ALGORITHM THEORETICAL BASIS DOCUMENT (ATBD):

SUBSURFACE MOORED TEMPERATURE CHAIN

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1   DESCRIPTION

Contained in this document are details concerning temperature measurements made at NEON lake sites using a subsurface moored vertical sensor array. Specifically, the processes necessary to convert "raw" sensor measurements into meaningful scientific units and their associated uncertainties are described. The subsurface moored temperature chains, which produce Water temperature and conductivity in lakes from subsurface moored array of sensors (DP1.20055.001), are deployed at all NEON Lake sites.

1.1   Purpose

This document details the algorithms used for creating NEON Level 1 data products for Water temperature and conductivity in lakes from Level 0 data, and ancillary data as defined in this document (such as calibration data) obtained via instrumental measurements made by the subsurface moored temperature chain. It includes a detailed discussion of measurement theory and implementation, appropriate theoretical background, data product provenance, quality assurance and control methods used, approximations and/or assumptions made, and a detailed exposition of uncertainty resulting in a cumulative reported uncertainty for this product.

1.2   Scope

The theoretical background and entire algorithmic process used to derive Level 1 data from Level 0 data for Water temperature and conductivity in lakes from subsurface moored array of sensors (DP1.20055.001) is described in this document. The subsurface moored temperature chains are comprised of several HOBO U24 conductivity/temperature loggers and an unvented levelTROLL 400. See NEON SENSOR COMMAND, CONTROL AND CONFIGURATION (C3) DOCUMENT: SUBSURFACE MOORED SENSOR CHAIN (NEON.DOC.005218) for more details about sensor configuration and installation. This document does not provide computational implementation details, except for cases where these stem directly from algorithmic choices explained here.

2   RELATED DOCUMENTS, ACRONYMS AND VARIABLE NOMENCLATURE

2.1   Applicable Documents

AD[01]	NEON.DOC.000001 NEON OBSERVATORY DESIGN
AD[02]	NEON.DOC.002652 NEON Level 1, Level 2 and Level 3 Data Products Catalog
AD[03]	NEON.DOC.000782 ATBD QA/QC Data Consistency
AD[04]	NEON.DOC.011081 ATBD QA/QC Plausibility Tests
AD[05]	NEON.DOC.000783 ATBD De-spiking and Time Series Analyses
AD[06]	NEON.DOC.000746 Calibration Fixture and Sensor Uncertainty Analysis (CVAL)
AD[07]	NEON.DOC.000785 TIS Level 1 Data Products Uncertainty Budget Estimation Plan
AD[08]	NEON.DOC.000927 NEON Calibration and Sensor Uncertainty Values[1]
AD[09]	NEON.DOC.001113 Quality Flags and Quality Metrics for TIS Data Products
AD[10]	NEON.DOC.005218 NEON SENSOR COMMAND, CONTROL AND CONFIGURATION (C3) DOCUMENT: SUBSURFACE MOORED SENSOR CHAIN
AD[11]	NEON.DOC.005290 STCDD - 0317730400 In-Situ Level TROLL 400
AD[12]	NEON.DOC.005289 STCDD - 0378610000 High-accuracy conductivity data logger

[1] Note that CI obtains calibration and sensor values directly from an XML file maintained and updated by CVAL in real time. This report is updated approximately quarterly such that there may be a lag time between the XML and report updates.

2.2   Reference Documents

RD[01]	NEON.DOC.000008	NEON Acronym List
RD[02]	NEON.DOC.000243	NEON Glossary of Terms

2.3   Acronyms

Acronym	Explanation
AIS	Aquatic Instrument System
ATBD	Algorithm Theoretical Basis Document
CI	NEON Cyberinfrastructure
CVAL	NEON Calibration, Validation, and Audit Laboratory
DAS	Data Acquisition System
DP	Data Product
FDAS	Field Data Acquisition System
Hz	Hertz
L0	Level 0
L1	Level 1
QA/QC	Quality assurance and quality control

2.4   Variable Nomenclature

The symbols used to display the various inputs in the ATBD, e.g., calibration coefficients and uncertainty estimates, were chosen so that the equations can be easily interpreted by the reader. However, the symbols provided will not always reflect NEON's internal notation, which is relevant for CI's use, and/or the notation that is used to present variables on NEON's data portal. Therefore, lookup tables are provided in order to distinguish what symbols specific variables can be tied to in the following document.

Lookup table for LevelTROLL 400

Symbol	Internal Notation	Description
C_{P0}	CVALA0	Calibration coefficient for LT400 Pressure sensor
C_{P1}	CVALA1	Calibration coefficient for LT400 Pressure sensor
C_{P2}	CVALA2	Calibration coefficient for LT400 Pressure sensor
$u_{A1,P}$	U_CVALA1	Combined, standard calibration uncertainty of the pressure measurement by LT400 sensor (kPa)

Lookup table for HOBO U24

Symbol	Internal Notation	Description
C_{L0}	CVALL0	Calibration coefficient for HOBO U24 low range conductivity sensor
C_{L1}	CVALL1	Calibration coefficient for HOBO U24 low range conductivity sensor
C_{L2}	CVALL2	Calibration coefficient for HOBO U24 low range conductivity sensor
C_{H0}	CVALH0	Calibration coefficient for HOBO U24 high range conductivity sensor
C_{H1}	CVALH1	Calibration coefficient for HOBO U24 high range conductivity sensor
C_{H2}	CVALH2	Calibration coefficient for HOBO U24 high range conductivity sensor
C_{T0}	CVALA0	Calibration coefficient for HOBO U24 temperature sensor

