

<i>Title:</i> NEON Algorithm Theoretical Basis Document (ATBD) – TIS Soil Temperature		<i>Date:</i> 06/13/2016
<i>NEON Doc. #:</i> NEON.DOC.001571	<i>Author:</i> E. Ayres	<i>Revision:</i> A

NEON ALGORITHM THEORETICAL BASIS DOCUMENT (ATBD)

TIS SOIL TEMPERATURE

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See configuration management system for approval history.

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Change Record

REVISION	DATE	ECO #	DESCRIPTION OF CHANGE
A	06/13/2016	ECO-03907	Initial Release

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1 DESCRIPTION

Contained in this document are details concerning temperature measurements made at all NEON sites. Specifically, the processes necessary to convert “raw” sensor measurements into meaningful scientific units and their associated uncertainties are described. Soil temperature profiles will be ascertained by installing sensors at various depths below the soil surface in each of the 5 TIS soil plots at NEON core and relocatable sites.

1.1 Purpose

This document details the algorithms used for creating NEON Level 1 data products for Soil Temperature from Level 0 data, and ancillary data as defined in this document (such as calibration data) obtained via instrumental measurements made by the soil temperature sensor. 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 Soil Temperature is described in this document. The soil temperature sensor employed is the Thermometrics Climate RTD 100 Ω Probe. This document does not provide computational implementation details, except for cases where these stem directly from algorithmic choices explained here.

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2 RELATED DOCUMENTS, ACRONYMS AND VARIABLE NOMENCLATURE

2.1 Applicable Documents

AD[01]	NEON.DOC.000782	ATBD QA/QC Data Consistency
AD[02]	NEON.DOC.011081	ATBD QA/QC plausibility tests
AD[03]	NEON.DOC.000783	ATBD De-spiking and time series analyses
AD[04]	NEON.DOC.000746	Evaluating Uncertainty (CVAL)
AD[05]	NEON.DOC.000442	NEON Sensor Command, Control and Configuration – Soil Temperature Profile
AD[06]	NEON.DOC.000723	Triple Point Temperature Calibration Fixture
AD[07]	NEON.DOC.002002	Engineering Master Location Sensor Matrix
AD[08]	NEON.DOC.000784	ATBD Profile Development
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.001606	System Integration and Verification Test Report: Soil Temperature Profile

2.2 Reference Documents

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

2.3 Acronyms

Acronym	Explanation
AIS	Aquatic Instrument System
ATBD	Algorithm Theoretical Basis Document
CI	NEON Cyberinfrastructure
CVAL	NEON Calibration, Validation, and Audit Laboratory
DAS	Data Acquisition System
DP	Data Product
FDAS	Field Data Acquisition System
GRAPE	Grouped Remote Analog Peripheral Equipment
Hz	Hertz
L0	Level 0
L1	Level 1

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PRT	Platinum resistance thermometer
N/A	Not Applicable
NOAA	National Oceanic Atmospheric Administration
RTD	Resistance Temperature Detectors
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 in order to distinguish what symbols specific variables can be tied to in the following document.

Symbol	Internal Notation	Description
C_0	CVALA0	CVAL PRT calibration coefficient
C_1	CVALA1	CVAL PRT calibration coefficient
C_2	CVALA2	CVAL PRT calibration coefficient
O_R	U_CVALR4	offset imposed by the FDAS for resistance readings (Ω)
u_{A1}	U_CVALA1	Combined, relative uncertainty of PRT sensor (%)
u_{A3}	U_CVALA3	Combined, relative uncertainty (truth and trueness only) of PRT sensor (%)
u_{R1}	U_CVALR1	Combined, relative uncertainty of Field DAS resistance readings (%)
u_{R3}	U_CVALR3	Combined, relative uncertainty (truth and trueness only) of Field DAS resistance readings (%)

3 DATA PRODUCT DESCRIPTION

3.1 Variables Reported

The Soil Temperature related L1 DPs provided by the algorithms documented in this ATBD are displayed in the accompanying file `stp_datapub_NEON.DOC.003785.txt`.

