NEON ALGORITHM THEORETICAL BASIS DOCUMENT (ATBD):

SURFACE WATER TEMPERATURE, ELEVATION AND SPECIFIC CONDUCTANCE

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Change Record

REVISION	DATE	ECO #	DESCRIPTION OF CHANGE
A	07/05/2018	ECO-04914	Initial Release
B	01/07/2019	ECO-05975	Added accurate description of named location data needed for z-offset in transition.
C	03/16/2022	ECO-06785	Update to reflect change in terminology from relocatable to gradient sites; revised logo.
D	2/8/2024	ECO-07087	Updated to add new surface water temperature and conductivity data products. Updated uncertainty and flagging. Added information related to processing in the pachyderm pipeline, including log files and 1-minute water column height output.
E	08/12/2024	ECO-07101	Update/clarify uncertainty calculation for specific conductance

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1 DESCRIPTION

Contained in this document are details concerning surface water temperature, elevation (stage), and specific conductance measurements made at all NEON aquatic sites. Specifically, the processes necessary to convert "raw" sensor measurements into meaningful scientific units and their associated uncertainties are described. Surface water temperature, elevation, and specific conductance measurements are continuously monitored by NEON at core and gradient aquatic sites using two sensors:1) In-Situ, Inc. LevelTroll 500, (LT500) at wadeable streams and river sites, and 2) In-Situ, Inc. AquaTroll 200, (AT200) at lake sites, Caribou Creek (CARI), and Oksrukuyik Creek (OKSR).

1.1 Purpose

This document details the algorithms used for creating NEON Level 1 data products for surface water elevation, temperature (digital thermistor), and specific conductance from Level 0 data, and ancillary data as defined in this document (such as calibration data) obtained via instrumental measurements made by the LevelTroll500 (here after LT500) or the AquaTroll200 (here after AT200). 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 surface water elevation, temperature (digital thermistor), and specific conductance is described in this document. The sensors employed are multiparameter probes which are mounted within a submerged sensor enclosure. The LT500 measures temperature and pressure of water above the sensor. The AT200, measures temperature, pressure, and the actual conductivity of the water. 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.005003	NEON Scientific Data Products Catalog
AD[03]	NEON.DOC.002652	NEON Level 1, Level 2, and Level 3 Data Products Catalog
AD[04]	NEON.DOC.005005	NEON Level 0 Data Products Catalog
AD[05]	NEON.DOC.000782	ATBD QA/QC Data Consistency
AD[06]	NEON.DOC.011081	ATBD QA/QC Plausibility Tests
AD[07]	NEON.DOC.000783	ATBD De-spiking and Time Series Analyses
AD[08]	NEON.DOC.000746	Calibration Fixture and Sensor Uncertainty Analysis (CVAL)
AD[09]	NEON.DOC.000785	TIS Level 1 Data Products Uncertainty Budget Estimation Plan
AD[10]	NEON.DOC.000927	NEON Calibration and Sensor Uncertainty Values
AD[11]	NEON.DOC.001113	Quality Flags and Quality Metrics for TIS Data Products
AD[12]	NEON.DOC.002556	L1A300 Aquatic Pressure Calibration Fixture Manual

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
AT200	AquaTroll200 Sensor
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
GRAPE	Grouped Remote Analog Peripheral Equipment
Hz	Hertz
L0	Level 0
L1	Level 1
LT500	LevelTroll500 Sensor
PRT	Platinum resistance thermometer
QA/QC	Quality assurance and quality control
SWE	Surface Water Elevation

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, a lookup table is provided in order to distinguish what symbols specific variables can be tied to in the following document.

Symbol	Internal Notation		Description
C_{T0}	CVALA0		Calibration coefficient for AT200 or LT500 Temperature sensor
C_{T1}	CVALA1		Calibration coefficient for AT200 or LT500 Temperature sensor
C_{T3}	CVALA2		Calibration coefficient for AT200 or LT500 Temperature sensor
C_{P0}	CVALB0		Calibration coefficient for AT200 or LT500 Pressure sensor
C_{P1}	CVALB1		Calibration coefficient for AT200 or LT500 Pressure sensor
C_{P2}	CVALB2		Calibration coefficient for AT200 or LT500 Pressure sensor
Conductivity has split calibration range:	IF X<100 µS	IF X>100 µS	
C_{C0}	CVALM0	CVALH0	Calibration coefficient for AT200 Conductivity sensor
C_{C1}	CVALM1	CVALH1	Calibration coefficient for AT200 Conductivity sensor
C_{C2}	CVALM2	CVALH2	Calibration coefficient for AT200 Conductivity sensor
$u_{A1,T}$	U_CVALA1		Combined, standard calibration uncertainty of the temperature

Symbol	Internal Notation	Description
		measurement by AT200 or LT500 sensor (°C)
$u_{A1,P}$	U_CVALA1	Combined, standard calibration uncertainty of the pressure measurement by AT200 or LT500 sensor (kPa)
$u_{A1,C}$	U_CVALA1	Combined, standard calibration uncertainty of the conductivity measurement by AT200 sensor (%)
$u_{A3,T}$	U_CVALA3	Combined, relative uncertainty (truth and trueness only) of the temperature measurement by AT200 or LT500 sensor (°C)
$u_{A3,P}$	U_CVALA3	Combined, relative uncertainty (truth and trueness only) of the pressure measurement by AT200 or LT500 sensor (kPa)
$u_{A3,C}$	U_CVALA3	Combined, relative uncertainty (truth and trueness only) of the conductivity measurement by AT200 sensor (%)
$E_{Sensor,i}$	Named Location Database: "ELEVATION" + "Z_OFFSET" for each sensor location	Elevation of the sensor measurement location (m – above sea level)
$u_c(E_{Sensor,i})$	Named Location Manager: "ELEVATION_UNCERTAINTY" for each sensor location	Combined uncertainty of elevation of the sensor (m)

3 DATA PRODUCT DESCRIPTION

3.1 Variables Reported

The surface water related L1 DPs provided by the algorithms documented in this ATBD are displayed in the accompanying files: *PublicationWorkbook_Elevation of surface water.txt*, *PublicationWorkbook_Temperature (digital thermistor) of surface water.txt*, and *PublicationWorkbook_Specific conductivity of surface water.txt*.