Symbol	Internal Notation	Description
C_{T1}	CVALA1	Calibration coefficient for HOBO U24 temperature sensor
C_{T2}	CVALA2	Calibration coefficient for HOBO U24 temperature sensor
$u_{A1,C}$	U_CVALA1 streams 0 & 1	Combined, standard calibration uncertainty of the low range conductivity measurement by HOBO U24 sensor. Un-averaged reading
$u_{A1,T}$	U_CVALA1 stream 2	Combined, standard calibration uncertainty of the temperature measurement by HOBO U24 sensor (degrees Celsius)

Lookup table for geolocation information

Symbol	Internal Notation	Description
$Z_{thermistor}$	Measured manually	Distance between the HOBO U24 and LT400 sensors (m), a positive value indicates that the HOBO U24 is closer to the water surface than the LT400 sensor.
$u_{Z_{thermistor}}$	Measured manually	Assumed to be 1 cm, conservatively. A meter tape with 1-mm resolution is used to record the measurement associated with this uncertainty estimate
Z_{LT400}	Measured manually	Distance of the LT400 above the anchor (m)
$u_{Z_{LT400}}$	Measured manually	Assumed to be 1 cm, conservatively. A meter tape with 1-mm resolution is used to record the measurement associated with this uncertainty estimate

3   DATA PRODUCT DESCRIPTION

3.1   Variables Reported

The Water temperature and specific conductance in lakes from subsurface moored array of sensors-related L1 DPs provided by the algorithms documented in this ATBD are displayed in the accompanying

file: PublicationWorkbook_Water temperature and conductivity in lakes from subsurface moored array of sensors.txt.

3.2 Input Dependencies

Table 1 details the Water temperature and conductivity in lakes from subsurface moored array of sensors -related L0 DPs used to produce L1 Water temperature and conductivity in lakes from subsurface moored array of sensors DPs in this ATBD.

Table 1. List of Water temperature and conductivity in lakes from subsurface moored array of sensors L0 DPs used to produce L1 Water temperature and conductivity in lakes from subsurface moored array of sensors DPs in this ATBD.

Description	Sample Frequency	Units	Source
Water pressure LT400	1/30 min.	kPa	LT400 log file
Barometric pressure	1/1 min.	kPa	DP1.0004.001
Water temperature HOBO U24	1/30 min.	^{o} C	HOBO U24 log file
Water conductivity low range HOBO U24	1/30 min.	µS/cm	HOBO U24 log file
Water conductivity high range HOBO U24	1/30 min.	µS/cm	HOBO U24 log file
LT400 height relative to anchor mooring	annually	m	Named location database
HOBO U24 position relative to LT400	annually	m	Named location database

3.3 Product Instances

One subsurface moored temp chain will be deployed at each NEON lake site. Each temperature chain is comprised of 4-10 temperature and conductivity loggers and a single pressure sensor to monitor the depth of the water over time. The temperature chains are deployed year-round including periods of time when thick ice covers some sites. Data is downloaded twice yearly and ingested into the NEON data processing pipeline using a file transfer system. No practical method is currently available to stream data from these sensors that are deployed below the water surface when ice is present.

3.4 Temporal Resolution and Extent

L0 data will be collected every 30 minutes and reported at native resolution.

3.5   Spatial Resolution and Extent

In lakes, the subsurface moored temp chain will be located at a fixed depth from the cable anchor and near where the surface mounted buoy is deployed. It is sufficiently far to avoid interfering with in situ surface-buoy mounted sensors and the profiling system, if present.

4   SCIENTIFIC CONTEXT

Water chemistry and aquatic communities are highly dependent on water temperature. Temperature profiles indicate whether or not the lake or river is thermally stratified, i.e. where the body of water is separated into two or more layers based on density. Typically, in a thermally stratified system, the top layer of water is warmer (epilimnion) while the lower layer is colder (hypolimnion). The area separating the two layers is known as the thermocline. The thermocline occurs when the rate of decreasing temperature with increasing depth is greatest, where there is a change of >1 degree Celsius per 1.0 m change in depth (USEPA 2012). Thermal stratification can dramatically change the water chemistry and biology of each layer. Frequent (1 per 30-minute) readings will be useful for determining the physical stratification status of lakes and rivers through time.
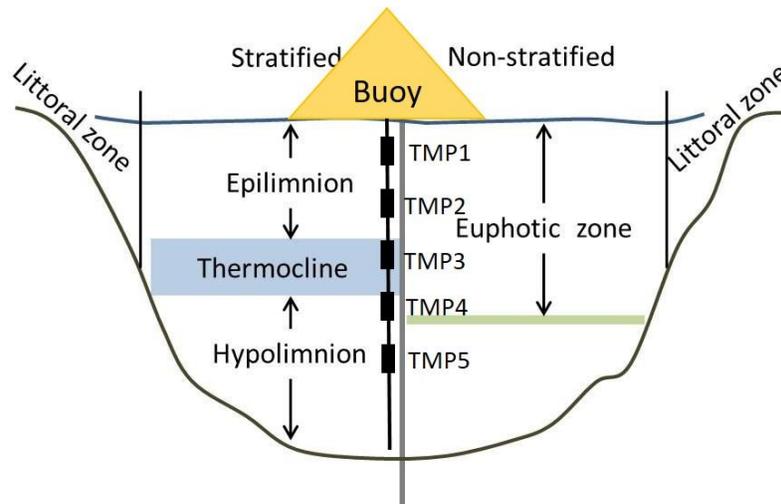
Figure 1. Diagram representing the zones in a thermally stratified and non-stratified lake.

4.1   Theory of Measurement

The subsurface moored temperature chain is comprised of several matching digital temperature/conductivity sensors and a single pressure sensor (Figure 2). The HOBO U24 converts thermistor measurements to digital signals internally and is the only output option from the sensor. Obtaining raw analog signals is not possible from this sensor. Temperature is derived from the HOBO U24, which uses a temperature dependent electrically resistive material coated in titanium pentoxide to

maintain rapid response to changes in temperature. The sensor applies a fixed current within the circuit and monitors changes in voltage which are directly induced by the temperature dependence of the resistor. Empirically the voltage changes are correlated to water temperature values internally by the sensor prior to data output. The HOBO U24 also contains a conductivity sensor that reports a digital signal.