3.2 Input Dependencies

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Table 1 details the Soil Temperature-related L0 DPs used to produce L1 Soil temperature DPs in this ATBD.

Table 3-1: List of Soil Temperature-related L0 DPs that are transformed into L1 Soil Temperature DPs in this ATBD.

Description	Sample Frequency	Units	Data Product Number
soilPRTresistance (R_t)	0.1 Hz	Ω	NEON.DOM.SITE.DP0.00041.001.01728.HOR.VER.000

3.3 Product Instances

Multiple soil temperature sensors will be deployed in each of the five TIS soil plots at NEON core and relocatable sites. At most NEON sites there will be 45 soil temperature sensors (9 sensors per soil plot); however, at sites with very shallow soils, fewer sensors will be deployed.

3.4 Temporal Resolution and Extent

One- and thirty-minute averages of temperature will be calculated to form L1 DPs.

Testing of the soil temperature assembly by NEON indicated a response time of between 318-1295 seconds to achieve a change of 63.2% of the way from temperature 1 to temperature 2 (AD[13]).

3.5 Spatial Resolution and Extent

Each TIS soil plot will contain a profile of soil temperature sensors ranging in depth from approximately 2 cm below the soil surface to 2 m deep at non-permafrost sites or shallower if the soil is shallower. At permafrost sites the profile will extend to approximately 3 m deep or shallower if the soil is shallower. At most TIS soil plots the soil temperature profile will consist of 9 sensors installed at different depths; however, at sites with very shallow soils, fewer soil temperature sensors may be installed.

The different installation depths of temperature sensors within an individual soil plot provide vertical spatial information. The temperature sensors installed across the five TIS soil plots at each NEON core and relocatable site provide horizontal spatial information.

Each soil temperature sensor will represent the point at which it is placed in the soil. Ultimately, a temperature profile will be developed for each soil plot from the soil temperature sensors installed at different depths (see AD[07] for detail on sensor placement for a specific site, and AD[08] for a description of the algorithms used for deriving this profile).

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4 SCIENTIFIC CONTEXT

Temperature is one of the most fundamental physical measurements. It is a primary driving factor for countless physical, chemical, and biological processes. Temperature measurements will provide NEON with ancillary data for numerous other environmental measurements.

4.1 Theory of Measurement

Ultimately, temperature is derived from a PRT. Changes in the PRT resistance due to temperature are determined using a four-wire measurement. The four-wire measurement was chosen due to its decreased dependence on cable length and resistors over the four-wire bridge method. Using a fixed current source the four-wire measurement detects a voltage drop across a resistor using a digital multi-meter (DMM) with high impedance, shown in Figure 1. The voltage drop across the PRT is used, in conjunction with known current source, to calculate the PRT resistance. This measurement technique accomplished by a DMM (i.e. GRAPE) will acquire resistance for NEON operated PRTs.

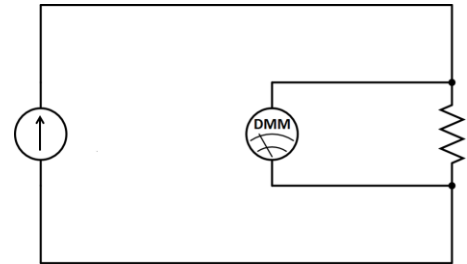


Figure 1. Four-wire measurement for PRT.

4.2 Theory of Algorithm

The PRT is one of the most widely used RTD because platinum has the best linear relationship for changes in resistance to temperature over the greatest temperature range (–200 to 650 °C). Normally, when evaluating temperatures over the entire range of the PRT, the relationship between temperature and resistance for a PRT is expressed by two equations due to a divergence from linearity. However, NEON is concerned with only a fraction of the PRT’s functional range. Thus, within NEON’s desired temperature range the relationship between temperature and resistance is simplified and temperature as a function of resistance is expressed by a single equation (AD[06]):

$$T_i = C_2 R_{T_i}^2 + C_1 R_{T_i} + C_0 \quad (1)$$

Where:

- T_i = Individual (0.1 Hz) Temperature (°C)
- C_0 = Calibration coefficients provided by CVAL (°C)
- C_1 = Calibration coefficients provided by CVAL (°C/Ω)
- C_2 = Calibration coefficients provided by CVAL (°C/Ω²)
- R_{T_i} = Individual (0.1 Hz) resistance at temperature T (Ω)

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After resistance is converted to temperature, one-minute and thirty-minute averages of temperature will be determined accordingly to Eq. (2) and (3) to create the L1 soil temperature DPs in the datapub_NEONDOC000781_1min.csv and datapub_NEONDOC000781_30min.csv files:

$$\bar{T}_1 = \frac{1}{n} \sum_{i=1}^n T_i \quad (2)$$

where, for each 1-minute average, n represents the number of measurements during the averaging period and T_i is a soil temperature measurement obtained during the 60-second averaging period, starting on the minute [hh:mm:00].

Similarly,

$$\bar{T}_{30} = \frac{1}{n} \sum_{i=1}^n T_i \quad (3)$$

where, for each 30-minute average, n represents the number of measurements during the averaging period and T_i is a soil temperature measurement obtained during the 1800-second averaging period, starting at the hour (hh:00:00) and at half past the hour (hh,30:00).

Note: The beginning of the first averaging period in a series shall be the nearest whole minute less than or equal to the first timestamp in the series.

5 ALGORITHM IMPLEMENTATION

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

1. 0.1 Hz resistance data will be converted to temperature, T_i , according to Eq. (1) using PRT calibration coefficients provided by CVAL.
2. QA/QC Plausibility tests will be applied to the data stream in accordance with AD[02], details are provided below.
3. Signal de-spiking will be applied to the data stream in accordance with AD[03].
4. One- and thirty-minute temperature averages will be calculated using Eq. (2) and (3).
5. Descriptive statistics, i.e. minimum, maximum, and variance, will be determined for both one- and thirty-minute averages.
6. Quality metrics, quality flags, and the final quality flag will be produced for one- and thirty-minute averages according to AD[12].

QA/QC Procedure:

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1. **Plausibility Tests AD[02]** – All plausibility tests will be determined for the soil temperature data. Test parameters will be provided by FIU and maintained in the CI data store. All plausibility tests will be applied to the sensor’s converted L0 DPs and associated quality flags (QFs) will be generated for each test.
2. **Signal De-spiking**– Time segments and threshold values for the automated despiking QA/QC routine will be specified by FIU and maintained in the CI data store. QFs from the despiking analysis will be applied according to AD[03].
3. **Quality Flags (QFs) and Quality Metrics (QMs) AD[12]** – If a datum has failed one of the following tests it will not be used to create a L1 DP, *range, de-spiking, and step*. α and β QFs and QMs will be determined using the flags listed in Table 2. In addition, all L1 DPs will have a QA/QC report and quality metric 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 5-1. Flags associated with soil temperature measurements.

Tests
Range
Persistence
Step
Null
Gap
Signal De-spiking
Final quality flag

Table 5-2. Information maintained in the CI data store for soil temperature.

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

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Null	Test limit
Gap	Test limit
Signal Despiking	Time segments and threshold values
Calibration	CVAL sensor specific calibration coefficients
Uncertainty	AD[11]
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 TIS measurements will provide a measure of the reliability and applicability of individual measurements and TIS data products. This portion of the document serves to identify, evaluate, and quantify sources of uncertainty relating to individual, calibrated soil temperature measurements as well as L1 mean soil temperature data products. It is a reflection of the information described in AD[09], and is explicitly described for the soil temperature assembly in the following sections.

1.1 Uncertainty of Temperature Measurements

Uncertainty of soil temperature is discussed in this section. The section is broken down into two topics. The first informs the sources of *measurement* uncertainty, i.e., those associated with *individual temperature measurements*. The second details uncertainties associated with temporally averaged temperature data products. A diagram detailing the data flow and known sources of uncertainty are displayed in Figure 2.