3.2 Input Dependencies

Table 1 details the LT500-related and AT200-related L0 DPs used to produce L1 surface water DPs in this ATBD.

Table 1. List of LT500-related and AT200-related L0 DPs that are transformed into L1 surface water DPs in this ATBD.

Description	Sample Frequency	Units	Data Product Number
Surface Water Pressure from LT500	0.0167 Hz	*kPa*	NEON.DOM.SITE.DP0.20016.001.01379.HOR.VER.000
Surface Water Pressure from AT200	0.0167 Hz	*kPa*	NEON.DOM.SITE.DP0.20054.001.01376.HOR.VER.000
Surface Water Temperature from LT500	0.0167 Hz	° C	NEON.DOM.SITE.DP0.20016.001.01378.HOR.VER.000
Surface Water Temperature from AT200	0.0167 Hz	° C	NEON.DOM.SITE.DP0.20054.001.01374.HOR.VER.000
Surface Water Conductance	0.0167 Hz	µS/cm	NEON.DOM.SITE.DP0.20015.001.01371.HOR.VER.000
Elevation of the sensor (above sea level, ASL)	NA	m	Geolocation database

3.3 Product Instances

Multiple LT500 sensors are located at each NEON aquatic site. LT500 and AT200 sensors are located in surface water at stream, river, and lake sites. Data from each LT500 and AT200 sensor are sent to the aquatic portal by two different methods, which is determined by site type. At stream sites data are ingested via GRAPE and Ethernet cable. At lake sites data are ingested via wireless transmission. When data transmission fails, data are manually retrieved via sensor log files when available.

3.4 Temporal Resolution and Extent

Surface water temperature, pressure, and conductivity (at locations with AT200 sensors) are measured at a rate of 0.0167 Hz (1 per minute) for L0 DPs, and these L0 DPs are used to calculate the instantaneous 1-minute surface water column height, and 5 and 30-minute averages of, stream temperature, elevation, and specific conductance. The sensors deployed within each site are internally programmed to perform simultaneous measurements. Each sensor is internally programmed to collect a "burst" of three individual measurements for each measurement parameter over a 15 second interval centered on the scheduled time of the measurement. The sensor will internally compute the average and will report this value as a single measurement in the data stream from the sensor. Retrieval of the individual measurements is not possible from the sensor, so the Level 0 data are the average of the burst measurements, hereafter considered the instantaneous measurement.

3.5 Spatial Resolution and Extent

A single LT500 or AT500 is located inside the aquatic enclosure assembly mounted to the aquatic anchor in the stream at both aquatic sensor set one (S1) and aquatic sensor set two (S2). At river sites, the sensors are located inside an aquatic enclosure assembly anchored at a static location near the riverbank below the annual mean low flow level. At lake sites, the sensors are located inside an aquatic enclosure assembly mounted to the aquatic anchor in the lake at both littoral sensor set locations. The sensors are located at a known elevation and the surface water level is determined by the height of the water surface above the sensor elevation.

4 SCIENTIFIC CONTEXT

Surface water elevation temperature, and specific conductance are fundamental parameters to measuring hydrology, biogeochemistry and aquatic ecology. Stream discharge is controlled by several hydrologic components as well as physical characteristics of the watershed. Figure 1 shows how stream discharge is determined by precipitation at both the landscape and channel scales, overland flow, interflow, and groundwater flow. Stream discharge is a critical variable of the hydrological cycle at the landscape scale and therefore essential to understanding how water moves through the environment. This is necessary to determine how both aquatic and terrestrial ecosystems respond to hydrologic changes. Changes in hydrologic cycles at the landscape and broader regional level are pervasive in the face of changing land use, resource management and climate change.

Tracking the cycle of nutrients through aquatic and terrestrial environment allows scientists to determine structure and function of ecosystems. Stream discharge is necessary to calculate carbon exports and other nutrient fluxes as well as to close the water budget at the watershed scale.

While it is not practical to directly measure discharge continuously at a stream site, discharge is correlated to surface water level. At NEON, surface water level is used to determine higher-level data products including stream discharge and nutrient flux, metabolism, and reaeration rating curves.

Surface water temperature in streams is critical to supporting aquatic life as many aquatic organisms can only survive in a limited temperature range. Temperature fluctuates between day and night (diurnal cycling) and more so during seasonal changes.

Surface water specific conductance is a measure of the concentration of ionic solutes dissolved in the water. This measurement is used as a proxy for water quality since provides a direct measurement of the presence of chemicals in the water and it's a simple measurement to make. Since pure water is electrically non-conductive, the lower the concentration of ionic chemical species in the water the lower the magnitude of the measurement is. The following section details how the sensor measures conductivity.