The LT400 contains an unvented pressure sensor. The LT400 converts the analog measurements to digital signals internally and is the only output option from sensor. Obtaining raw analog signals is not possible from this sensor. Water column height is determined by first knowing the pressure of the water above the sensor measurement point and barometric pressure at the time of the measurement. This is done through the use for a pressure transducer in the LT400, which determines pressure by measuring the slight voltage change that occurs when a variable resistor is compressed or deflected due to the hydrostatic pressure of the water.
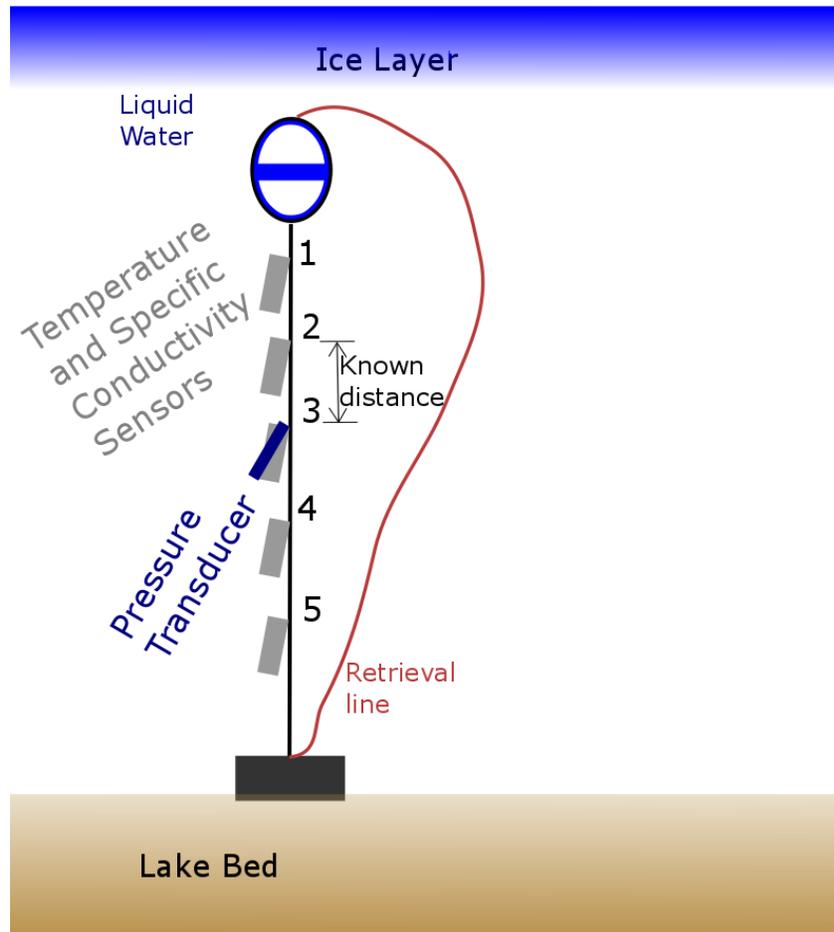

Figure 2. A float and anchor create a taut line. Precise measurements between temperature and conductivity sensors (HOBO U24) and the pressure transducer (LevelTROLL 400) allows sensor depths to be determined when data are coupled with barometric pressure.

4.2 Theory of Algorithm

The following sections detail the theory of the algorithm for measuring water temperature (section 4.2.1), converting conductivity to specific conductance (section 4.2.2), and calculating sensor depth using LT400 pressure and riparian barometric pressure measurements (section 4.2.3).

4.2.1 Surface Water Temperature Algorithm

Surface water temperature (digital thermistor) is reported as a 30-minute instantaneous value. The instantaneous temperature measurements are calculated according to:

$$T_{SW,i} = C_{T2} * T_i^2 + C_{T1} * T_i + C_{T0}$$

Equation 1

Where:

$T_{SW,i}$ = Individual (1/30-minute) surface water temperature (°C)
C_{T2} = Calibration coefficient provided by CVAL ((°C)$^{-1}$)
C_{T1} = Calibration coefficient provided by CVAL (unitless)
C_{T0} = Calibration coefficient provided by CVAL (°C)
T_i = Individual (1/30-minute) temperature output from sensor (°C)

4.2.2 Surface Water Specific Conductance Algorithm

Specific conductance is the water's ability to conduct electricity which is related to dissolved solute concentrations. The higher the concentration of dissolved ions is in the water, the less resistive the water is, i.e. higher specific conductance. Along with dissolved ion concentrations, temperature directly affects the ability of electricity to flow through water. Actual conductivity is the term given to an electrical conductivity measurement of water that is not normalized for temperature effects; whereas specific conductance is the value at a water temperature normalized to 25°C. Normalization of the conductivity measurement allows for comparison of the metric without temperature bias and is calculated according to Wilde et al (various dates).

The HOBO logger records a "high" and "low" conductivity reading measurement ranges. The low range is used for readings below 1000 µS/cm and high range is used for readings from 1,000 to 10,000 µS/cm. Actual surface water conductivity is determined by applying the calibration coefficients, supplied by CVAL, to the "raw" sensor output as follows:

$$\text{Low Range: } C_{SW,i} = C_{L2} * C_i^2 + C_{L1} * C_i + C_{L0}$$

Equation 2

or

$$\text{High Range: } C_{SW,i} = C_{H2} * C_i^2 + C_{H1} * C_i + C_{H0}$$

Equation 3

Specific conductance will then be calculated from actual conductivity and temperature using the calibrated 1-minute values according to Low Range: $C_{SW,i} = C_{L2} * C_i^2 + C_{L1} * C_i + C_{L0}$
Equation 2 and High Range: $C_{SW,i} = C_{H2} * C_i^2 + C_{H1} * C_i + C_{H0}$
Equation 3.

$$SpC_{SW,i} = \frac{C_{SW,i}}{1+0.0191(T_{SW,i}-25)}$$ **Equation 4**

where:

$SpC_{SW,i}$ = Individual Conductivity at 25 °C, known as Specific Conductance (µS/cm)
$C_{SW,i}$ = Individual Conductivity as measured at the ambient temperature (µS/cm)
$T_{SW,i}$ = Individual surface water (ambient) temperature (°C)

If the synchronous temperature measurements are not available, then specific conductance shall not be calculated, and missing data is flagged.

