



DATA PRODUCT SPECIFICATION FOR VENT FLUID CHLORIDE CONCENTRATION

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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 Chief Systems Engineer:  _____

Date: 2012-03-19

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

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1 Abstract

This document describes the computation used to calculate the OOI Level 2 Vent Fluid Chloride Concentration, from resistivity and temperature measurements made using the Resistivity-Temperature Probe Instrument (TRHPH) placed in a high-temperature hydrothermal vent. This data product is calculated from temperature and resistivity, using a temperature-conductivity-chloride reference surface developed by Larson et al. (2007). The primary intended use of this document is for OOI programmers to construct appropriate processes to create the L2 Chloride Concentration data product.

2 Introduction

2.1 Author Contact Information

Please contact the Data Product Specification lead (DPS@lists.oceanobservatories.org) or the authors Giora Proskurowski (giora@uw.edu) and Benjamin Larson (blarson@ocean.washington.edu) for more information concerning the computation and other items in this document.

2.2 Metadata Information

2.2.1 Data Product Name

The OOI Core Data Product Name for this product is

- TRHPHCC

The OOI Core Data Product Descriptive Name for this product is

- Vent Fluid Chloride Concentration

2.2.2 Data Product Abstract (for Metadata)

The OOI Level 2 Vent Fluid Chloride Concentration core data product is computed using a reference surface of temperature-conductivity-chloride to determine chloride from temperature and resistivity. Temperature is an input from TRHPHTE, an OOI Level 1 product, and resistivity is an input from OOI Level 0 product input from the TRHPH instrument.

2.2.3 Computation Name

- Vent Fluid Chloride Concentration Algorithm

2.2.4 Computation Abstract (for Metadata)

This computation computes the OOI Level 2 Vent Fluid Chloride Concentration core data product, which is calculated from OOI Level 1 Temperature Vent Fluid-TRHPH core data product and conductivity, the inverse of resistivity, an OOI Level 0 data product output from the TRHPH instrument.

2.2.5 Instrument-Specific Metadata

See Section 4.4 for instrument-specific metadata fields that must be part of the output data.

2.2.6 Data Product Synonyms

Synonyms for this data product are

- Chlorinity

2.2.7 Similar Data Products

N/A

2.3 Instruments

For information on the instruments from which the Level 2 Vent Fluid Chloride Concentration core data product inputs are obtained, see the TRHPH Processing Flow document (DCN 1342-00150), which describes the flow of data from the TRHPH through all of the relevant QC, calibration, and data product computations and procedures.

Please see the Instrument Application in the OOI Software Application Framework (SAF) for specifics of instrument locations and platforms.

2.4 Literature and Reference Documents

Larson, B.I., Olson, E.J, and Lilley M.D. (2007). "In situ measurement of dissolved chloride in high temperature hydrothermal fluids." *Geochimica et Cosmochimica Acta* **71**, 2510-2523. (see *DPS Artifacts* >> *TRHPHCC* >> *TRHPHCC_Larson_2007.pdf*)
Temperature-Conductivity-Chloride calibration surface from above paper, saved as a Matlab .mat file. (see *DPS Artifacts* >> *TRHPHCC* >> *Larson_2007surface.mat*)

2.5 Terminology

2.5.1 Definitions

Chloride concentration: Concentration of chloride ion in mmol/kg.

2.5.2 Acronyms, Abbreviations and Notations

N/A

2.5.3 Variables and Symbols

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

T	Temperature (°C) – from TRHPHTE
V_R	Resistivity- Inverse of conductivity (V)
C	Conductivity- Inverse of measured resistivity (1/V)
TCSsurf	Temperature-Conductivity-Chloride surface
Tdat	Temperature (°C) calibration data in TCSsurf
Sdat	Chloride concentration (mol/kg) data in TCSsurf
Cdat	Conductivity data (1/V) data in TCSsurf
S	Chloride concentration (mol/kg) as derived from the TCSsurf surface
Cl	Chloride concentration (mmol/kg) additional secondary calibration to be applied using POLYVAL QC routine

