NEON ALGORITHM THEORETICAL BASIS DOCUMENT (ATBD): GROUNDWATER TEMPERATURE, ELEVATION AND SPECIFIC CONDUCTANCE

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Change Record

REVISION	DATE	ECO #	DESCRIPTION OF CHANGE
A	08/10/2016	ECO-03872	Initial Release
B	12/06/2019	ECO-05976	Update to sensor elevation algorithm and information
C	03/16/2022	ECO-06785	Update to reflect change in terminology from relocatable to gradient sites.
D	02/14/2024	ECO-07087	Updated uncertainty and flagging. Added information related to processing in the pachyderm pipeline including log files.
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 groundwater temperature, elevation (stage), and specific conductance measurements made in groundwater observation wells at all NEON aquatic sites. Specifically, the processes necessary to convert "raw" sensor measurements into meaningful scientific units and their associated uncertainties are described. Groundwater temperature, elevation and specific conductance are continuously monitored by NEON at core and gradient aquatic sites using a single sensor (In-Situ, Inc. Aqua Troll 200, AT200).

1.1 Purpose

This document details the algorithms used for creating NEON Level 1 data products for groundwater temperature, elevation, 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 Aqua Troll 200 (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 groundwater temperature, elevation, and specific conductance is described in this document. The AT200 is a multiparameter probe, which 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.005004	NEON Level 1-3 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.000751	CVAL Transfer of standard procedure
AD[11]	NEON.DOC.000927	NEON Calibration and Sensor Uncertainty Values
AD[12]	NEON.DOC.001113	Quality Flags and Quality Metrics for TIS Data Products
AD[13]	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
PRT	Platinum resistance thermometer
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, a lookup table is provided 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 Temperature sensor
C_{T1}	CVALA1		Calibration coefficient for AT200 Temperature sensor
C_{T3}	CVALA2		Calibration coefficient for AT200 Temperature sensor
C_{P0}	CVALB0		Calibration coefficient for AT200 Pressure sensor
C_{P1}	CVALB1		Calibration coefficient for AT200 Pressure sensor
C_{P2}	CVALB2		Calibration coefficient for AT200 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

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

3 DATA PRODUCT DESCRIPTION

3.1 Variables Reported

The groundwater related L1 DPs provided by the algorithms documented in this ATBD are displayed in the accompanying files: *PublicationWorkbook_Elevation of groundwater.txt, PublicationWorkbook_Temperature of groundwater.txt,* and *PublicationWorkbook_Specific conductivity in groundwater.txt*.

3.2 Input Dependencies

Table 1 details the AT200-related L0 DPs used to produce L1 groundwater DPs in this ATBD.

Table 1. List of AT200-related L0 DPs that are transformed into L1 groundwater DPs in this ATBD.

Description	Sample Frequency	Units	Data Product Number
Groundwater Pressure	.00333 Hz	kPa	NEON.DOM.SITE.DP0.20015.001.01376.HOR.VER.000
Groundwater Temperature	.00333 Hz	° C	NEON.DOM.SITE.DP0.20015.001.01374.HOR.VER.000
Groundwater Conductance	.00333 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 AT200 sensors are located at each NEON aquatic site. AT200 sensors are in each of groundwater observation well, hereafter referred to as a well, at NEON aquatic sites. Data from each AT200 are sent to the aquatic portal for ingest through wireless data transmission. Special case scenarios will exist in the network where wireless data transmission is not feasible, in which case the data will need to be manually downloaded from each sensor approximately every3 months.

3.4 Temporal Resolution and Extent

Measurement of temperature, level, and conductivity (TLC) will occur every 5 minutes in each well. The AT200s are programmed to obtain data simultaneously from all wells and will measure and report the specific TLC parameters as a linear average. Each sensor is internally programmed to collect three individual measurements for each TLC 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 averaged measurements.