The missing temperature flag will be set to 1 when specific conductance cannot be calculated due to a missing temperature value.

4.2.3 Sensor Depth Algorithm

Calibrated, measured pressure is used to calculate the sensor depth. Pressure is determined by applying the calibration coefficients, supplied by CVAL, to the "raw" sensor output as follows:

$$P_{meas} = C_{P2} * P_i^2 + C_{P1} * P_i + C_{P0}$$ **Equation 5**

Where:

C_{P2} = Calibration coefficient provided by CVAL ((kPa)$^{-1}$)
C_{P1} = Calibration coefficient provided by CVAL (unitless)
C_{P0} = Calibration coefficient provided by CVAL (kPa)
P_i = Individual (1/30 minute) pressure output from sensor (kPa)

The surface water pressure is determined by subtracting the air pressure of the atmosphere from the measured pressure.

$$P_{SW,i} = P_{meas,i} - P_{air,i}$$ **Equation 6**

Where:

$P_{SW,i}$ = Individual (1/30 minute) surface water pressure (kPa)

$P_{meas,i}$ = Individual (1/30 minute), calibrated surface water pressure (kPa)

$P_{air,i}$ = 30-minute averaged, calibrated air pressure (kPa) from riparian barometric pressure sensor

Surface water column height, or the height of water above the sensor, is critical for determining the depth of the HOBO U24 temperature and conductivity sensors. Surface water column height is calculated using the calibrated surface water pressure by:

$$WC_{SW,i} = 1000 \times (P_{SW,i} / (\rho_{water} \times g))$$

Equation 7

Where:

$WC_{SW,i}$ = Individual surface water column height measurement (m)

$P_{SW,i}$ = Individual pressure measurement (kPa)

ρ_{water} = Density of water = 999.0 (kg/m³)

g = Acceleration due to gravity = 9.81 (m/s²)

The depth of the temperature and conductivity sensors will be determined using the distance between the temperature and conductivity sensor and the pressure sensor along with surface water column height.

$$D_{sensor,i} = WC_{SW,i} - Z_{thermistor}$$

Equation 8

Where:

$D_{sensor,i}$ = Sensor depth below the water surface (m)

$WC_{SW,I}$ = Individual surface water column height measurement (m)

$Z_{thermistor}$ = Distance between the HOBO U24 and LT400 sensors (m), a positive value indicates that the HOBO U24 is closer to the water surface than the LT400 sensor.

Sensor depth is reported as a 30-minute instantaneous values.

In instances where barometric pressure is unavailable, the missing barometric pressure flag is set to 1 and depth is not calculated.

4.2.4   Sensor Height Above the Anchor Algorithm

Measurements made of the assembled sensors and cables are used to determine the individual sensor/thermistor height above the anchor (see AD[10] for sensor physical configuration). This height is constant over time unless the sensors are manually moved to new locations along the cable. The calculation is made as follows:

$$H_{meas} = Z_{LT400} + Z_{thermistor}$$

Equation 9

Where:

H_{meas} = Calculated thermistor height above the anchor (m)
Z_{LT400} = Distance of the LT400 above the anchor (m)
$Z_{thermistor}$ = Distance between the HOBO U24 and LT400 sensors (m), a positive value indicates that the HOBO U24 is closer to the water surface than the LT400 sensor.

The thermistor height above the anchor is determined by adding the Z_{LT400} of the LT400 relative to the anchor to the $Z_{thermistor}$ of the thermistor relative to the LT400. This information is stored in the NEON named location database as part of the geolocation history.

NOTE: This value is likely to be the same for long periods of time since it reflects the dimensions of the temperature chain as deployed. Changes to the height above anchor is only expected when the cable supporting the sensors is modified. These modifications are expected infrequently, likely due to changes in water level, e.g. when lake levels drop and the expected winter ice depth would entrap the top of the cable, sensors, or floats.

The Missing Thermistor Height flag is set to 1 when either Z_{LT400} or $Z_{thermistor}$ are missing and thermistor height will not be populated.

5   ALGORITHM IMPLEMENTATION

Data flow for signal processing of L1 DPs will be treated in the following order.

1.   Calibration coefficients will be applied to instantaneous 30-minute surface water temperature (T_i) according to $T_{SW,i} = C_{T2} * T_i^2 + C_{T1} * T_i + C_{T0}$ Equation 1.

2.   Calibration coefficients will be applied to instantaneous 30-minute surface water conductivity (C_i) according to Low Range: $C_{SW,i} = C_{L2} * C_i^2 + C_{L1} * C_i + C_{L0}$

Equation 2 and High Range: $C_{SW,i} = C_{H2} * C_i^2 + C_{H1} * C_i + C_{H0}$
Equation 3 .

3.   Surface water conductivity (C_{SW}) will be converted to Specific Conductance (SpC_{SW}) according to $SpC_{SW,i} = \dfrac{C_{SW,i}}{1+0.0191(T_{SW,i}-25)}$ Equation 4.

4.   Calibration coefficients will be applied to instantaneous 30-minute surface water pressure value (P_i) according to $P_{meas} = C_{P2} * P_i^2 + C_{P1} * P_i + C_{P0}$
Equation 5.