3 Theory

3.1 Description

Resistivity, measured in volts by the Temperature-Resistivity Instrument, is the inverse of conductivity. While neither resistivity nor conductivity data from this instrument have been precisely calibrated to their respective SI units (ohm*m and siemens/m), extensive laboratory work allows for the calculation of chloride concentration from the measured resistivity and temperature data. Conductivity can be transformed into chloride concentration based on methods published by Larson et al. (2007), utilizing a temperature-conductivity-chloride calibration surface. The intersection of the measured temperature, conductivity (reciprocal of measured resistivity), and the calibration surface define the chloride concentration. The 3-dimensional calibration surface is provided to OOI Cyberinfrastructure as a Matlab file (*Larson_2007surface.mat*) consisting of three 200 x 200 matrices describing temperature (°C), conductivity (1/V) and chloride concentration (mol/kg). This calibration surface, and the method by which it was developed, is described in Larson et al. (2007), and pictured in Figure 1. If, in the future an

improved calibration surface is developed, the updated surface will be provided to OOI Cyberinfrastructure.

The Temperature-Resistivity instrument measures resistivity using four gold electrodes imbedded in a magnesium stabilized ZrO₂ ceramic rod. Two of the four gold electrodes are connected to 'drive' terminals on the electronics package and the other two are connected to 'sensor' terminals. The drive electrodes establish an electric field across a packet of fluid, which behaves as a resistor, by sending a constant alternating current of 100 μA at 1 kHz across a 10kΩ resistor. The resistance of the fluid is dependent on its temperature and salt content and is measured by monitoring the potential difference across two sensor electrodes immersed in the fluid. The potential across the resistivity electrodes is amplified using three different circuits, resulting in three data values between 0-4V reflecting gains of 1, 5 and 25. The computation described here chooses the most highly resolved, on-scale, resistivity data value, assigns a chloride concentration based on the surface, and then converts this value to standard concentration units (mmol/kg). Although not a part of this algorithm, secondary calibration is applied to the output using the POLYVAL QC routine (DCN 1341-10003), with the offset and scalar determined by laboratory analysis of chloride from fluid samples taken at deployment and recovery.

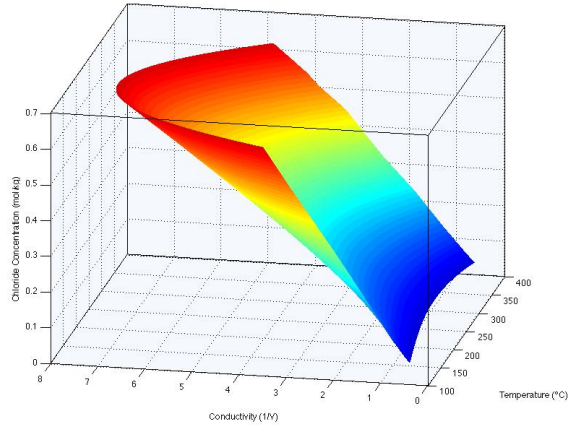


Figure 1. Temperature-Conductivity-Chloride calibration surface

3.2 Mathematical Theory

The following formulae are used to calculate the L2 Vent Fluid Chloride Concentration data product, Cl.

Chloride concentration is determined from the calibration surface, with units mol/kg. This concentration is converted to mmol/kg units. This value must be ground-truthed to physical samples using a simple linear correction (offset and scale factor). These physical samples will be acquired post-deployment, pre-recovery, and when mid-deployment opportunities allow. The scale and offset secondary calibrations will be applied using the algorithms described by the POLYVAL QC Data Product Specification (DCN 1341-10003).

3.3 Known Theoretical Limitations

The current T-C-Cl calibration surface is only valid for the following ranges for the inputs:

Temperature (°C): 103 to 382

Resistivity (V): 0.135 to 2.350

However, due to the curvature of the calibration surface values of Temperature and Resistivity at the bounds of the range may not always yield a Chloride Concentration value. It is recommended that instead of a range check, errors in the subroutine due to out-of-bounds input values be stored as NaN or similar. In the future, when a new calibration surface is developed, the range will also change. The Matlab code provided in Appendix A forgoes a range check, instead outputs a NaN if either the temperature or conductivity value is outside the bounds of the calibration surface.

3.4 Revision History

No revisions to date.

4 Implementation

4.1 Overview

The computation of temperature is implemented using a series of simple mathematical equations to convert from raw voltages to temperature, and then adjust for a laboratory calibration. The example Matlab code presented in the Appendix A illustrates the sequence of calculations.