3.5 Spatial Resolution and Extent

A single AT200 is in each well at each aquatic site. The number of wells will vary between sites due to various reasons, but will range from 6-8 per site, and are positioned around or on one side of the aquatic feature (stream, river, lake) based on site dependent constraints such as topography or landowner permission. Within each well the AT200 sensor is positioned near the lower portion of the screened casing of the well, to minimize the potential that the sensor goes above the water table surface in the well. Figure 1 shows a cross-section of a typical well illustrating the positioning of the sensor with respect to the well screen and the water table. Details to sensor function and why this is important are presented in Section 4.1 below.

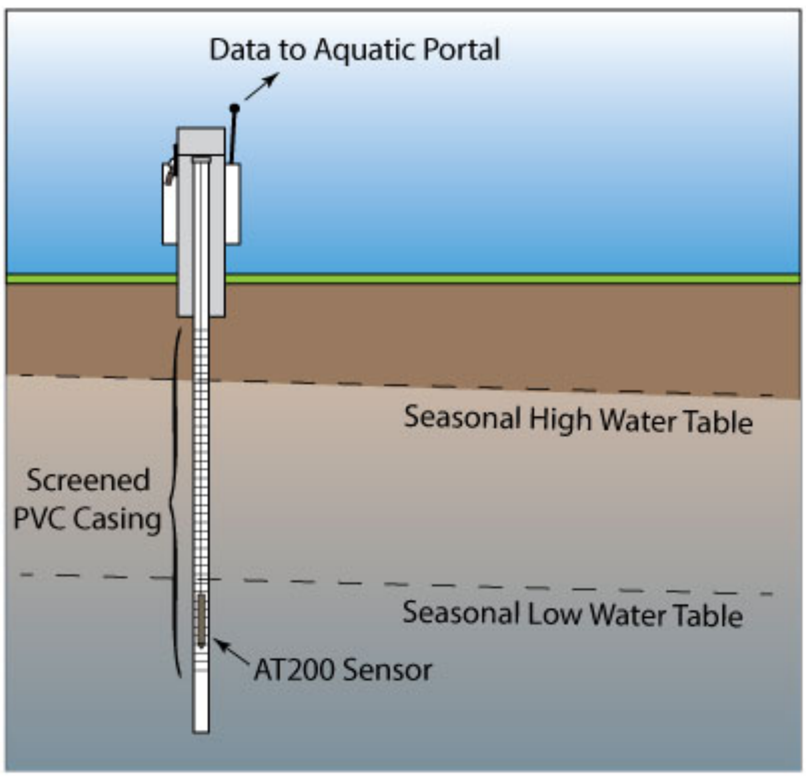

Figure 1. Cross-section of a typical well illustrating the location of the sensor compared to the well screen and the water table, including seasonal variations.

4 SCIENTIFIC CONTEXT

Groundwater level, temperature, and specific conductance are fundamental parameters to monitor as a proxy for determining groundwater movement and quality. Groundwater is the water contained in the soils beneath the surface of the earth. Typically, this water has fallen on the surface of the earth in some form of precipitation (rain/snow), has percolated into the soils or rocks, and has seeped downward into the earth until it hit a relatively impermeable layer of soil or rock. This layer creates a lower bound for further infiltrating water to pool up on creating a layer of saturation in the soils and rocks beneath the earth's surface. Due to gradients (e.g., topographical, pressure) groundwater moves, albeit very slowly, through the soils beneath our feet. The zone of saturated media is bounded at the top by air and the interface between the fully saturated media and the unsaturated media is termed the water table. Technically it's defined as the point in the vertical soil profile where the hydrostatic pressure of water is zero, since just above this point there a negative hydrostatic pressure due to capillary action, and below this point the depth below water table surface increases and thus the hydrostatic pressure increases.

Water table elevation is the key parameter used in tracking the rate and/or volume of groundwater movement through the subsurface. This is done by comparing the water table elevation between several wells; and relies on accurately knowing the spatial orientation of an array of groundwater wells and sensor positioning in each well. Water flows in the direction of decreasing hydrostatic gradient and as such, knowing the water table elevations in each well and the distance between wells allows for mapping and calculating the seasonal rates and variations in groundwater flow paths, volumes, and movement rates. Knowing groundwater flow rate is critical in the ability to calculate ecosystem processes such as estimating water budgets, calculating nutrient fluxes, or examining surface water groundwater interactions.

