DATA PRODUCT SPECIFICATION FOR WATER TEMPERATURE

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Document Control Sheet

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Signature Page

This document has been reviewed and approved for release to Configuration Management.

OOI Senior Systems Engineer: ____________________

Date:2012-01-13

This document has been reviewed and meets the needs of the OOI Cyberinfrastructure for the purpose of coding and implementation.

OOI CI Signing Authority: ____________________

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Table of Contents

1 Abstract

This document describes the computation used to calculate the OOI Level 1 Water Temperature data product, which is calculated using data from the Sea-Bird Electronics conductivity, temperature and depth (CTD) family of instruments. This document is intended to be used by OOI programmers to construct appropriate processes to create the L1 water temperature product.

2 Introduction

2.1 Author Contact Information

Please contact Lorraine Heilman (lheilman@oceanleadership.org), Sarah Webster (swebster@oceanleadership.org) or the Data Product Specification lead (DPS@lists.oceanobservatories.org) for more information concerning this document.

2.2 Metadata Information

2.2.1 Data Product Name

The OOI Core Data Product Name for this data product is

- TEMPWAT

The OOI Core Data Product Descriptive Name for this data product is

- Water temperature

2.2.2 Data Product Abstract (for Metadata)

The OOI Level 1 Water Temperature data product is computed by converting raw hexadecimal temperature data from the conductivity, temperature and depth (CTD) family of instruments into °C.

2.2.3 Computation Name

Not required for data product algorithms.

2.2.4 Computation Abstract (for Metadata)

This algorithm computes the OOI Level 1 Water Temperature data product, which is calculated by converting raw hexadecimal temperature data from the conductivity, temperature and depth (CTD) family of instruments into °C.

2.2.5 Instrument-Specific Metadata

There are no instrument-specific metadata that need to be added for the algorithm.

2.2.6 Synonyms

Synonyms for this data product are

- Temperature
- Water Temperature
- *In situ* Water Temperature
- ITS-90 Water Temperature

2.2.7 Similar Data Products

Prior to 1990, when the ITS-90 standard was adopted (Sea-Bird App Note 42, 2010), a different calibration, the IPTS-68 standard, was in use. The relationship between T_90 and T_68 is a simple, linear one (T_68 = 1.00024 * T_90).

2.3 Instruments

The CTD Processing Flow document (DCN 1342-00001) describes the instrument classes and make/models that produce the data from which the L1 temperature data product is calculated. This document also describes the flow of data from the CTDs through all of the relevant QC, calibration, and data product algorithms.

Note that the raw data from the GPCTD make/model—the CTDs on board the gliders and autonomous underwater vehicles (AUVs)—are processed onboard the vehicles with proprietary software from the vehicle vendors. These data are presented already in decimal format in appropriate units (°C, Siemens/meter, decibars), therefore processing raw hexadecimal data from the CTDGP is not included in the algorithm described in this document.

Please see the Instrument Application in the SAF for specifics of instrument locations and platforms.

2.4 Literature and Reference Documents

IOC, et al. (2010). The international thermodynamic equation of seawater-2010: Calculation and use of thermodynamic properties, UNESCO.

Sea-Bird (2009), SBE 16*plus* V2 SEACAT User's Manual. Manual Version #005.

Sea-Bird (2011), SBE 37-IM MicroCAT User's Manual. Manual Version #027.

Sea-Bird (2010), Application Note 42. ITS-90 Temperature Scale. Revision February 2010. Sea-Bird Electronics, Inc..

Sea-Bird (2010), Application Note 31. Computing Temperature and Conductivity Slope and Offset Correction Coefficients from Laboratory Calibrations and Salinity Bottle Samples. Revision February 2010. Sea-Bird Electronics, Inc..

2.5 Terminology

2.5.1 Definitions

The following terms are defined here for use throughout this document. Definitions of general OOI terminology are contained in the Level 2 Reference Module in the OOI requirements database (DOORS).

Potential temperature: "Potential temperature is the temperature that a fluid parcel would have if its pressure was changed to a fixed reference pressure in an isentropic and isohaline matter." (IOC et al, 2010)

2.5.2 Acronyms, Abbreviations and Notations

General OOI acronyms, abbreviations and notations are contained in the Level 2 Reference Module in the OOI requirements database (DOORS).). The following acronyms and abbreviations are defined here for use throughout this document.