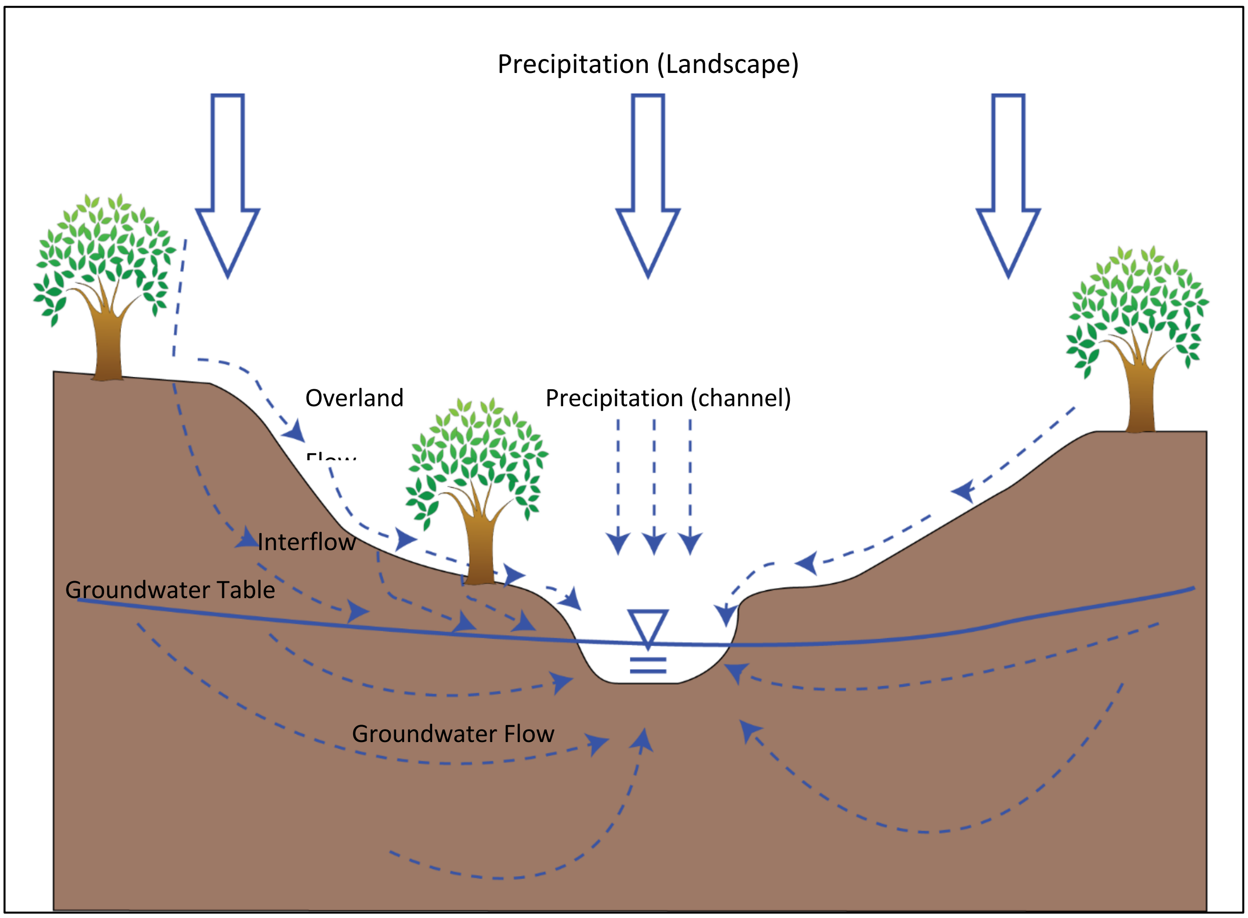

Figure 1. Components of streamflow.

4.1 Theory of Measurement

Pressure gauges to measure surface water elevation have been in use by the United States Geological Survey (USGS) for several decades (Rantz and others, 1982). Recent technological improvements have provided commercially available pressure sensors that meet NEON's accuracy and precision requirements (AD[05]).

The LT500 uses a pressure transducer to measure the pressure exerted by water and the atmosphere and a silicon bandgap sensor to measure temperature. The AT200 contains three sensors, one for each parameter - level, temperature, and conductance. The AT200 and LT500 internally convert the analog measurements to digital output, as a result it is not possible to obtain raw analog signals from this sensor. These individual measurements are addressed separately below.

In instances where remote data transmission fails, sensor data may be manually retrieved via sensor log files and used to gap fill the raw data prior to algorithm implementation. Logged data are expected to be identical to streamed data except it is possible for the readout time on the sensor to experience drift. Thus, logged data are reported with an accompanying flag and are recognized to have higher temporal uncertainty.

4.1.1 Surface Water Pressure

NEON will report the elevation of surface water based on the measured water level using the pressure gauge within the LT500 or AT200. The pressure gauge senses changes in pressure, measured in force per square unit of surface area, exerted on a strain gauge. Surface Water Elevation is determined by knowing the pressure of the water and atmosphere above the sensor measurement point and the precise elevation of the sensor measurement point.

Figure 2. Photo of a Level Troll 500 with dashed red line indicating the location of the sensing mechanism underneath the nose cone.

This LT500 and AT200 determine pressure by measuring the slight voltage change that occurs when a variable resistor is compressed due to the hydrostatic pressure of the water. The sensor head is a diaphragm-like impermeable membrane that is in direct contact with the water on one side and vented to the atmosphere on the other side via a small tube that is contained in power and communication cable. The imbalance between the pressure of the water and the air pressure on the two sides of the membrane cause it to be deflected towards the air side. The membrane is part of an electrical circuit and is made of a variable resistor material, which when deflected by the water pressure changes the resistance of the circuit and causes a drop in electrical voltage in the circuit. Through calibrations these changes in electrical voltage can be equated directly to changes in hydrostatic pressure, when the LT500 or AT200 are spatially fixed. Since changes in atmospheric pressure will directly result in changes in the hydrostatic pressure at a given point in the water column, venting the sensor to the atmospheric pressure changes eliminates the need to compensate for the pressure of the atmosphere in the measurement stream.

Surface water pressure is used to determine surface water elevation. Non-vented pressure measurements are useful in vacuum testing, in short-term testing when atmospheric pressure would not be expected to change, in very deep aquifers where the effects of atmospheric pressure are negligible, and in unconfined aquifers that are open to the atmosphere.

With vented or "gauged" pressure sensors, a vent tube in the cable applies atmospheric pressure to the back of the strain gauge. The basic unit for vented measurements is PSIG (pounds per square inch "gauge"), measured with respect to atmospheric pressure. Vented sensors thus exclude the atmospheric or barometric pressure component.

The difference between absolute and gauged measurements may be represented by a simple equation:

$$P_{gauge} = P_{absolute} - P_{atmosphere} \tag{1}$$

4.1.2 Surface Water Temperature

Temperature is derived from the LT500 or AT200, which uses a temperature dependent electrically resistive material. 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.