Groundwater temperature plays an important role in regulating surface water temperature in streams, which is critical to supporting aquatic life as many aquatic organisms can only survive in a limited temperature range. Groundwater temperature fluctuates slightly between day and night (diurnal cycling) and more so during seasonal changes but below about 4 meters tends to stay relatively consistent throughout the year.

Groundwater specific conductance is a measure of the concentration of ionic solutes dissolved in the groundwater. 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.

4.1 Theory of Measurement

The AT200 contains three sensors, one for each parameter - level, temperature, and conductance. The AT200 converts the analog measurements to digital signals internally and is the only output option from sensor. Obtaining raw analog signals are not possible from this sensor. The following paragraphs in this section detail how the sensor makes each measurement.

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 is 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 Groundwater Pressure

Groundwater elevation is determined by first knowing the pressure of the water above the sensor measurement point. This is done through the use for a pressure transducer in the AT200, 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. The sensor head is a diaphragm-like impermeable membrane, which 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 AT200 is 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.

4.1.2 Groundwater Temperature

Temperature is derived from the 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 Groundwater 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 below 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 Groundwater Surface Elevation Algorithm

Calibrated groundwater pressure is used to calculate the groundwater elevation. Groundwater pressure is determined by applying the calibration coefficients, supplied by CVAL, to the "raw" sensor output as follows:

$$\boldsymbol{P_{GW,i} = C_{P2} * P_i^2 + C_{P1} * P_i + C_{P0}} \quad (1)$$

Where:

P_{GW,i_i} = Individual (1/300 Hz) groundwater 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 (1/300 Hz) pressure output from sensor (kPa)

The elevation of the water table surface is the key point to measuring the hydrostatic pressure in the well and is calculated by knowing the depth from the ground surface at the well to the sensor in the well. The water pressure can be converted to a length term by:

$$\boldsymbol{E_{GW,i} = E_{sensor,i} + 1000 \times (P_{GW,i} / (\rho_{water} \times g))} \quad (2)$$

Where:

$E_{GW,i}$ = Individual (1/300 Hz) elevation of the water table (m-ASL)
$E_{sensor,i}$ = Elevation of the sensor within the i^{th} well (m-ASL) = ELEVATION + Z_OFFSET in the Named Location Database
$P_{GW,i}$ = Individual (1/300 Hz) hydrostatic pressure (from sensor) (kPa)
ρ_{water} = Density of water, 999 (kg/m^3)
g = *Acceleration due to* gravity, 9.81 (m/s^2)

During the construction of each aquatic site, groundwater wells are surveyed and the ground surface elevation ($GS_{well,i}$) at each well is determined. The surveyed location information is stored in the Named Location Database as an ELEVATION of the survey point. In addition, the depth of the sensor below ground surface is measured and stored in the Named Location Database as a Z_OFFSET. These values of the sensor depth are combined to provide the elevation of the sensor ($E_{sensor,i}$). The locations as well as the longitude and latitude for each groundwater well will are stored in the Named Location Database for each NEON AQU site. Based on the design of the wells and AT200 mounting hardware, removal of the sensor should not interfere with the ability to replace the sensor in the same location in the well.