5.   Sensor depth will be calculated from surface water pressure (P_{SW}) and sensor relative positions from the named location database according to the following: $P_{SW,i} = P_{meas,i} - P_{air,i}$ Equation 6, Equation 7, and $D_{sensor,i} = WC_{SW,i} - Z_{thermistor}$ Equation 8.

6.   Thermistor height will be calculated from surface water pressure (P_{SW}) and sensor relative positions from the named location database according to $H_{meas} = Z_{LT400} + Z_{thermistor}$
Equation 9.

7.   QA/QC Plausibility tests will be applied to the HOBO U24 temperature and specific conductance data streams and LT400 sensor depth in accordance with AD[06]. The details are provided below.

8.   Signal de-spiking will be applied to the HOBO U24 temperature and conductivity data streams and LT400 sensor depth in accordance with AD[07].

QA/QC Procedure:

1. **Plausibility Tests** – All plausibility tests will be determined for surface water temperature and conductivity AD[06]). Test parameters will be provided by AQU and maintained in the CI data store. All plausibility tests will be applied to the sensor's L0 DP and associated quality flags (QFs) will be generated for each test.

   Sensor depth will not have the persistence test applied.

2. **Signal De-spiking** – The time series de-spiking routine will be run according to AD[07]. Test parameters will be specified by AQU and maintained in the CI data store. Quality flags resulting from the de-spiking analysis will be applied according to AD[07].

3. **Quality Flags (QFs) and Quality Metrics (QMs)** AD[16] – If a datum fails one of the following tests it will not be used to create a L1 DP: *range*, *spike*, *null and gap*. Ancillary information needed for the algorithm and other information maintained in the CI data store.
   a. **Specific Conductance** – The calculation of Specific Conductance from actual conductivity and temperature shall be done before the QA/QC procedure. If the input temperature value is null or erroneous, the corresponding Specific Conductance value should also likely fail the QA/QC tests and produce a final QF flag of 1 and therefore not be used in the development of the L1 DP.

Table 2. Flags associated with HOBO U24 measurements.

Tests
Range
Persistence
Step
Null
Gap
Signal Despiking
Missing Temperature
Final quality flag

Table 3. Flags associated with levelTROLL 400 measurements.

Tests
Range
Step
Null
Gap
Signal Despiking
Missing Barometric Pressure
Missing Thermistor Height From Anchor
Final quality flag

Table 4. Information maintained in the CI data store for LT400 and HOBO U24.

Tests/Values	CI Data Store Contents
Range	Minimum and maximum values
Persistence	Window size, threshold values and maximum time length

Tests/Values	CI Data Store Contents
Step	Threshold values
Null	Test limit
Gap	Test limit
Signal Despiking	Time segments and threshold values
Calibration	CVAL sensor specific calibration coefficients
Uncertainty	AD[14]
Final Quality Flag	AD[16]

6 UNCERTAINTY

Uncertainty of measurement is inevitable (JCGM 2008, 2012; Taylor 1997). It is crucial that uncertainties are identified and quantified to determine statistical interpretations about mean quantity and variance structure; both are important when constructing higher level data products (e.g. L1 DP) and modeled processes. Uncertainty related to the subsurface moored sensor array and associated data products is provided in detail in the Aquatics Uncertainty Document AD[07], which serves to identify, evaluate, and quantify sources of uncertainty relating to L1 Water temperature and conductivity in lakes from subsurface moored array of sensors. It is a reflection of the information described in AD[07] and is explicitly described for the subsurface moored sensors in AD[08].