ITS-90 International Temperature Scale of 1990

2.5.3 Variables and Symbols

The following variables and symbols are defined here for use throughout this document.

T_L1, T_90	L1 temperature data product, using the ITS-90 temperature scale
t_{dec}, `t_dec`	instrument temperature data in decimal
t_{hex}, `t_hex`	instrument temperature data in hexadecimal
T_68	Temperature calculated using the older IPTS_68 temperature scale (not used for the OOI Water Temperature data product)
a0,a1,a2,a3	calibration coefficients

3 Theory

3.1 Description

Water temperature is one of the variables directly measured by CTD instruments and is calculated from the raw hexadecimal data provided by the instrument. The SBE 16plusV2 model will output “raw frequencies and voltages in hexadecimal" as it is referred to in the Sea-Bird manuals. The 37IM model will output “engineering units in hexadecimal". The hexadecimal string is converted to decimal and scaled according to the CTD manual (different for each CTD make/model). Conversion and scaling (described herein) results in water temperature in °Celsius.

Note that which temperature standard to use (IPTS-68 or ITS-90) is an option on the Sea-Bird CTDs, and all OOI CTDs are set to use the ITS-90 standard (Sea-Bird 2010, App Note 42).

3.2 Mathematical Theory

The CTD is received by OOI calibrated from Sea-Bird before its initial deployment. Post-initial deployment calibration checks and/or recalibrations will be performed at Sea-Bird. This is done using the ITS-90 temperature standards, which have been in use by Sea-Bird since 1995. The calibrated temperature is scaled into an efficient, memory-saving hexadecimal string aboard the CTD instrument. This hexadecimal string, after it is separated from the rest of the data stream by the CTD driver, is the L0 temperature data product. The parsing instructions for the instrument hexadecimal string can be found in Appendix A.

The L1 temperature data product algorithm takes the L0 temperature data product and converts it into °Celcius (°C). Once the hexadecimal string is converted to decimal, the following steps are necessary to produce the correct decimal representation of the data in °Celsius. The conversion function differs by CTD make/model as described below.

SBE 16plus V2, Output Format 0 (running either its native firmware or the 19plus V2 firmware)

1) Standard conversion from 6-character hex string (t_{hex}) to decimal (t_{dec})
2) Calculate MV: MV = (t_{dec} – 524288) / 1.6e+007
3) Calculate R: R = (MV * 2.900e+009 + 1.024e+008) / (2.048e+004 – MV * 2.0e+005)
4) Calculate T_L1: T_L1 [°C] = $1/(a0 + a1[\ln(R)] + a2[\ln^2(R)] + a3[\ln^3(R)]) – 273.15$

where a0, a1, a2, and a3 are calibration coefficients provided on individual instrument calibration sheets and stored as metadata.

SBE 37IM, Output Format 0

1) Standard conversion from 5-character hex string (t_{hex}) to decimal (t_{dec})
2) Scaling: T_L1 [°C] = (t_{dec} / 10,000) - 10

3.3 Known Theoretical Limitations

None.

3.4 Revision History

No revisions to date.

4 Implementation

4.1 Overview

The conversion from the L0 temperature data product to the L1 temperature data product consists of a simple conversion from hex to decimal and a scaling operation. Existing code to perform these operations is not available, but modified examples from the CTD manuals are provided herein.

4.2 Inputs

Inputs

- L0 Water Temperature as a hexadecimal string
- a0, a1, a2, a3 calibration coefficients (from instrument calibration sheets, retrieved from metadata)

Input Data Formats
The L0 temperature data product is a hexadecimal string, the number of digits varies by instrument make/model:

SBE 16plus V2 (Output Format 0) 6 character hex string
(applies to all 16plus V2, running either its native firmware or the 19plus V2 firmware)

SBE 37IM (Output Format 0) 5-character hex string

4.3 Processing Flow

The specific steps necessary to create all calibrated and quality controlled data products for the CTD are described in the CTD Processing Flow document (DCN 1342-00001). This processing flow document contains a flow diagram showing all of the specific algorithms (data product and QC) necessary to compute all data products from the CTD and the order that the algorithms must be applied.