4.1.3 Surface Water Conductivity

The sensor uses the electrodes to create an electrical circuit in the water and applies a fixed current to the circuit. The electrical conductance of the water is then determined by monitoring the voltage in the circuit after it passes through the water. Electrical conductivity of water is a function of the spacing between the electrodes and the temperature of the system. The sensor has accounted for these parameters by having a spatially fixed electrode placement and by monitoring the water temperature. Actual conductivity is the rawest form of the measurement that the sensor can send to the NEON DAS (GRAPE) and is the conductivity measurement that accounts for electrode spacing but does not correct for temperature effects. Section 4.2 defines the algorithm to convert actual conductivity (actual measurement) to specific conductivity (temperature corrected).

4.2 Theory of Algorithm

The following sections detail the theory of the algorithm for converting water pressure to water table elevation (Section 4.2.1) and to normalize conductivity measurements for temperature effects.

4.2.1 Surface Water Elevation Algorithm

Calibrated surface water pressure is used to calculate the surface water column height and surface water elevation. Surface water pressure is determined by applying the calibration coefficients, supplied by CVAL, to the “raw” sensor output as follows:

$$P_{SW,i} = C_{P2} * P_i^2 + C_{P1} * P_i + C_{P0} \quad (2)$$

Where:

P_{SW,i_i} = Individual (0.0167 Hz) surface water pressure (kPa)
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 (0.0167 Hz) pressure output from sensor (kPa)

Surface water column height, or the height of water above the sensor, is useful for calculating stage-discharge relationships. Surface water column height is calculated using the calibrated surface water pressure by:

$$WC_{SW,i} = 1000 \times (P_{SW,i} / (\rho_{water} \times g)) \quad (3)$$

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/m^3)
g = Acceleration due to gravity = 9.81 (m/s^2)

Surface water column height is converted to surface water elevation above sea level by:

$$E_{SW,i} = E_s + WC_{SW,i} \tag{4}$$

Where:

$E_{SW,i}$ = Individual surface water elevation measurement (m-asl)
E_s = Elevation of sensor (m-asl) = elevation + z-offset in named location database
$WC_{SW,i}$ = Individual surface water column height measurement (m)

*m-asl = meters above sea level

During the construction of each aquatic site, the in-stream infrastructure was surveyed and the precise geospatial locations of the LT500 were determined. The surveyed location data are stored in the named location database as an elevation of a survey point and a z-offset from the survey point to the location of the pressure sensor. The named location database includes the sensor's latitude, longitude, elevation, offsets, and its associated uncertainties. Removal of the sensor from the mounting disc should not interfere with the ability to replace the sensor in the same location in the stream.

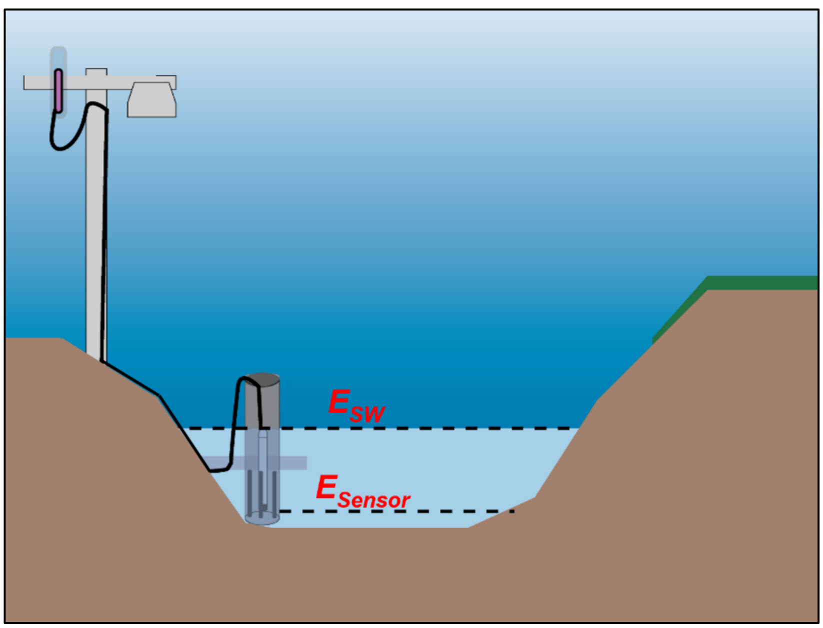

Figure 3. Illustration showing the elevation of the sensor (E_{Sensor}) which is measured by NEON staff and the calculated surface water elevation (E_{SW}).

Surface water elevation is reported as a 5-minute and a 30-minute average. Surface water column height is reported as 1-minute instantaneous measurement for use in calculating stage-discharge relationships. The 0.01667Hz instantaneous L0 measurement ($E_{SW,i}$) shall be used to calculate the 5-minute average as:

$$\overline{E_{SW5}} = \frac{1}{n}\sum_{i=x}^{n} E_{SW,i} \quad (5)$$

Where for each 5-minute average, n is the number of measurements in the averaging period and $E_{SW,i}$ is the calibrated surface water elevation calculated from the 0.0167 Hz measurements according to Equations 2-4 above during the 5-minute averaging period. For a 5-minute average, n = 5 if all points are included [0,5).

The 0.0167Hz instantaneous L0 measurement ($E_{SW,i}$) shall be used to calculate the 30-minute average as:

$$\overline{E_{SW30}} = \frac{1}{n}\sum_{i=x}^{n} E_{SW,i} \quad (6)$$

Where for each for a 30-minute average, n = 30 if all points are are included [0, 30).

4.2.2 Surface Water Temperature Algorithm

Surface water temperature (digital thermistor) is reported as a 5-minute and a 30-minute average. The instantaneous (0.01667Hz) temperature measurements are calculated according to:

$$\boldsymbol{T_{SW,i} = C_{T2} * T_i^2 + C_{T1} * T_i + C_{T0}} \quad (7)$$

Where:

$T_{SW,i}$ = Individual (0.01667Hz) 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 (0.01667Hz) temperature output from sensor (°C)

The instantaneous temperature measurement is used to calculate the 5-minute average according to:

$$\boldsymbol{\overline{T_{30}} = \frac{1}{n} \sum_{i=x}^{n} T_{SW,i}} \quad (8)$$

Where for each 5-minute averaging, n is the number of measurements in the averaging period and $T_{SW,i}$ is the surface water temperature calculated from the 0.01667Hz temperature measurement according to Equation 7 above during the 5-minute averaging period. For a 5-minute average, n = 5 if all points are included [0,5).