Uncertainty of the subsurface moored temperature chain assembly is discussed in this section. The section is broken down into two topics. The first informs the sources of *measurement* uncertainty, i.e., those associated with *individual temperature, conductivity, and pressure measurements*. A diagram detailing the data flow and known sources of uncertainty are displayed in Figure 3 and Figure 4.
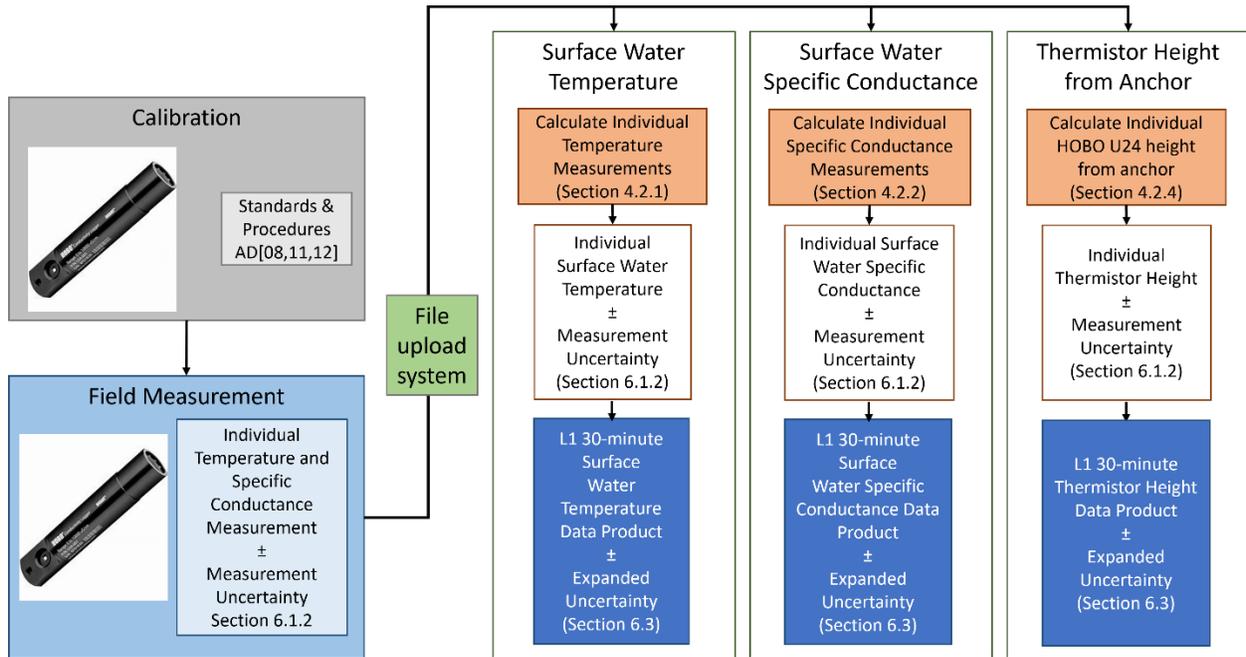
Figure 3. Displays the data flow and associated uncertainties of individual HOBO U24 measurements of temperature, specific conductance, sensor height above anchor, and associated L1 DPs.
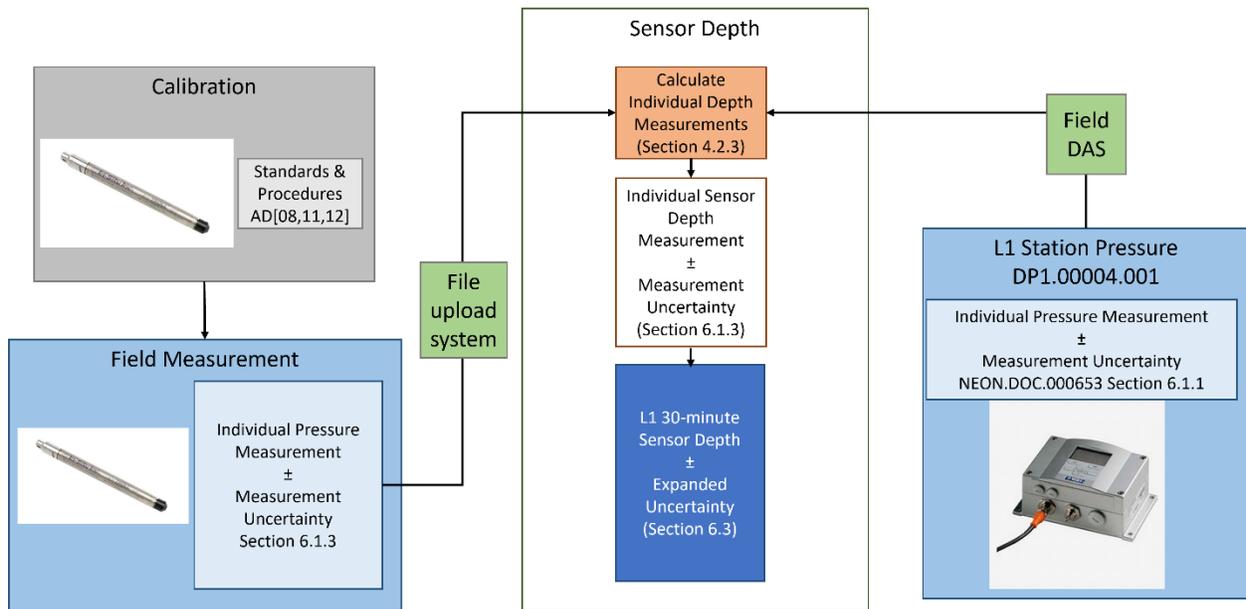

Figure 4. Displays the data flow and associated uncertainties of individual LT400 measurements of sensor depth below the water surface and associated L1 DPs.

6.1   Measurement Uncertainty

The following subsections present the uncertainties associated with *individual observations*. It is important to note that the uncertainties presented in the following subsections are *measurement uncertainties*, that is, they reflect the uncertainty of an *individual* measurement. Because the L1 data product is an instantaneous measurement the L1and measurement uncertainties are identical.

NEON calculates measurement uncertainties according to recommendations of the Joint Committee for Guides in Metrology (JCGM) 2008. In essence, if a measurand *y* is a function of *n* input quantities

x_i $(i = 1, …, n)$, $i.e., y = f(x_1, x_2, …, x_n)$, the combined measurement uncertainty of *y*, assuming the inputs are independent, can be calculated as follows:

$$u_c(y) \ = \left(\sum_{i=1}^{N} \left(\frac{\partial f}{\partial x_i} \right)^2 u^2(x_i) \right)^{\frac{1}{2}}$$ **Equation 10**

where

$\frac{\partial f}{\partial x_i}$ =partial derivative of *y* with respect to x_i

$u(x_i)$ =combined standard uncertainty of x_i.

Thus, the uncertainty of the measurand can be found by summing the input uncertainties in quadrature. For the subsurface moored sensor array, the sources of uncertainty are discussed below.

6.1.1   DAS

The HOBO U24 temperature and conductivity sensor and levelTROLL 400 pressure sensor have internal Analog to Digital (A/D) converters and output data in digital form. Therefore, no data conversions occur within the DAS, and uncertainty introduced by the DAS can be considered negligible.

6.1.2   Calibration

Uncertainties associated with the calibration process of the HOBO U24 for surface water temperature and conductivity measurements are provided by CVAL as individual standard combined uncertainty values. These uncertainties $\{u_{A1}\}$ (see Section 2.4) represent i) the repeatability and reproducibility of the sensor and the lab DAS and ii) uncertainty of the calibration procedures and coefficients including uncertainty in the standard (truth). Both are constant values that are provided by CVAL and stored in the CI data store.