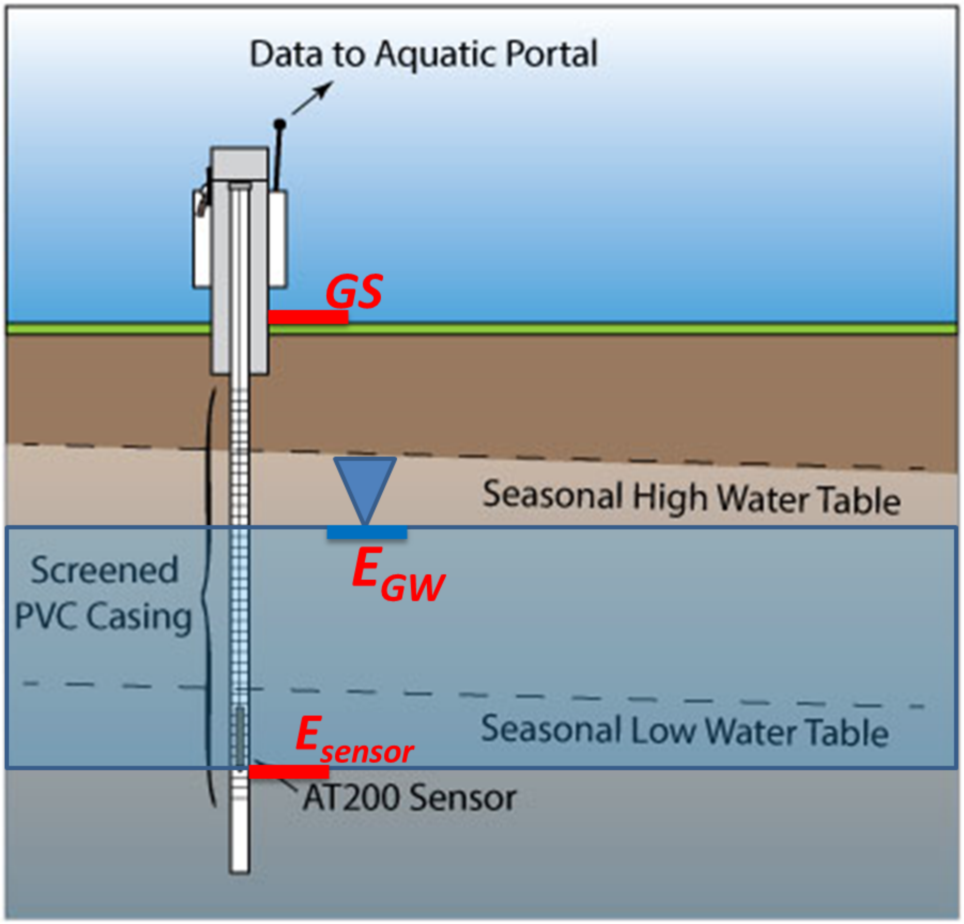

Figure 2. Picture showing the reference points for the elevation of the ground surface (*GS*), elevation of the sensor (E_{sensor}) and the groundwater elevation (E_{GW}).

Groundwater elevation is reported as the instantaneous 5-minute measurement and a 30-minute average. The instantaneous groundwater surface elevation ($E_{GW,i}$) shall be calculated to create the 30-minute average as:

$$\overline{E_{30}} = \frac{1}{n} \sum_{i=1}^{n} E_{GW,i} \tag{3}$$

Where for each 30-minute averaging, n is the number of measurements in the averaging period and $E_{GW,i}$ is the groundwater elevation calculated from the 1/300 Hz pressure measurement according to equations 1-2 above during the 30-minute averaging period. For a 30-minute average, n = 6 if all points are included [0,6).

4.2.2 Groundwater Temperature Algorithm

Groundwater temperature is reported as the instantaneous 5-minute measurement and a 30-minute average. The instantaneous (0.003 Hz) temperature is determined accordingly to create additional L1 DPs:

$$\boldsymbol{T_{GW,i} = C_{T2} * T_i^2 + C_{T1} * T_i + C_{T0}} \tag{4}$$

Where:

$T_{GW,i}$ = Individual (1/300 Hz) groundwater 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 (1/300 Hz) temperature output from sensor (°C)

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

$$\boldsymbol{\overline{T_{30}} = \frac{1}{n} \sum_{i=x}^{n} T_{GW,i}} \tag{5}$$

Where for each 30-minute averaging, n is the number of measurements in the averaging period and $T_{GW,i}$ is the groundwater temperature calculated from the 1/300 Hz temperature measurement according to equation 4 above during the 30-minute averaging period. For a 30-minute average, n = 6 if all points are included [0,6).