The instantaneous temperature measurements are used to calculate the 30-minute average according to:

$$\overline{T_{30}} = \frac{1}{n}\sum_{i=x}^{n} T_{SW,i} \quad (9)$$

Where for each 30-minute averaging, n is the number of measurements in the averaging period and $T_{SW,i}$ is the surface water temperature calculated from the 0.01667Hz temperature measurement according to Equations 7 above during the 30-minute averaging period. For a 30-minute average, n = 30 if all points are included [0,30).

4.2.3 Surface Water Specific Conductivity Algorithm

Specific conductance is the water's ability to conduct electricity which was detailed above as a proxy for water quality. The higher the concentration of dissolved ions is in the water, the less resistive the water is. The measurement is made by the sensor through a set of 4 equally spaced electrodes near the sensor tip which are in contact with the water. 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 as (Wilde et al, various dates).

Actual surface water conductivity is determined by applying the calibration coefficients, supplied by CVAL, to the "raw" sensor output as follows:

$$C_{SW,i} = C_{C2} * C_i^2 + C_{C1} * C_i + C_{C0} \quad (10)$$

Specific conductivity will then be calculated from actual conductivity and temperature using the calibrated 1-minute values according to Equation 10.

$$SpC_{SW,i} = \frac{C_{SW,i}}{1+0.0191(T_{SW,i}-25)} \quad (11)$$

where:

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

After conductivity is temperature corrected to produce specific conductance (SpC_{SW}), 5-minute averages of specific conductance ($\overline{SpC_5}$) is determined accordingly to create L1 DPs:

$$\overline{SpC_5} = \frac{1}{n}\sum_{i=x}^{n} SpC_{SW,i} \tag{12}$$

Where for each 5-minute averaging, n is the number of measurements in the averaging period and $SpC_{SW,i}$ is the surface water specific conductivity calculated from the 0.01667Hz conductivity measurement according to Equation 11 above during the 5-minute averaging period. For a 5-minute average, n = 5 if all points are included [0,5).

The instantaneous conductivity measurements are used to calculate the 30-minute average according to:

$$\overline{SpC_{30}} = \frac{1}{n}\sum_{i=x}^{n} SpC_{SW,i} \tag{13}$$

Where for each 30-minute averaging, n is the number of measurements in the averaging period and $SpC_{SW,i}$ is the surface water specific conductivity calculated from the 0.01667Hz conductivity measurement according to Equation 11 above during the 30-minute averaging period. For a 30-minute average, n = 30 if all points are included [0,30).

5 ALGORITHM IMPLEMENTATION

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

1. Calibration coefficients are applied to instantaneous 0.0167 Hz surface water pressure value (P_i) according to Equation 2.
2. Calibration coefficients are applied to instantaneous 0.0167 Hz surface water temperature (T_i) according to Equation 7.
3. Calibration coefficients are applied to instantaneous 0.0167 Hz surface water conductivity (C_i) according to Equation 10.
4. Surface water pressure values are converted to surface water column height according to Equation 3 and surface water elevation according to Equation 4 using the pressure from the sensor and the elevation of the sensor.
5. Surface water conductivity (C_{SW}) is converted to Specific Conductivity (SpC_{SW}) according to Equation 11*.
6. QA/QC Plausibility tests are applied to the data streams in accordance with AD[07].
7. Signal de-spiking and time series analysis are applied to the data stream in accordance with AD[08].
8. 5-minute and 30-minute averages for surface water elevation ($\overline{E_{30}}$), temperature ($\overline{T_{30}}$), and specific conductivity ($\overline{SpC_{30}}$) is calculated using Equations 5, 6, 8, 9, 12, and 13 respectively.
9. Descriptive statistics, i.e., minimum, maximum, and variance, are determined 5-minute and 30-minute averages.
10. Quality metrics, quality flags, and the final quality flag are produced for 5-minute and 30-minute averages according to AD[11].

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

<u>**QA/QC Procedure**</u>:

1. **Plausibility Tests** – All plausibility tests are determined for surface water pressure, temperature, and conductivity (AD[07]). Test parameters is provided by AQU and maintained in the CI data store. All plausibility tests are applied to the sensor's L0 DP and associated quality flags (QFs) are generated for each test.

2. **Signal De-spiking and Time Series Analysis** – The time series de-spiking routine is run according to AD[08]. Test parameters are specified by AQU and maintained in the CI data store. Quality flags resulting from the de-spiking analysis are applied according to AD[07].

3. **Placeholder for Consistency Analysis** (see Section 7 for future implementation).

4. **Quality Flags (QFs) and Quality Metrics (QMs)** AD[11] – In addition to the quality flags described in AD[11], data-product-specific flags are included for the data products described in this document.

    a. **zeroPressure** flag - applied to elevation, temperature, and specific conductivity of surface water when the sensor raw pressure value is below 0 kPa, indicating a dry sensor.
    b. **missingTemp** flag - applied to specific conductivity of surface water when the sensor temperature data is unavailable.
    c. **logData** flag - applied to elevation, temperature, and specific conductivity of surface water when log files have been used to gap fill missing data. Log data have a higher temporal uncertainty than streamed data.
    d. **logDateError** flag - applied to elevation, temperature, and specific conductivity of surface water when log data have corrupted dates. These data may have been assigned a date using best guess scenarios. Data with a logDateError flag may have a high temporal uncertainty.

All flagged data will still be included in the L1 DP. α and β QFs and QMs are determined using the flags in Table 2. In addition, L1 DPs will have a QA/QC report and quality metrics associated with each flag listed in Table 2 as well as a final quality flag, as detailed in AD[11]. Ancillary information needed for the algorithm and other information maintained in the CI data store is shown in Table 3.

