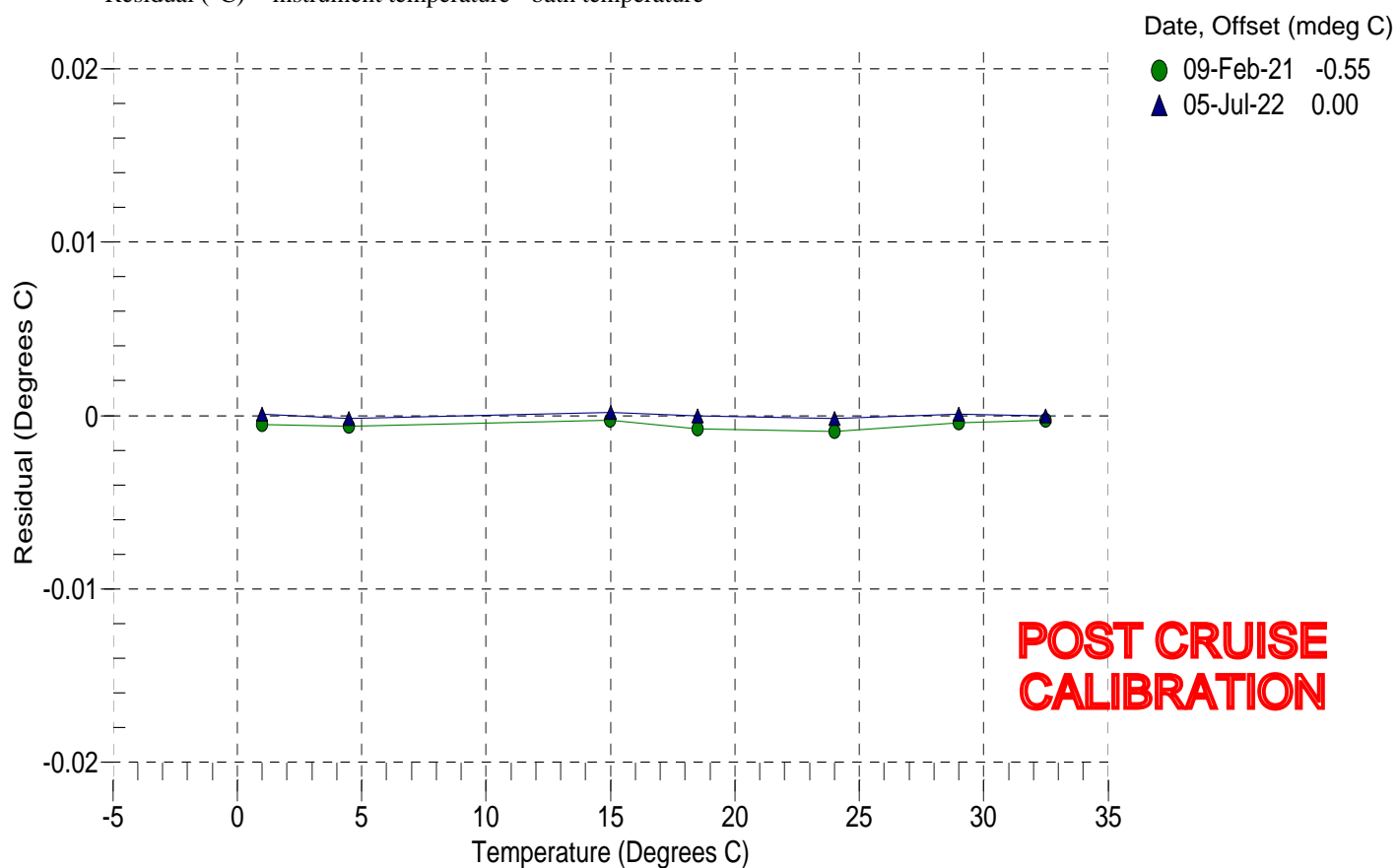
$g = 4.19460189e-003$
 $h = 6.21277186e-004$
 $i = 1.95623982e-005$
 $j = 1.55419974e-006$
 $f0 = 1000.0$

BATH TEMP (° C)	INSTRUMENT OUTPUT (Hz)	INST TEMP (° C)	RESIDUAL (° C)
1.0000	2470.168	1.0001	0.00008
4.5000	2670.889	4.4998	-0.00016
15.0000	3343.868	15.0002	0.00019
18.5000	3592.858	18.5000	-0.00003
24.0000	4010.275	23.9998	-0.00018
29.0000	4418.368	29.0001	0.00010
32.5000	4720.684	32.5000	-0.00001

f = Instrument Output (Hz)

Temperature ITS-90 (°C) = $1 / \{g + h[\ln(f0 / f)] + i[\ln^2(f0 / f)] + j[\ln^3(f0 / f)]\} - 273.15$

Residual (°C) = instrument temperature - bath temperature





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SENSOR SERIAL NUMBER: 3189
CALIBRATION DATE: 05-Jul-22

SBE 21 CONDUCTIVITY CALIBRATION DATA
PSS 1978: C(35,15,0) = 4.2914 Siemens/meter

COEFFICIENTS:

g = -4.30872287e+000
h = 5.08754547e-001
i = -4.05195018e-004
j = 4.66093451e-005

CPcor = -9.5700e-008 (nominal)
CTcor = 3.2500e-006 (nominal)

BATH TEMP (° C)	BATH SAL (PSU)	BATH COND (S/m)	INSTRUMENT OUTPUT (kHz)	INSTRUMENT COND (S/m)	RESIDUAL (S/m)
22.0000	0.0000	0.00000	2.91243	0.00000	0.00000
1.0000	34.8343	2.97736	8.18643	2.97738	0.00002
4.5000	34.8143	3.28455	8.54628	3.28454	-0.00002
15.0000	34.7721	4.26676	9.60552	4.26676	-0.00000
18.5000	34.7634	4.61211	9.95065	4.61208	-0.00003
24.0000	34.7539	5.17037	10.48411	5.17039	0.00003
29.0000	34.7487	5.69249	10.95892	5.69253	0.00003
32.5000	34.7460	6.06512	11.28516	6.06509	-0.00003

f = Instrument Output (kHz)

t = temperature (°C); p = pressure (decibars); δ = CTcor; ϵ = CPcor;

Conductivity (S/m) = $(g + h * f^2 + i * f^3 + j * f^4) / 10 (1 + \delta * t + \epsilon * p)$

Residual (Siemens/meter) = instrument conductivity - bath conductivity