4.2.3 Groundwater 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 groundwater conductivity is determined by applying the calibration coefficients, supplied by CVAL, to the "raw" sensor output as follows:

$$\boldsymbol{C_{GW,i} = C_{C2} * C_i^2 + C_{C1} * C_i + C_{C0}} \tag{6}$$

Specific conductivity will then be calculated from actual conductivity and temperature using the calibrated 5-minute values according to Eq.7.

$$\boldsymbol{SpC_{GW,i} = \frac{C_{GW,i}}{1+0.0191(T_{GW,i}-25)}} \tag{7}$$

where:

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

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

After conductivity is temperature corrected to produce specific conductance (SpC_{GW}), 30-minute average of specific conductance ($\overline{SpC_{30}}$) is determined accordingly to create L1 DPs:

$$\overline{\boldsymbol{SpC_{30}}} = \frac{1}{n}\sum_{i=x}^{n} \boldsymbol{SpC_{GW,i}} \qquad (8)$$

Where for each 30-minute averaging, n is the number of measurements in the averaging period and $SpC_{GW,i}$ is the groundwater specific conductivity calculated from the 1/300 Hz conductivity measurement according to equation 6 above during the 30-minute averaging period. For a 30-minute average, n = 6 if all points are included [0,6).

5 ALGORITHM IMPLEMENTATION

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

1. Calibration coefficients are applied to instantaneous 5-minute groundwater pressure value (P_i) according to Equation 1.
2. Calibration coefficients are applied to instantaneous 5-minute groundwater temperature (T_i) according to Equation 3.
3. Calibration coefficients are applied to instantaneous 5-minute groundwater conductivity (C_i) according to Equation 6.
4. Groundwater pressure (P_{GW}) is converted to groundwater Surface Elevation (E_{GW}) according to Equation 2.
5. Groundwater conductivity (C_{GW}) is converted to Specific Conductivity (SpC_{GW}) according to Equation 7*.
6. QA/QC Plausibility tests are applied to the AT200 pressure, temperature, and conductivity data streams in accordance with AD[06]. The details are provided below.
7. Signal de-spiking is applied to the AT200 pressure, temperature, and conductivity data stream in accordance with AD[07].
8. 30-minute averages are calculated for Groundwater Temperature ($\overline{T_{30}}$), Groundwater Surface Elevation ($\overline{E_{30}}$) and Specific Conductivity ($\overline{SpC_{30}}$) according to Equations 3, 5, and 8 respectively.
9. Descriptive statistics, i.e., minimum, maximum, and variance, are determined for thirty-minute averages.
10. Quality metrics, quality flags, and the final quality flag is produced for thirty-minute average according to AD[12].

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

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

1. **Plausibility Tests** – All plausibility tests are determined for groundwater pressure, temperature, and conductivity (AD[06]). Test parameters are provided by AQU and maintained in the CI data store. All plausibility tests are applied to the sensor's L0 DP and an 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[07]. 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[12] – In addition to the quality flags described in AD[12], 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.

    If a datum fails one of the following tests it will not be used to create a L1 DP: ***zeroPressure, missingTemp, range***, ***persistence***, ***step, null and gap***. 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[12]. 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 AT200 measurements.

Tests	Groundwater Elevation	Groundwater Temperature	Groundwater Specific Conductance
zeroPressure	x	x	x
missingTemp			x
Range	x	x	x
Persistence	x		
Step	x	x	x
Null	x	x	x
Gap	x	x	x
LogData	x	x	x
LogDateError	x	x	x

Tests	**Groundwater Elevation**	**Groundwater Temperature**	**Groundwater Specific Conductance**
Alpha	x	x	x
Beta	x	x	x
Final quality flag	x	x	x

Table 3. Information maintained in the CI data store for with AT200.

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[9]
Final Quality Flag	AD[12]

6 UNCERTAINTY

Uncertainty of measurement is inevitable; therefore, measurements should be accompanied by a statement of their uncertainty for completeness (JCGM 2008; Taylor 1997). To do so, it is imperative to identify all sources of measurement uncertainty related to the quantity being measured. Quantifying the uncertainty of AIS measurements will provide a measure of the reliability and applicability of individual measurements and AIS data products. This portion of the document serves to identify, evaluate, and quantify sources of uncertainty relating to individual, calibrated groundwater measurements as well as L1 mean groundwater DPs. It reflects the information described in AD[11] and is explicitly described for the In-Situ AT200 in the following sections.