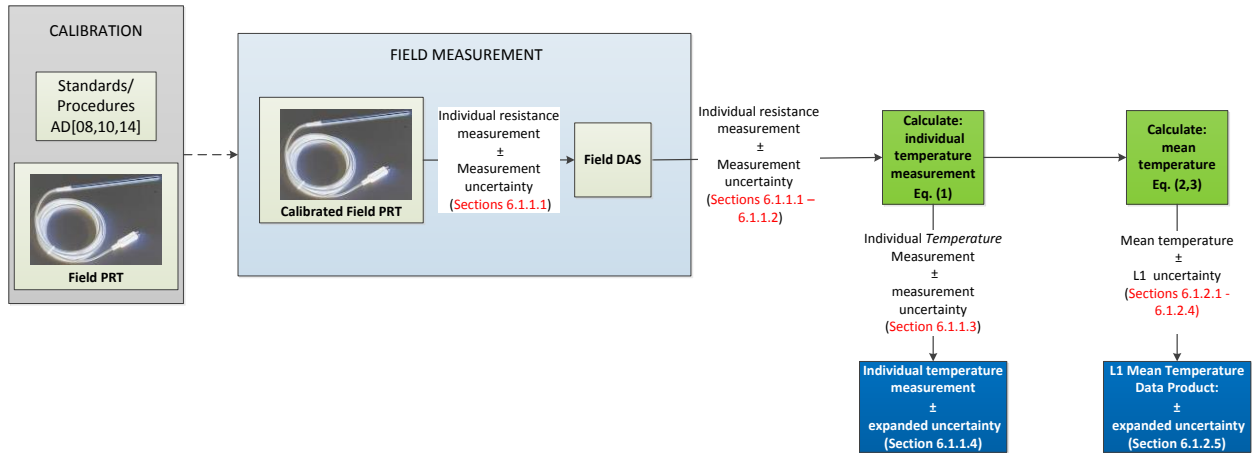


Figure 2: Displays the data flow and associated uncertainties of individual temperature measurements and L1 mean soil temperature DPs. A detailed explanation of the PRT calibration procedures, please refer to AD[08,10,14].

1.1.1 Measurement Uncertainty

The following subsections present the uncertainties associated with *individual temperature 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* temperature measurement. These uncertainties should not be confused with those presented in Section 6.1.2. We urge the reader to refer to AD[09] 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:

$$u_c(y) = \left(\sum_{i=1}^N \left(\frac{\partial f}{\partial x_i} \right)^2 u^2(x_i) \right)^{\frac{1}{2}} \quad (4)$$

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 .

The calculation of these input uncertainties is discussed below.

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1.1.1.1 Calibration

Uncertainties associated with the PRT calibration process propagate into a standard, combined measurement uncertainty. This combined uncertainty, u_{A1} , represents 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). (refer to Eq. (1)). It is a constant value that will be provided by CVAL (AD[11]), stored in the CI data store, and applied to all *individual temperature measurements* (that is, it does not vary with any specific sensor, DAS component, location, etc.). A detailed summary of the calibration procedures and corresponding uncertainty estimates can be found in AD[08,10,14].

1.1.1.2 Field DAS

The uncertainty introduced by the Field DAS (FDAS) through the resistance reading is:

$$u_{FDAS}(R_{Ti}) = (u_{R1} * R_{Ti}) + O_R \quad (5)$$

Where:

- $u_{FDAS}(R_{Ti})$ = standard uncertainty of the resistance measurement introduced by the Field DAS (Ω)
- R_{Ti} = *individual*, raw, resistance measurement (Ω)
- u_{R1} = combined, relative Field DAS uncertainty for resistance measurements provided by CVAL (unitless)
- O_R = offset imposed by the FDAS for resistance readings, provided by CVAL (Ω)

The partial derivative of a temperature measurement with respect to the resistance reading is:

$$\frac{\partial T_i}{\partial R_{Ti}} = (2 * C_2 * R_{Ti}) + C_1; \quad (6)$$

therefore, the uncertainty of a temperature measurement due to the FDAS is:

$$u_{FDAS_{RT}}(T_i) = \left| \frac{\partial T_i}{\partial R_{Ti}} \right| u_{FDAS}(R_{Ti}) \quad (7)$$

where:

- $\frac{\partial T_i}{\partial R_{Ti}}$ = partial derivative of Eq. (1) with respect to R_{Ti} ($^{\circ}\text{C}/\Omega$)
- C_2 = calibration coefficient provided by CVAL ($^{\circ}\text{C}/\Omega^2$)
- C_1 = calibration coefficient provided by CVAL ($^{\circ}\text{C}/\Omega$)

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$u_{FDAS_{RT}}(T_i)$ = standard uncertainty of temperature introduced by the Field DAS through the resistance measurement (°C)

1.1.1.3 Combined Measurement Uncertainty

The combined, standard, measurement uncertainty for an individual temperature measurement, $u_c(T_i)$, is given in units of °C and computed by summing the individual uncertainties in quadrature (Eq. (4)):

$$u_c(T_i) = \left(u_{A1}^2 + u_{FDAS_{RT}}^2(T_i) \right)^{\frac{1}{2}} \quad (8)$$

1.1.1.4 Expanded Measurement Uncertainty

The expanded measurement uncertainty is calculated as:

$$U_{95}(T_i) = k_{95} * u_c(T_i) \quad (9)$$

Where:

$U_{95}(T_i)$ = expanded measurement uncertainty at 95% confidence (°C)
 $k_{95} = 2$; coverage factor for 95% confidence (unitless)

1.1.2 Uncertainty of L1 Mean Temperature Data Product

The following subsections discuss uncertainties associated with L1 mean temperature 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.

1.1.2.1 Repeatability (natural variation)

To determine the validity of the L1 mean temperature DP, its uncertainty must be calculated. The distribution of the individual measurements is used as a metric to quantify this uncertainty. Specifically, the *estimated standard error of the mean (natural variation)* is computed. This value reflects the repeatability of temperature measurements for the specified time period:

$$u_{NAT}(\bar{T}) = \frac{s(T_i)}{\sqrt{n}} \quad [^{\circ}\text{C}] \quad (10)$$

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where $s(T_i)$ is the experimental standard deviation of the temperature observations during the averaging period, and n is the number of observations made over the same time period.

1.1.2.2 Calibration

The uncertainty detailed here is similar to that described in Section 6.1.1.1. However, the relevant uncertainty for the mean DPs, u_{A3} , does not consider i) individual sensor repeatability, or ii) the variation of sensors’ responses over a population of sensors (reproducibility). This component of uncertainty estimates the uncertainty due to the accuracy of the instrumentation in the form of *Truth* and *Trueness*, a quantity which is not captured by the standard error of the mean. It is a constant value that will be provided by CVAL (AD [11]) and stored in the CI data store. Please refer to AD[09] for further justification regarding evaluation and quantification of this combined uncertainty.

1.1.2.3 Field DAS

Since the L1 mean temperature DP is a function of the individual temperature measurements, any measurement bias introduced by the Field DAS will be reflected in the L1 mean data product. Here, the raw measurement(s) that maximize the combined uncertainty of an individual measurement is used in the calculation of the L1 mean DP uncertainty. Uncertainty components due to random effects, whether a function of the environment or the measurement assembly, are quantified via the natural variation of the mean (see Section 6.1.2.1). For more information regarding the justification of this approach, please see AD[09].

The accuracy of the Field DAS in the form of *Truth* and *Trueness* propagates through to the uncertainty of the mean DP similarly to how the Field DAS uncertainty associated with a raw resistance propagates through to the uncertainty of the measurement attributable to the Field DAS (Eqs.(5)-(7)).

$$u_{FDAS(TT)}(R_{T_{MAX}}) = (u_{R3} * R_{T_{MAX}}) + O_R \tag{11}$$

Where, the subscript “MAX” represents the index, i , where the *maximum*, combined, standard, measurement uncertainty of soil temperature is observed over a set (averaging period) of observations. Mathematically, this can be defined as:

$$MAX = \{i: u_c(T_i) = \max[u_c(T_1), \dots, u_c(T_n)]\}. \tag{12}$$

Also,

- $u_{FDAS(TT)}(R_{T_{MAX}})$ = Field DAS *Truth* and *Trueness* uncertainty of $R_{T_{MAX}}(\Omega)$
- $R_{T_{MAX}}$ = individual, raw, resistance measurement observed at MAX index (Ω)
- u_{R3} = relative, combined, Field DAS *Truth* and *Trueness* for resistance measurements, provided by CVAL (unitless)
- O_R = offset imposed by the FDAS for resistance measurements, provided by CVAL (Ω)