6.1.3 Combined Measurement Uncertainties

6.1.3.1 Surface Water Temperature

There is no additional uncertainty beyond the measurement and calibration uncertainties that are considered for this analysis. The combined uncertainty is simply equal to the standard uncertainty values provided by CVAL.

$$u_{c_{temp}} = u_{A1,T} \quad \textbf{Equation 11}$$

6.1.3.2 Surface Water Specific Conductance

The calculation of Specific Conductance from actual conductivity and ambient temperature in

$$SpC_{SW,i} = \frac{C_{SW,i}}{1+0.0191(T_{SW,i}-25)} \qquad \text{Equation 4 is a normalization process}$$

that compounds the standard errors of both measurements. The uncertainty of individual Specific Conductance measurements is calculated as follows:

$$u(SpC_{SW,i}) = \left[\frac{\partial SpC_{SW,i}}{\partial C_{SW,i}}^2 \times (u_{A1,C} \times C_{SW,i})^2 + \frac{\partial SpC_{SW,i}}{\partial T_{SW,i}}^2 \times u_{A1,T}^2 \right]^{\frac{1}{2}} \qquad \textbf{Equation 12}$$

Where the partial derivatives of the components are:

$$\frac{\partial SpC_{SW,i}}{\partial C_{SW,i}}^2 = \left(\frac{1}{1+0.0191(T_{SW,i}-25)} \right)^2 \qquad \textbf{Equation 13}$$

$$\frac{\partial SpC_{SW,i}}{\partial T_{SW,i}}^2 = \left(\frac{0.0191C_{SW,i}}{(1+0.0191(T_{SW,i}-25))^2} \right)^2 \qquad \textbf{Equation 14}$$

Taking the partial derivatives in $u(SpC_{SW,i}) = \left[\frac{\partial SpC_{SW,i}}{\partial C_{SW,i}}^2 \times (u_{A1,C} \times C_{SW,i})^2 + \frac{\partial SpC_{SW,i}}{\partial T_{SW,i}}^2 \times u_{A1,T}^2 \right]^{\frac{1}{2}}$

Equation 12 yields:

$$u(SpC_{SW,i}) = \left[\left(\frac{1}{1+0.0191(T_{SW,i}-25)} \right)^2 \times (u_{A1,C} \times C_{SW,i})^2 + \left(\frac{0.0191C_{SW,i}}{(1+0.0191(T_{SW,i}-25))^2} \right)^2 \times u_{A1,T}^2 \right]^{\frac{1}{2}}$$

$$\textbf{Equation 15}$$

Where:

$u(SpC_{SW,i})$ = uncertainty of individual Specific Conductance measurements

6.1.3.3 Surface Water Sensor Depth

Because the LT400 is an unvented pressure transducer, the barometric pressure of the atmosphere must be accounted for to determine water depth since the sensor measures pressure from both the atmosphere and water column. Uncertainty of the L1 Barometric pressure data product (DP1.00004.001) is added as a term in the uncertainty of the reported sensor depth.

Spatial error is another source of uncertainty in the calculation of the surface water elevation. Each sensor's location is measured upon installation of the sensor infrastructure. The measured location information and associated uncertainties are stored in the named location database. The sensor depth uncertainties include the physical measurement uncertainty ($u_C(E_{Sensor})$), which accounts for the uncertainty of the sensor's location in relation to other sensors at that NEON site.

Density of water is a function of temperature, pressure, and dissolved ions (conductivity). The density of pure water at 4°C is 1000 kg/m³. Conductivity over the range expected across the range of NEON aquatic sites will have a negligible effect on the density of water. Temperature in the typical range of 5-20°C can affect the density by up to 1 kg/m³. The density of water is part of the calculation of surface water sensor depth. A change of 1 kg/m³ in density translates to an error of nearly 4mm. This is below the 1 cm accuracy requirement; therefore the error associated with using the precise density of water is considered negligible. The density of water is considered constant at 999.0 kg/m³. The uncertainty of individual sensor is calculated as follows:

$$u(D_{sensor,i}) = \left[\frac{\partial D_{sensor,i}}{\partial P_{meas,i}}^2 \times (u_{A1,Pwat})^2 + \frac{\partial D_{sensor,i}}{\partial P_{air,i}}^2 \times (u_{A1,Pair})^2 + u_c{}^2(E_{sensor})\right]^{\frac{1}{2}} \qquad \textbf{Equation 16}$$

$u(D_{sensor,i})$ = uncertainty of individual sensor depth measurements

$u_{A1,pwat}$ = uncertainty of the pressure measurement in water

$u_{A1,pair}$ = uncertainty of the air pressure measurement

$u_C(E_{Sensor})$ = uncertainty of the sensor's measured position relative to the TROLL (m)

Where the partial derivatives of the components are:

$$\frac{\partial D_{sensor,i}}{\partial P_{meas,i}}^2 = \left(\frac{1000}{\rho_{water} \times g}\right)^2 \qquad \textbf{Equation 17}$$

$$\frac{\partial D_{sensor,i}}{\partial P_{air,i}}^2 = \left(\frac{-1000}{\rho_{water} \times g}\right)^2 \qquad \textbf{Equation 18}$$

The partial derivatives in $u(D_{sensor,i}) = \left[\frac{\partial D_{sensor,i}}{\partial P_{meas,i}}^2 \times (u_{A1,Pwat})^2 + \frac{\partial D_{sensor,i}}{\partial P_{air,i}}^2 \times (u_{A1,Pair})^2 + u_c^2(E_{sensor})\right]^{\frac{1}{2}}$ Equation 16 become:

$$u(D_{sensor,i}) = \left[\left(\frac{1000}{\rho_{water} \times g}\right)^2 \times (u_{A1,Pwat})^2 + \left(\frac{-1000}{\rho_{water} \times g}\right)^2 \times (u_{A1,Pair})^2 + u_c^2(E_{sensor})\right]^{\frac{1}{2}} \textbf{Equation 19}$$

6.1.3.4 Height Above Anchor

There is no additional uncertainty beyond the measurement uncertainty associated with the relative position measurements that are considered for this analysis. Those are combined in quadrature as follows:

$$u(H_{sensor,i}) = \sqrt{u_{Z_{LT400}}^2 + u_{Z_{thermistor}}^2} \qquad \textbf{Equation 20}$$