The processing flow for the temperature algorithm code is as follows:

1) The algorithm input is the L0 temperature data product (t_hex).

2) Convert the hexadecimal string to a decimal number
   SBE 16plus V2 (running either its native firmware or the 19plus V2 firmware)
   Convert 6-character hex string (t_hex) to decimal (t_dec)

   SBE 37IM
   Convert 5-character hex string (t_hex) to decimal (t_dec)

3) Convert from counts to Celcius
   SBE 16plus V2 (running either its native firmware or the 19plus V2 firmware)
   L1 temperature data product (in °C):
   a) Calculate MV: MV = (t_dec – 524288) / 1.6e+007

b) Calculate R: $R = (MV * 2.900e{+}009 + 1.024e{+}008) / (2.048e{+}004 - MV * 2.0e{+}005)$

c) Calculate T_L1: $T\_L1 = 1/(a0 + a1[\ln(R)] + a2[\ln^2(R)] + a3[\ln^3(R)]) - 273.15$

where a0, a1, a2, and a3 are calibration coefficients provided on individual instrument calibration sheets and stored as metadata.

SBE 37IM

L1 temperature data product (in °C): T_L1 = (t_dec / 10,000) – 10

4) The final product is the L1 temperature data product in °C.

Examples taken from the CTD manuals are included in Appendix A.

4.4 Outputs

The outputs of the temperature algorithm are

- *In situ* water temperature in °C as a floating point number with four decimal places %.4f

The metadata that must be included with the output of this algorithm are

- There is no additional metadata that need to be included with this data product

See Appendix B for a discussion of the accuracy of the algorithm output.

4.5 Computational and Numerical Considerations

4.5.1 Numerical Programming Considerations

There are no numerical programming considerations for this algorithm. No special numerical methods are used.

4.5.2 Computational Requirements

Computation estimate not required for algorithms that are not computationally intensive.

4.6 Code Verification and Test Data Sets

The code will be verified using the test data set provided, which contains inputs and their associated correct outputs. CI will verify that the code is correct by checking that the temperature output, generated using the test data inputs, is identical to the test data temperature output.

A test data set below provides a few data points over the extent of the water column. It includes inputs and outputs.

A spreadsheet (CTD16plusv2_outputformat0_v2.xls) that can be used to verify all calculations for the 16plusV2 data is included with references in the DPS Artifacts folder on Alfresco, along with a copy of the 16plusV2 calibration sheet (SVE+16plusV2+SEACAT+RS232+SN+16P66805-6943.pdf): Alfresco (https://alfresco.oceanobservatories.org)
REFERENCE > Data product Specification Artifacts > 1341-00020_TEMPWAT

SBE 37-IM Test Data	
Inputs	**Output**
raw temperature in hex	Water Temperature [°C]
4E200	22
493E0	20
445C0	18
3F7A0	16
3A980	14
35B60	12
30D40	10
2BF20	8
27100	6
222E0	4
1D4C0	2
186A0	0

SBE 16plus V2 Test Data*

rawHex	L1_T (ITS-90 °C)	L1_C (S/m)	P (psi) interim calc.	L1_P (dbar)	thermistor T (°C)
0461FC0A609208064F591F	18.9288	0.005771	0.225	0.158	18.55
0461FD0A609208064F591F	18.9287	0.005771	0.225	0.158	18.55
0461FC0A609208064F591F	18.9288	0.005771	0.225	0.158	18.55
03CCC50A67860801B35E7B	22.4892	0.010898	-18.609	-12.828	23.76
03CADB0A67860801B35E82	22.5379	0.010898	-18.610	-12.828	23.79
03CA3D0A67830801B25E8B	22.5536	0.010890	-18.627	-12.840	23.82
03C8EC0A677E0801B35E9B	22.5872	0.010875	-18.613	-12.830	23.88
03C7F90A677C0801B25E91	22.6114	0.010869	-18.628	-12.841	23.84
03C63B0A677E0801B25E95	22.6559	0.010875	-18.628	-12.841	23.86
03BFBA199F150803D05EAD	22.8227	5.011614	-10.095	-6.957	23.95
03CA971987D70810225EEF	22.5447	4.969069	39.565	27.282	24.20
04E0FB1806AB08437C5D5E	16.2108	4.286307	246.510	169.965	22.68
0637351688F90883725798	9.9227	3.651432	504.146	347.599	17.07
0778CA156B7F08CED05130	4.9768	3.203659	807.345	556.648	10.83
07DF9415254B08F7984E66	3.5383	3.097099	971.188	669.613	8.11
08281415013E094EEE4B2C	2.5580	3.042976	1321.399	911.075	4.97

* This test data set applies for both SBE 16plus V2 running its native firmware and the 16plus V2 running the 19plus V2 firmware.