4.2 Inputs

- L1 Vent Fluid Temperature-TRHPH (T, TRHPHTE)
- L0 Resistivity V1 (V_R1, TRHPHR1, word 1)
- L0 Resistivity V2 (V_R2, TRHPHR2, word 2)
- L0 Resistivity V3 (V_R3, TRHPHR3, word 3)
- TCSsurf (name of file should be included in metadata)

L0 inputs are five character, fixed width, floating point numbers, %5.3f.

L1 TRHPHTE input is a 5 character floating point number, %.1f.

In addition, the 3-dimensional calibration surface is provided as a Matlab file (Larson_2007surface.mat) consisting of three 200 x 200 matrices (Temperature, Conductivity, Chloride) of double precision formatted data.

Input Data Formats:

Instrument provides a single line of ASCII text data with X “words”. V_R1 is word 1, V_R2 is word 2, V_R3 is word 3. Each input word of interest is a fixed width five character number, including the decimal point, floating point value (%5.3f).

4.3 Processing Flow

The specific steps necessary to create all calibrated and quality controlled data products for each OOI core instrument are described in the instrument-specific Processing Flow documents (DCN 1342-00150). These processing flow documents contain flow diagrams detailing all of the specific procedures (data product and QC) necessary to compute all levels of data products from the instrument and the order in which these procedures.

The processing flow for the Chloride Concentration computation is as follows (in Matlab syntax):

Step 1:

Choose the optimal L0 Resistivity voltage:

```
if V_R2 < 0.75
    V_R = V_R3/5;
elseif 0.75 <= V_R2 < 3.90
    V_R = V_R2;
else V_R = V_R1*5;
end
```

Step 2:

Convert resistivity to conductivity:

$$C = 1/V_R$$

Step 3:

Using T from TRHPHTE and Conductivity, determine Chloride (mol/kg) from surface: define an isotherm of conductivity vs chloride at the observed temperature (T), and compute Chloride from the observed conductivity (C).

Step 4:

Convert Chloride (mol/kg) from surface to units mmol/kg. Cl is the final data product output by this computation; however, a scale and offset determined from field verification physical samples will be applied using the algorithms described by the POLYVAL QC DPS (DCN 1341-10003).

$$Cl = (S*1000)$$

The following function encompasses Steps 1-4:

```
[V_R, C, S, Cl] = Chloride(V_R1,V_R2,V_R3,T,Tdat,Sdat,Cdat);
(See example code in appendix A.)
```

If one of the inputs is outside the range of the calibration surface a “NaN” value will be returned. A global range check is applied to the output “Cl” and flagged if equal to “NaN”.

4.4 Outputs

The outputs of the chloride concentration computation are

- Chloride concentration, Cl, in mmol/kg, as a 4 character floating point number, %.0f.

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

4.5 Computational and Numerical Considerations

4.5.1 Numerical Programming Considerations

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

4.5.2 Computational Requirements

- One TRHPH probe, sample rate of 1 sample every 12s.

4.6 Code Verification and Test Data Set

The code will be verified using the test data set provided, which contains inputs and their associated correct outputs. Cl will verify that the code is correct by checking that the output, generated using the test data inputs, is identical to the test data chloride concentration output. Inputs to Vent Fluid Chloride Concentration product, V_R1, V_R2, V_R3 are highlighted in red, and TRHPHTE, T, is in blue.

Example TRHPH Raw Data Output (with TRHPHTE appended)