6.1 Uncertainty of Groundwater Measurements

Uncertainty of the AT200 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 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 3.

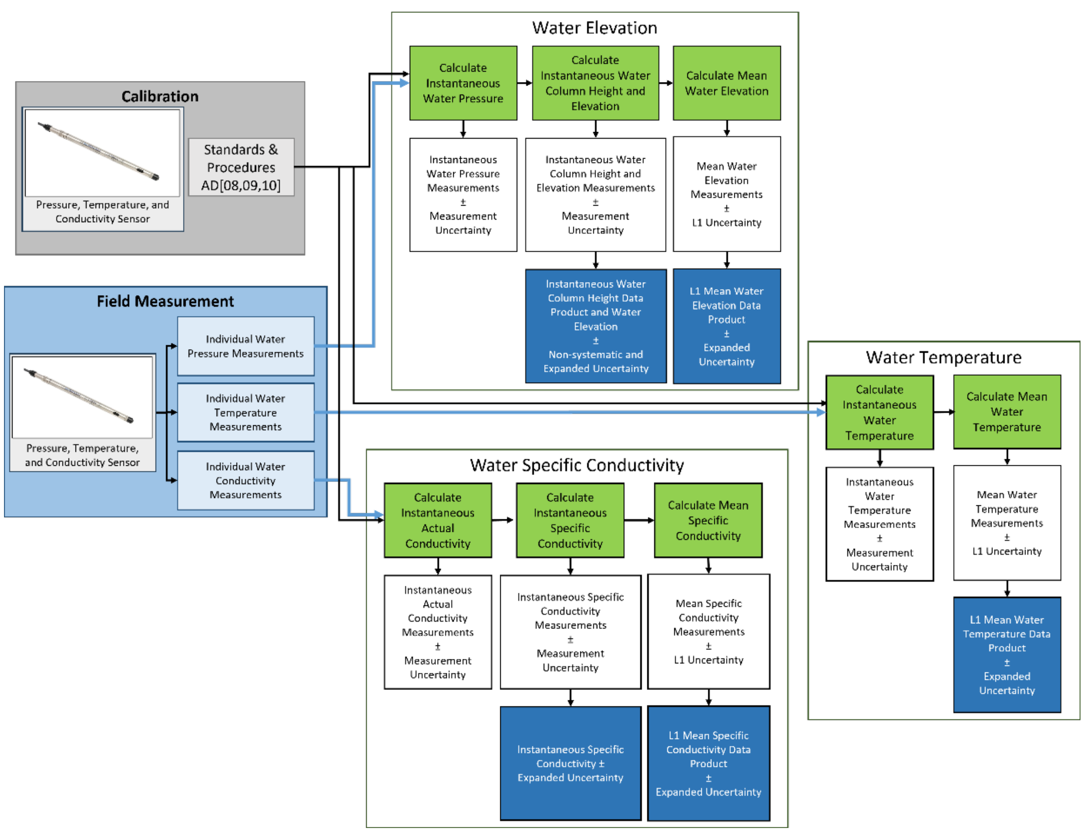

Figure 3. Displays the data flow and associated uncertainties of individual measurements of groundwater pressure, temperature, and conductivity and associated L1 DPs.

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:

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

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

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 be summing the input uncertainties in quadrature. For groundwater pressure, temperature and conductivity measurements, the sources of uncertainty are discussed below.

6.1.1.1 DAS

The In-Situ AT200 sensor has an internal Analog to Digital (A/D) converter and outputs 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 AT200 for groundwater 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 Groundwater data product (DP1.20100.001) 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[8,9,13].