Table 2. Flags associated with surface water elevation, temperature, and specific conductance measurements.

Tests	**Surface Water Elevation**	**Surface Water Temperature**	**Surface Water Specific Conductance**
zeroPressure	x	x	x
missingTemp			x
Range	x	x	x
Persistence	x	x	x
Step	x	x	x
Null	x	x	x
Gap	x	x	x
LogData	x	x	x

Tests	Surface Water Elevation	Surface Water Temperature	Surface Water Specific Conductance
LogDateError	x	x	x
Alpha	x	x	x
Beta	x	x	x
Final quality flag	x	x	x

Table 3. Information maintained in the CI data store for surface water pressure.

Tests/Values	CI Data Store Contents
Range	Minimum and maximum values
Persistence	Window size, threshold values and maximum time length
Step	Threshold values
Null	Test limit
Gap	Test limit
Signal Despiking	Time segments and threshold values
Calibration	CVAL sensor specific calibration coefficients
Log Data	Log data files
Uncertainty	AD[8]
Final Quality Flag	AD[12]

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. This portion of the document serves to identify to identify, evaluate, and quantify sources of uncertainty relating to individual measurements, calibrated measurements, and L1 mean surface water DPs. It is a reflection of the information described in AD[10] and is explicitly described for the In-Situ LT500 and AT200 in the following sections.

6.1 Uncertainty of Surface Water Measurements

Uncertainty of the LT500 and AT200 assemblies 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 pressure, temperature, and conductivity measurements*. The second details uncertainties associated with temporally averaged data products. A diagram detailing the data flow and known sources of uncertainty are displayed in Figure 6.

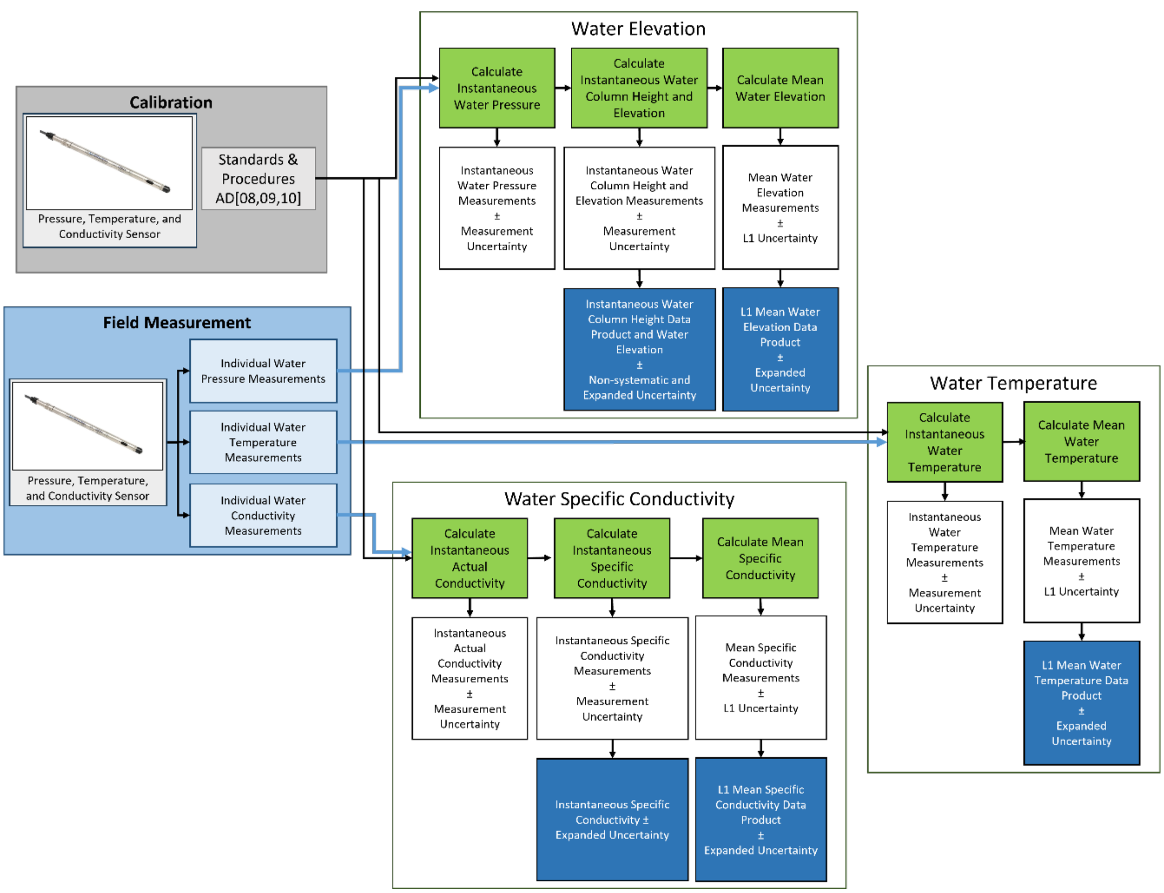

Figure 4. Displays the data flow and associated uncertainties of individual measurements of surface water pressure, temperature, conductivity, and associated L1 DPs.

6.1.1 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. These uncertainties should not be confused with those presented in Section 6.1.2. We urge the reader to refer to AD[8] for further details concerning the discrepancies between quantification of measurement uncertainties and L1 uncertainties.

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

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

$$u_c(y) = \left(\sum_{i=1}^{N} \left(\frac{\partial f}{\partial x_i} \right)^2 u^2(x_i) \right)^{\frac{1}{2}} \tag{14}$$

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 measurement can be found by summing the input uncertainties in quadrature. For surface water pressure, temperature, and conductivity measurements, the sources of uncertainty are discussed below.

6.1.1.1 DAS

The In-Situ LT500 and AT200 sensors 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.

6.1.1.2 Calibration

Uncertainties associated with the calibration process of the LT500 for surface water pressure, 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, stored in the CI data store, and applied to all *individual pressure, temperature, and conductivity measurements* (that is, the uncertainty values do not vary with any specific sensor, DAS component, etc.).