6.2 Expanded Uncertainty

We assume the measurement variability is normally distributed (Gaussian). The combined uncertainty represents plus or minus one standard deviation or a confidence interval of 68%. This confidence level is below the industry standard and is therefore expanded to a 95% confidence interval. This is typically calculated by multiplying the combined uncertainty, $u_{c,r}(y)$, by a coverage factor, k_p.

$$U_p = k_p \, u_{c,r}(y) \qquad \textbf{Equation 21}$$

Where $k_{95} = 1.96$ for $p = 95$ for a given degrees of freedom. k_p is approximated by a t-distribution with an effective degrees of freedom, v_{eff}, obtained from the Welch-Saterwaite formula:

$$v_{eff} = \frac{u_c^4(y)}{\sum_{i=1}^{n} \frac{u_i^4(y)}{v_i}} \qquad \textbf{Equation 22}$$

The coverage factor then becomes $k_p = t_p(v_{eff})$, where $t_p(v_{eff})$ is obtained from a table.

However to simplify the calculations further, we can conservatively estimate the expanded uncertainty at a 95% confidence level to be two times the combined uncertainty.

$$U_{Expanded} = 2 \times u_c \qquad \textbf{Equation 23}$$

This expansion is to be applied to all combined uncertainties for the L1 DP described herein.

6.3   Communicating Precision

L1 water temperature will be reported to 0.01 °C. The sensor is capable of measuring temperature at a resolution of 0.01 °C and accuracy of 0.1 °C. The resolution of individual temperature measurements is 0.01 °C, as this maintains the proper significant figures, despite the reported resolution being greater than the 0.1 °C accuracy and limit of detection.

L1 specific conductance will be reported to 1 µS/cm. The sensor is capable of measuring conductivity at a resolution of 1 µS/cm and accuracy of 5 µS/cm for low range and 20 µS/cm for high range. The resolution of individual specific conductance measurements is 1 µS/cm, as this maintains the proper significant figures, despite the reported resolution being greater than the accuracy and limit of detection.

L1 sensor depth will be reported to 0.01 m. This digital sensor is capable of measuring pressure at a resolution of 0.005% of full scale, which in this case is 0.03 kPa. This pressure sensitivity equates to 0.0035m in water height. The largest source of uncertainty is related to the positioning of the sensor. The reported resolution is consistent with the NEON scientific requirement for accurate determination of the water level.

6.4   Uncertainty Budget

The uncertainty budget is a visual aid detailing i) quantifiable sources of uncertainty, ii) means by which they are derived, and iii) the order of their propagation. Uncertainty values denoted in this budget are either derived within this document or are provided by other NEON teams (e.g., CVAL) and stored in the CI data store.

Table 5. Uncertainty budget for individual temperature measurements.

Source of Measurement Uncertainty	Measurement uncertainty Component $u(x_i)$	Measurement Uncertainty Value	$\frac{\partial f}{\partial x_i}$	$u_{x_i}(Y) \equiv \left|\frac{\partial f}{\partial x_i}\right| u(x_i)$
Temperature	$u_{A1,T}$	$u_{A1,T}$	1	$u_{c_{temp}} = u_{A1,T}$ Equation 11

Table 6. Uncertainty budget for individual specific conductance measurements.

Source of Measurement Uncertainty	Measurement uncertainty Component $u(x_i)$	Measurement Uncertainty Value	$\frac{\partial f}{\partial x_i}$	$u_{x_i}(Y) \equiv \left|\frac{\partial f}{\partial x_i}\right| u(x_i)$

Temperature	$u_{A1,T}$	$u_{A1,T}$	n/a	$\frac{\partial SpC_{SW,i}}{\partial C_{SW,i}}^2 = \left(\frac{1}{1+0.0191(T_{SW,i}-25)}\right)^2$ **Equation 13**
Conductivity	$u_{A1,L}$ or $u_{A1,H}$	$u_{A1,C}$	n/a	$\frac{\partial SpC_{SW,i}}{\partial T_{SW,i}}^2 = \left(\frac{0.0191 C_{SW,i}}{(1+0.0191(T_{SW,i}-25))^2}\right)^2$ **Equation 14**

Table 7. Uncertainty budget for individual sensor depth measurements.

Source of Measurement Uncertainty	Measurement uncertainty Component $u(x_i)$	Measurement Uncertainty Value	$\frac{\partial f}{\partial x_i}$	$u_{x_i}(Y) \equiv \left|\frac{\partial f}{\partial x_i}\right| u(x_i)$
Water pressure	$u_{A1,Pwater}$	$u_{A1,Pwater}$	n/a	$\frac{\partial D_{sensor,i}}{\partial P_{meas,i}}^2 = \left(\frac{1000}{\rho_{water} \times g}\right)^2$ **Equation 17**
Air Pressure	$u_{A1,Pair}$	$u_{A1,Pair}$	n/a	$\frac{\partial D_{sensor,i}}{\partial P_{air,i}}^2 = \left(\frac{-1000}{\rho_{water} \times g}\right)^2$ **Equation 18**
Sensor position	$Z_{thermistor}$	1 cm	1	1 cm

Table 8. Uncertainty budget for individual thermistor height measurements.

Source of Measurement Uncertainty	Measurement uncertainty Component $u(x_i)$	Measurement Uncertainty Value	$\frac{\partial f}{\partial x_i}$	$u_{x_i}(Y) \equiv \left|\frac{\partial f}{\partial x_i}\right| u(x_i)$
Sensor position	$Z_{thermistor}$	1 cm	1	$Z_{thermistor}$
Thermistor height	$u_{Z_{LT400}}$	1 cm	1	$u_{Z_{LT400}}$

7 FUTURE PLANS AND MODIFICATIONS

Create data tables for AIS maintenance data associated with the subsurface moored temperature chain.

8   BIBLIOGRAPHY

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