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Thus, analogous to Eq. (7),

$$u_{FDAS(TT)}(\bar{T}) = \left. \frac{\partial T_i}{\partial R_{T_i}} \right|_{R_{T_{MAX}}} u_{FDAS(TT)}(R_{T_{MAX}}), \quad (13)$$

where:

$$\left. \frac{\partial T_i}{\partial R_{T_i}} \right|_{R_{T_{MAX}}} = \text{partial derivative of } T_i \text{ with respect to } R_{T_i} \text{ (Eq. (6)) evaluated at } R_{T_{MAX}} \text{ (}^\circ\text{C}/\Omega\text{)}$$

$$u_{FDAS(TT)}(\bar{T}) = \text{Truth and Trueness uncertainty of the mean DP introduced by the Field DAS (}^\circ\text{C)}$$

1.1.2.4 Combined Uncertainty

The combined uncertainty for our L1 mean temperature data product, $u_c(\bar{T})$, is given in units of $^\circ\text{C}$ and computed by summing the uncertainties from Sections 6.1.2.1 through 6.1.2.3 in quadrature:

$$u_c(\bar{T}) = \left(u_{NAT}^2(\bar{T}) + u_{A3}^2 + u_{FDAS(TT)}^2(\bar{T}) \right)^{\frac{1}{2}} \quad (14)$$

1.1.2.5 Expanded Uncertainty

The expanded uncertainty is calculated as:

$$U_{95}(\bar{T}) = k_{95} * u_c(\bar{T}) \quad (15)$$

Where:

$$U_{95}(\bar{T}) = \text{expanded L1 mean data product uncertainty at 95\% confidence (}^\circ\text{C)}$$

$$k_{95} = 2; \text{ coverage factor for 95\% confidence (unitless)}$$

1.2 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 6-1. Uncertainty budget for individual temperature measurements. Shaded rows denote the order of uncertainty propagation (from lightest to darkest).

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Source of measurement uncertainty	Measurement uncertainty component $u(x_i)$	Measurement uncertainty value	$\frac{\partial f}{\partial x_i}$	$u_{x_i}(Y) \equiv \left \frac{\partial f}{\partial x_i} \right u(x_i)$ [°C]
0.1 Hz temp.	$u_c(T_i)$	Eq. (8) [°C]	n/a	n/a
Sensor/calibration	u_{A1}	AD[11] [°C]	1	u_{A1}
FDAS	$u_{FDAS}(R_{T_i})$	Eq. (5) [Ω]	Eq. (6)	Eq. (7)

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

Source of uncertainty	Uncertainty component $u(x_i)$	Uncertainty value	$\frac{\partial f}{\partial x_i}$	$u_{x_i}(Y) \equiv \left \frac{\partial f}{\partial x_i} \right u(x_i)$ [°C]
L1 mean temp	$u_c(\bar{T})$	Eq. (14) [°C]	n/a	n/a
Natural variation	$u_{NAT}(\bar{T})$	Eq. (10) [°C]	1	Eq. (10)
Sensor(TT)	u_{A3}	AD[11] [°C]	1	u_{A3}
FDAS(TT)	$u_{FDAS(TT)}(R_{T_{MAX}})$	Eq. (11) [Ω]	Eq. (6)	Eq. (13)

7 FUTURE PLANS AND MODIFICATIONS

Details concerning the evaluation and quantification of Sensor and Field DAS drift will be added to the uncertainty section.

QA/QC tests may be expanded to include consistency analyses among similar measurement streams. QA/QC consistency tests will be applied to one- and thirty-minute averages in accordance with AD[01].

8 BIBLIOGRAPHY

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