A change in pressure calibration set points was implemented in January 2024 when it was determined that lower pressure set points were necessary to obtain low pressure accuracy that met observatory objectives. Calibrations and deployments of sensors from 2024 onward include calibration set points of 10, 5, and 1 kPa and a verification at atmospheric (0 kPa gauge). All pressures are verified to not exceed an error of 0.1 kPa. Uncertainty values published in the Elevation of Surface Water data product (DP1.20016.001) for data collected prior to 2024 were verified to represent the impacts from this change and uncertainty will be reassessed to characterize this improvement. A detailed summary of the calibration procedures and corresponding uncertainty estimates can be found in AD[8,9,12].

6.1.1.3 Surface Water Temperature

There is no additional uncertainty beyond the measurement and calibration uncertainties that needs to be considered.

6.1.1.4 Surface Water Sensor Elevation

Spatial error is a principal source of uncertainty in the calculation of the surface water elevation. Each sensor's location is surveyed upon installation of the sensor infrastructure. The surveyed location information and associated uncertainties are stored in the named location database. The sensor elevation uncertainties include the survey uncertainty ($u_C(E_{Sensor})$), which accounts for the uncertainty of the sensor's location in relation to other sensors at that NEON site. The named location database also contains the real-world uncertainty, which is the uncertainty of the GPS coordinates used to transform the sensor elevation to meters above sea level.

6.1.1.4.1 Density of Water

Density of water is a function of temperature, pressure, and dissolved ions (conductivity). The density of pure water at 4°C is 1000 kg/m^3. 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/m^3. The density of water is part of the calculation of surface water column height as shown in Equation 3. A change of 1 kg/m^3 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/m^3.

6.1.1.5 Surface Water Specific Conductivity

The calculation of specific conductivity from actual conductivity and ambient temperature in Equation 11 is a normalization process that compounds the standard errors of both measurements. The uncertainty of individual specific conductivity measurements is calculated as follows:

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

Taking the partial derivatives in Equation 15yields:

$$\boldsymbol{u(SpC_{SW,i}) = \left[\left(\frac{1}{1 + 0.0191(T_{SW,i} - 25)}\right)^{2} \times (u_{A1,C} \times C_{SW,i})^{2} + \left(\frac{0.0191 C_{SW,i}}{(1 + 0.0191(T_{SW,i} - 25))^{2}}\right)^{2} \times u_{A1,T}{}^{2}\right]^{\frac{1}{2}}} \tag{16}$$

Where:

$u(SpC_{SW,i})$ = uncertainty of individual specific conductivity measurements

6.1.1.6 Combined Measurement Uncertainty

Temperature:
Because the only known quantifiable uncertainties are those provided by CVAL, the combined uncertainty of temperature is equal to the standard uncertainty values provided by CVAL (See Section 2.4).

Pressure:
Because the only known quantifiable uncertainties are those provided by CVAL, the combined uncertainty of actual conductivity is equal to the standard uncertainty values provided by CVAL (See Section 2.4).

Surface Water Elevation:
Because surface water elevation is derived from the pressure measurement and the known elevation of the sensor, the combined uncertainty for individual measurements takes into account the survey elevation uncertainty and the measurement uncertainty provided by CVAL according to:

$$\boldsymbol{u_c(E_{SW,i}) = \left[u_c{}^{2}(E_{sensor}) + u_{A1,P}^{2}\right]^{\frac{1}{2}}} \tag{17}$$

where

$u_c(E_{SW,i})$ = uncertainty of individual surface water elevation measurements

$u_C(E_{Sensor}))$ = uncertainty of the sensor's surveyed elevation

Conductivity:
Because the only known quantifiable uncertainties are those provided by CVAL, the combined uncertainty of actual conductivity is equal to the standard uncertainty values provided by CVAL (See Section 2.4).

Specific Conductivity:
Because specific conductivity is derived from the actual conductivity and temperature measurements, which have uncertainties that are provided by CVAL, the uncertainty of the individual specific conductivity measurements is calculated according to Equation 15 (Section 6.1.1.5).

6.1.2 Uncertainty of the L1 Mean Data Products

The following subsections discuss uncertainties associated with temporally averagedL1 mean data products. As stated previously, it is important to note the differences between the *measurement uncertainties* presented in Section 6.1.1 and the uncertainties presented in the following subsections. The uncertainties presented in the following subsections reflect the uncertainty of a time-averaged mean value, that is, they reflect the uncertainty of a distribution of measurements collected under non-controlled conditions (i.e., those found in the field), as well as any uncertainties in the form of *Truth* and *Trueness* related to the accuracy of the field assembly.

6.1.2.1 Repeatability (Natural Variation)

To quantify the uncertainty attributable to random effects, the distribution of the individual measurements is used. Specifically, the *estimated standard error of the mean (natural variation)* is computed. This value reflects the repeatability of measurements for a specified time period:

$$u_{NAT}(\bar{X}) = \sqrt{\frac{\sigma^2}{n}} \tag{18}$$

Where:

X = measurement, *e.g., surface water pressure, temperature, or conductivity*
$u_{NAT}(\bar{X})$ = standard error of the mean (natural variation)
σ = experimental standard deviation of individual observations for a defined time period
n = number of observations made during the defined period

6.1.2.2 Calibration

The calibration uncertainty for an L1 mean DP is similar to that described in Section 6.1.1.1. However, the uncertainties provided by CVAL (see Section 2.4) do not account for i) individual sensor repeatability, or ii) the variation of sensors' responses over a population (reproducibility). These components estimate the uncertainties due to the accuracy of the instrumentation in the form of *Truth* and *Trueness*, a quantity that is not captured by the standard error of the mean. All values (i.e., conductivity, temperature, and pressure) are constant values that are provided by CVAL and stored in the CI data store. Please refer to AD[10] for further justification regarding evaluation and quantification of this combined uncertainty.