V_R1	V_R2	V_R3				ORP_V	V_s	T_s	V_c	T_u		TRHPHTE T
0.906	4.095	4.095	0.000	0.019	0.076	1.806	1.506	12.01	0.000	12.0	9.2	11.8
0.890	4.095	4.095	0.000	0.021	0.077	1.541	1.479	12.67	0.015	16.3	9.2	15.9
0.891	4.095	4.095	0.000	0.021	0.079	1.810	1.926	2.47	0.001	2.7	9.2	3.2
0.184	0.915	4.064	0.000	0.022	0.074	0.735	1.932	2.34	0.274	69.5	9.2	67.7
0.198	1.002	4.095	0.000	0.020	0.075	0.745	1.927	2.45	0.306	77.4	9.2	75.8
0.172	0.857	4.082	0.000	0.022	0.073	0.715	1.930	2.38	0.393	98.7	9.2	97.5
0.183	0.926	4.076	0.000	0.020	0.079	0.775	1.929	2.40	0.383	96.2	9.2	95.0
0.233	1.182	4.072	0.000	0.021	0.075	0.799	1.930	2.38	0.388	97.4	9.2	96.2
0.146	0.747	3.634	0.000	0.018	0.078	0.757	1.930	2.38	0.469	117.3	9.2	116.8
0.134	0.681	3.405	0.000	0.021	0.078	0.542	1.931	2.36	1.077	266.2	9.2	272.8
0.131	0.673	3.293	0.000	0.021	0.078	0.831	1.926	2.47	1.288	318.0	9.2	325.8
0.133	0.678	3.396	0.000	0.019	0.077	0.867	1.926	2.47	1.305	322.2	9.2	330.0
0.135	0.681	3.409	0.000	0.021	0.079	0.911	1.928	2.43	1.319	325.5	9.2	333.4
0.135	0.681	3.426	0.000	0.021	0.079	0.911	1.929	2.40	1.318	325.3	9.2	333.2

The test data set below provides the results of the Temperature Vent Fluid calculation for the above example data set.

Inputs				Intermediate Calculations			Output
V_R1	V_R2	V_R3	T	V_R	C	S	Cl
[V]	[V]	[V]	[°C]	[V]	[1/V]	[mol/kg]	mmol/kg
0.906	4.095	4.095	11.8	4.530	0.2208	NaN	NaN
0.890	4.095	4.095	15.9	4.450	0.2247	NaN	NaN
0.891	4.095	4.095	3.2	4.455	0.2245	NaN	NaN
0.184	0.915	4.064	67.7	0.915	1.0929	NaN	NaN
0.198	1.002	4.095	75.8	1.002	0.9980	NaN	NaN
0.172	0.857	4.082	97.5	0.857	1.1669	NaN	NaN
0.183	0.926	4.076	95.0	0.926	1.0799	NaN	NaN
0.233	1.182	4.072	96.2	1.182	0.8460	NaN	NaN
0.146	0.747	3.634	116.8	0.727	1.3759	0.19507	195
0.134	0.681	3.405	272.8	0.681	1.4684	0.10893	109
0.131	0.673	3.293	325.8	0.659	1.5184	0.12813	128
0.133	0.678	3.396	330.0	0.679	1.4723	0.12664	127
0.135	0.681	3.409	333.4	0.682	1.4667	0.12878	129
0.135	0.681	3.426	333.2	0.685	1.4594	0.12802	128

Appendix A Example Code

This Appendix contains an example Matlab subroutine to calculate L2 Vent Fluid Chloride Concentration. This code has been verified by the originators using examples from raw TRHPH data.

```
function [V_R, C, S, Cl] = Chloride(V_R1,V_R2,V_R3,T,Tdat,Sdat,Cdat);
%This function uses resistivity and temperature inputs to calculate
Chloride
%concentration based on the surface data developed in Larson et al
2007.

%load Larson_2007surface.mat %this loads Tdat, Cdat, Sdat

if V_R2 < 0.75
    V_R = V_R3/5;
elseif 0.75 <= V_R2 < 3.90
    V_R = V_R2;
else V_R = V_R1*5;
end

V_R;

C=1/V_R; %conductivity from resistivity

%extract a curve of constant temperature out of the data surface
Scurve = linspace(min(min(Sdat)),max(max(Sdat)),100);
Tcurve = Scurve*0+T;
Ccurve = interp2(Tdat,Sdat,Cdat,Tcurve,Scurve);

if isfinite(Ccurve)
    %now interpolate onto the Scurve/Ccurve
    S = interp1(Ccurve,Scurve,C);

    Cl = (S*1000);

else
    S = NaN;
    Cl = NaN;
end

end
```

Appendix B Output Accuracy

The accuracy of the Chloride Concentration calculated as described herein is a function of the accuracy of the sensor measurements (temperature and resistivity) and the applied calibration. The specified accuracy outlined in the Technical Specification document (4320-00022) is:

10 mmol/kg

Accuracy Requirement in DOORS

Chloride concentration shall be measured with an accuracy of 10 mmol/kg.

< L4-RSN-IP-RQ-582 >