Note that the conductivity data were calculated using the temperature (in degrees C) and pressure (in dbar), both of which were calculated from the original rawHex. See the TEMPWAT DPS (DCN 1341-00010) and PRESWAT DPS (1341-00020) for more details.

Appendix A Example Data Processing

Following are three examples, one for each CTD make/model. These are examples modified from those provided in the CTD manuals.

SBE 16plus V2 with internally mounted strain gauge pressure sensor
(OutputFormat = 0)

Example: 16plus V2 with internally mounted strain gauge pressure sensor and 2 external voltages sampled,
Hex scan = ttttttccccccppppppvvvvssssssss
= 0A53711BC7220C14C17D820EC4270B

•EC4270B1BC7220C14C17D82internally mounted strain
temperature A/D counts = 676721
•emperature A/D counts = 0A5371 (676721 dec
conductivity frequency = 1820450 / 256 = 7111.133 Hz
•onductivity frequency = 1820450 / 256 = 7111.133 Hzuge pressure sensor and 2
Strain gauge pressure A/D counts = 791745
•train gauge pressure A/D counts = 791745ge pressuHzuge pressvvvv = 7D82 (32,130 decimal);
Strain gauge temperature = 32,130 / 13,107 = 2.4514 volts
•train gauge temperature = 32,130 / 13,107 = 2.4514
seconds since January 1, 2000 = 247,736,075

SBE 37IM with internally mounted strain gauge pressure sensor
(OutputFormat = 0)

Hex scan = tttttccccccppppTTTTTTTT
= 531850c355e50a805F0C14

- Temperature: ttttt = 53185 hex = 340357 decimal
  temperature (°C) = (ttttt / 10000) – 10 = (340357 / 10000) – 10 = 24.0357 °C
- Conductivity: ccccc = 0c355 hex = 50005 decimal
  conductivity (S/m) = (ccccc / 100000) – 0.5 = (50005 / 100000) – 0.5 = 0.00005 S/m
- Pressure range: From file header (metadata for OOI), the pressure range is 1000 psia.
  P_range (dbar) = 0.6894757 * [P_range (psia) – 14.7] = 679.34040721
- Pressure: pppp = e50a in hex (bytes in reverse order) = 0ae5 in hex = 2789 decimal
  pressure (dbar) = [pressure number * P_range / (0.85 * 65536)] – (0.05 * P_range)
  = [2789 * 679.34040721 / (0.85 * 65536)] – (0.05 * 679.34040721)
  = 0.045 dbar
- Time: TTTTTTTT = 805F0C14 hex (bytes in reverse order) = 140C5F80 = 336355200 decimal
  seconds since January 1, 2000 = 336355200

Appendix B Output Accuracy

The algorithm output accuracy for the OOI L1 Temperature core data product calculated by this algorithm is equivalent to the accuracy of the instrument:

SBE 16plus V2	±0.005 °C with stability of ±0.0002 °C/month
SBE 37IM	±0.002 °C with stability of ±0.0002 °C/month
SBE GPCTD	±0.002 °C

The following requirements in the DOORS database describe temperature accuracy requirements and are consistent with these calculations:

L2-SR-RQ-3465 Temperature measurements shall have an accuracy of ±0.002º C, inclusive.

L2-SR-RQ-3462 Temperature measurement shall have an annual drift of no more than 0.01º C per year.

Note that the accuracy requirements for the GPCTD, the CTD on the gliders and AUVs, are included here for completeness, but data from this make/model of instrument will be processed onboard the vehicles and presented already in decimal format in appropriate units (°C, Siemens/meter, decibars). Therefore processing “raw” data from the CTDGP is not included in the algorithm described in this document.

Appendix C Sensor Calibration Effects

None.