The temperature and conductivity uncertainties provided by CVAL will propagate through to the specific conductivity. This propagation is identical to that shown in 6.1.1.5, however, the uncertainties shown in equations 15 and 16 are replaced with $u_{A3,C}$ and $u_{A3,T}$ respectively such that:

$$u(\overline{SpC_{GW}}) = \left[\frac{\partial \overline{SpC_{GW}}}{\partial \overline{C_{GW}}}^2 \times (u_{A3,C} \times C_{SW,i})^2 + \frac{\partial \overline{SpC_{GW}}}{\partial \overline{T_{GW}}}^2 \times u_{A3,T}{}^2\right]^{\frac{1}{2}} \quad (3)$$

6.1.2.3 Combined Uncertainty

The combined uncertainties for L1 LT500 and AT200 data products are computed by summing the uncertainties from Section 6.1.2.1 and the CVAL provided uncertainties in quadrature:

Conductivity:

$$u_c(\overline{C_{SW}}) = \left[u_{NAT}^2(\overline{C}_{SW}) + u_{A3,C}^2\right]^{\frac{1}{2}} \quad (20)$$

Temperature:

$$u_c(\overline{T_{SW}}) = \left[u_{NAT}^2(\overline{T}_{SW}) + u_{A3,T}^2\right]^{\frac{1}{2}} \quad (21)$$

Pressure:

$$u_c(\overline{P_{SW}}) = \left[u_{NAT}^2(\overline{P}_{SW}) + u_{A3,P}^2\right]^{\frac{1}{2}} \quad (22)$$

6.1.2.4 Surface Water Elevation

The combined uncertainty for surface water elevation includes the combined uncertainties for sensor depth and ground surface. These are discussed above in Section 6.1.1.3.

$$u_c(\overline{E_{SW}}) = \left[u_c{}^2(E_{sensor}) + u_c^2(\overline{P_{SW}})\right]^{\frac{1}{2}} \quad (23)$$

6.1.2.5 Surface Water Specific Conductivity

The combined uncertainty for specific conductivity includes the uncertainties for temperature and conductivity. Thus, the combined uncertainty for specific conductivity is given as:

$$u_c(\overline{SpC_{SW}}) = \left[u_{NAT}^2(\overline{SpC_{SW}}) + \left(\frac{\partial SpC_{SW}}{\partial C_{SW}}^2\right)(u_{A3,C} \times C_{SW})^2 + \left(\frac{\partial SpC_{SW}}{\partial T_{SW}}^2\right) u_{A3,T}{}^2\right]^{\frac{1}{2}} \quad (24)$$

6.1.2.6 Communicating Precision

L1 surface water elevation data products is 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.

6.2 Expanded Uncertainty

The expanded measurement uncertainty is calculated as:

$$U_p = k_p\, u_c \quad (25)$$

Where:

$$U_p = \text{expanded measurement uncertainty at 95\% confidence (°C)}$$
$$K_p = 2;\ \text{coverage factor for 95\% confidence (unitless)}$$
$$u_c = \text{combined uncertainty}$$

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

6.3 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 4. Uncertainty budget for individual measurements. Shaded rows denote the order of uncertainty propagation (from lightest to darkest).

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	$u_{A1,T}$	AD[9]	n/a	n/a
Conductivity	$u_{A1,C}$	AD[9]	n/a	n/a
Pressure	$u_{A1,P}$	AD[9]	n/a	n/a

Table 5. Uncertainty budget for L1 mean DPs. Shaded rows denote the order of uncertainty propagation (from lightest to darkest).

Source of Uncertainty	Uncertainty Component $u(x)$	Uncertainty Value	$\frac{\partial f}{\partial x_i}$	$u_{u_{x_i}}(Y) \equiv \left\lvert\frac{\partial f}{\partial x_i}\right\rvert u(x_i)$
Temperature (individual combined)	$u_c(\bar{T}_{SW})$	Eq. (21)	n/a	n/a
Calibration	$u_{A3,T}$	AD[8]	n/a	n/a
Natural variation	$u_{NAT}(\bar{T}_{SW})$		n/a	n/a
Conductivity (individual combined)	$u_c(\bar{C}_{SW})$	Eq. (20)	n/a	n/a
Calibration	$u_{A3,C}$	AD[8]	n/a	n/a
Natural variation	$u_{NAT}(\bar{C}_{SW})$		n/a	n/a
Specific Conductivity (individual combined)	$u_c(\overline{SpC}_{SW})$	Eq. (24)	Eq. 15,16	Eq. 15,16,24
Temperature (combined truth and trueness)	$u_{A3,T}$	AD[8]	n/a	n/a
Conductivity (combined truth and trueness)	$u_{A3,C}$	AD[8]	n/a	n/a
Pressure (individual combined)	$u_c(\bar{P}_{SW})$	Eq. (22)	n/a	n/a
Calibration	$u_{A3,P}$	AD[8]	n/a	n/a
Natural variation	$u_{NAT}(\bar{P}_{SW})$		n/a	n/a
Surface Water Elevation (individual combined)	$u_c(\bar{E}_{SW})$	Eq. (23)	n/a	n/a

Pressure (individual combined)	$u_{A3,P}$	AD[8]	n/a	n/a
Sensor Elevation	$u_c(E_{sensor})$	Site metadata	n/a	n/a

7 FUTURE PLANS AND MODIFICATIONS

Future system flags may be incorporated into the data stream and included in the QA/QC summary DP ($Qsum_{5min}$) that summarizes any flagged data that went into the computation of the L1 DP.

It is planned that a QA/QC flag for data consistency is applied according to a developed consistency analysis (AD[05) and a pass/fail flag will be generated to reflect this activity. Pressure at each surface water level measurement location in at a given NEON aquatic site will have the time series data compared against the measurement variance at co-located water level measurement locations. If a difference between the measurements is less than the defined limits, provided by AQU and maintained in the CI data store, then the sensor will have passed the consistency analysis. Alternatively, a difference outside the defined limits will result in a failed test and will be flagged as such. L1 DPs that fail the consistency analysis will continue to be reported, but will have an associated failed flag that will be include in the QA/QC summary.

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