6.1.1.3 Groundwater Temperature

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

6.1.1.4 Groundwater Sensor Elevation

Spatial error is a principal source of uncertainty in the calculation of the groundwater 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 equals 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. Groundwater in non-coastal areas has relatively low conductance and does not affect the density of water beyond .001 kg/m^3. Temperature of 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 groundwater surface elevation as shown in Equation 2. 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 Groundwater Specific Conductivity

The calculation of specific conductivity from actual conductivity and ambient temperature in Equation 7 is a normalization process that compounds the standard errors of both measurements. The uncertainty of individual specific conductivity measurements is calculated as follows:

$$u(SpC_{GW,i}) = \left[\frac{\partial SpC_{GW,i}}{\partial C_{GW,i}}^2 \times (u_{A1,C} \times C_{GW,i})^2 + \frac{\partial SpC_{GW,i}}{\partial T_{GW,i}}^2 \times u_{A1,T}{}^2\right]^{\frac{1}{2}} \tag{10}$$

Taking the partial derivatives in Equation 10 yields:

$$u(SpC_{GW,i}) = \left[\left(\frac{1}{1 + 0.0191(T_{GW,i} - 25)}\right)^2 \times (u_{A1,C} \times C_{GW,i})^2 + \left(\frac{0.0191C_{GW,i}}{(1 + 0.0191(T_{GW,i} - 25))^2}\right)^2 \times u_{A1,T}{}^2\right]^{\frac{1}{2}} \tag{11}$$

Where

$u(SpC_{GW,i})$ = 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 simply 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 pressure is simply equal to the standard uncertainty values provided by CVAL (See Section 2.4).

Groundwater Surface Elevation:
Because groundwater surface elevation is derived from the pressure measurement and the known elevation of the sensor, the combined uncertainty for individual measurements considers the positional uncertainty stored in the Named Location Database and the pressure measurement uncertainty provided by CVAL according to:

$$u_c(E_{GW,i}) = \left[\frac{\partial E_{GW,i}}{\partial E_{sensor}}^2 \times u_C{}^2(E_{sensor}) + \frac{\partial E_{GW,i}}{\partial P_{GW,i}}^2 \times u_{A1,P}{}^2\right]^{\frac{1}{2}} \tag{12}$$

The partial derivatives in Equation 14 become:

$$\boldsymbol{u_c(E_{GW,i})} = \left[\mathbf{1} \times \boldsymbol{u_C}^2(\boldsymbol{E_{sensor}}) + \left(\frac{\mathbf{1000}}{\boldsymbol{\rho g}}\right)^{\mathbf{2}} \times \boldsymbol{u_{A1,P}}^2\right]^{\frac{1}{2}} \tag{13}$$

Where:

$u_c\left(E_{GW,i}\right)$ = uncertainty of individual groundwater 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 simply 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 10 (Section 6.1.1.5).

6.1.2 Uncertainty of the L1 Mean Data Products

The following subsections discuss uncertainties associated with temporally averaged, i.e., L1 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:

$$u_{NAT}(\bar{X}) = \sqrt{\frac{\sigma^2}{n}} \quad (14)$$

Where

X = measurement, *e.g., groundwater 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 a 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 10 and 11 are replaced with $u_{A3,C}$ and $u_{A3,T}$ respectively such that:

$$\boldsymbol{u(\overline{SpC_{GW}})} = \left[\frac{\boldsymbol{\partial \overline{SpC_{GW}}}}{\boldsymbol{\partial \overline{C_{GW}}}}^2 \times (\boldsymbol{u_{A3,C}} \times \boldsymbol{C_{SW}})^2 + \frac{\boldsymbol{\partial \overline{SpC_{GW}}}}{\boldsymbol{\partial \overline{T_{GW}}}}^2 \times \boldsymbol{u_{A3,T}}^2\right]^{\frac{1}{2}} \quad (15)$$

6.1.2.3 Combined Uncertainty

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

Conductivity:

$$\boldsymbol{u_c(\overline{C_{GW}})} = \left[\boldsymbol{u^2_{NAT}(\overline{C}_{GW})} + \boldsymbol{u^2_{A3,C}}\right]^{\frac{1}{2}} \quad (16)$$

Temperature:

$$\boldsymbol{u_c(\overline{T_{GW}})} = \left[\boldsymbol{u^2_{NAT}(\overline{T}_{GW})} + \boldsymbol{u^2_{A3,T}}\right]^{\frac{1}{2}} \quad (17)$$

Pressure:

$$u_c(\overline{P_{GW}}) = \left[u_{NAT}^2(\overline{P}_{GW}) + u_{A3,P}^2 \right]^{\frac{1}{2}} \quad (18)$$

6.1.2.4 Groundwater Elevation

The combined uncertainty for groundwater elevation includes the combined uncertainties for sensor depth and ground surface. These are discussed above in Section 6.1.1.4.

$$u_c(\overline{E_{GW}}) = \left[u_c{}^2(E_{sensor}) + \left(\frac{1000}{\rho g}\right)^2 u_c^2(\overline{P_{GW}}) \right]^{\frac{1}{2}} \quad (19)$$

6.1.2.5 Groundwater 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:

$$u_c(\overline{SpC_{GW}}) = \left[u_{NAT}^2(\overline{SpC_{GW}}) + \left(\frac{\partial SpC_{GW}{}^2}{\partial C_{GW}}\right)(u_{A3,C} \times C_{GW})^2 + \left(\frac{\partial SpC_{GW}{}^2}{\partial T_{GW}}\right) u_{A3,T}{}^2 \right]^{\frac{1}{2}} \quad (20)$$

6.1.2.6 Communicating Precision

L1 groundwater elevation data products are 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:

$$U_p = k_p \, u_c \quad (21)$$

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	$\frac{\partial f}{\partial x_i}$	$u_{u_{x_i}}(Y) \equiv \left\|\frac{\partial f}{\partial x_i}\right\| u(x_i)$
Temperature (individual combined)	$u_c(\bar{T}_{GW})$	Eq. (17)	n/a	n/a
Calibration	$u_{A3,T}$	AD[8]	n/a	n/a
Natural variation	$u_{NAT}(\bar{T}_{GW})$		n/a	n/a
Conductivity (individual combined)	$u_c(\bar{C}_{GW})$	Eq. (16)	n/a	n/a
Calibration	$u_{A3,C}$	AD[8]	n/a	n/a
Natural variation	$u_{NAT}(\bar{C}_{GW})$		n/a	n/a
Specific Conductivity (individual combined)	$u_c(\overline{SpC}_{GW})$	Eq. (20)	Eq. 10,11	Eq. 10,11,20

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)	$u_c(\bar{P}_{GW})$	Eq. (18)	n/a	n/a
Calibration	$u_{A3,P}$	AD[8]	n/a	n/a
Natural variation	$u_{NAT}(\bar{P}_{GW})$		n/a	n/a
Groundwater Elevation (individual combined)	$u_c(\bar{E}_{GW})$	Eq. (19)	n/a	n/a
Pressure (individual combined)	$u_{A3,P}$	AD[9]	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 are applied according to a developed consistency analysis (AD[05) and a pass/fail flag are generated to reflect this activity. Pressure, temperature, and conductivity measurements from each well 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 are flagged as such. L1 DPs that fail the consistency analysis will continue to be reported, but will have an associated failed flag that are include in the QA/QC summary.

8 BIBLIOGRAPHY

In-Situ, Inc. (2012) In-Situ Level TROLL 300, 500, 700 and BaroTROLL Operator's Manual http://www.in-situ.com/manuals

JCGM (2012) International vocabulary of metrology – Basic and general concepts and associated terms (VIM). 3rd Edition. pp. 92

Joint Committee for Guides in Metrology (JCGM) (2008) Evaluation of measurement data – Guide to the expression of uncertainty in measurement. pp. 120.

Taylor, J. R. (1997) An Introduction to Error Analysis: The Study of Uncertainties in Physical Measurements. University Science Books, Mill Valley, California. 2nd Ed. pp. 327.

Wilde, F.D., ed., variously dated, Field measurements: U.S. Geological Survey Techniques of Water-Resources Investigations, book 9, chap. A6, with sec. 6.0–6.8, accessed September 30, 2013, at http://pubs.water.usgs.gov/twri9A6/