NEON ALGORITHM THEORETICAL BASIS DOCUMENT (ATBD) - IR BIOLOGICAL TEMPERATURE

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1 DESCRIPTION

1.1 Purpose

This document details the algorithms used for creating NEON Level 1 Data Products (L1 DP) from Level 0 Data Products (L1 DP), and ancillary data as defined in this document (such as calibration data), obtained via instrumental measurements made by the Apogee SI-111 infrared 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

This document describes the theoretical background and entire algorithmic process for creating L1 DP from L0 DP for biological temperature. Specifically, the processes necessary to convert "raw" sensor measurements into meaningful scientific units, the QA/QC procedures involved, and an assessment of the measurement uncertainties are described. The biological temperature sensor employed is the Apogee SI-111 infrared (IR) temperature sensor. 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 1-3 Data Products Catalog
AD[04]	NEON.DOC.005005	NEON Level 0 Data Products Catalog
AD[05]	NEON.DOC.000746	Evaluating Uncertainty (CVAL)
AD[06]	NEON.DOC.000927	NEON Calibration and Sensor Uncertainty Values[1]
AD[07]	NEON.DOC.000782	NEON ATBD QA/QC data consistency
AD[08]	NEON.DOC.011081	ATBD QA/QC plausibility tests
AD[09]	NEON.DOC.000783	ATBD QA/QC Automated Time Series Signal Despiking for TIS Level 1 Data Products
AD[10]	NEON.DOC.002768	SCMB Baseline - TIS Subsystem Architecture, Site Configuration and Subsystem Demand by Site
AD[11]	NEON.DOC.000785	TIS Level 1 Data Products Uncertainty Budget Estimation Plan
AD[12]	NEON.DOC.000744	IR Radiation Calibration Fixture
AD[13]	NEON.DOC.001113	Quality Flags and Quality Metrics for TIS Data Products

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
ATBD	Algorithm Theoretical Basis Document
BTS	Biological Temperature Sensor
CVAL	NEON Calibration, Validation, and Audit Laboratory
DAS	Data Acquisition System
FDAS	Field Data Acquisition System
FIU	Fundamental Instrument Unit
DP	Data Product
IR	Infrared

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

L0	Level 0
L1	Level 1

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_{M_0}	CVALM0	CVAL Calibration coefficient to determine the slope
C_{M_1}	CVALM1	CVAL Calibration coefficient to determine the slope
C_{M_2}	CVALM2	CVAL Calibration coefficient to determine the slope
C_{B_0}	CVALB0	CVAL Calibration coefficient to determine the intercept
C_{B_1}	CVALB1	CVAL Calibration coefficient to determine the intercept
C_{B_2}	CVALB2	CVAL Calibration coefficient to determine the intercept
O_R	U_CVALR4	offset imposed by the FDAS for resistance readings, provided by CVAL (Ω)
O_V	U_CVALV4	offset imposed by the FDAS for voltage readings, provided by CVAL (V)
u_{A1}	U_CVALA1	Combined, relative uncertainty of infrared temperature sensor (%)
u_{A3}	U_CVALA3	Combined, relative uncertainty (truth and trueness only) of infrared temperature 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 (%)
u_{V1}	U_CVALV1	Combined, relative uncertainty of Field DAS voltage readings (%)
u_{V3}	U_CVALV3	Combined, relative uncertainty (truth and trueness only) of Field DAS voltage readings (%)
$V_{eff_{A1}}$	U_CVALD1	Effective degrees of freedom relating to U_CVALA1 (unitless)
$V_{eff_{A3}}$	U_CVALD3	Effective degrees of freedom relating to U_CVALA3 (unitless)
$V_{eff_{R1}}$	U_CVALF1	Effective degrees of freedom relating to U_CVALR1 (unitless)
$V_{eff_{R3}}$	U_CVALF3	Effective degrees of freedom relating to U_CVALR3 (unitless)
$V_{eff_{V1}}$	U_CVALG1	Effective degrees of freedom relating to U_CVALV1 (unitless)
$V_{eff_{V3}}$	U_CVALG3	Effective degrees of freedom relating to U_CVALV3 (unitless)

3 DATA PRODUCT DESCRIPTION

3.1 Variables Reported

Biological temperature related L1 DPs provided by the algorithms documented in this ATBD are displayed in the accompanying file irb_datapub_NEONDOC002853.txt. Throughout the body of the ATBD, descriptive, mathematical notation will be used to define and derive variables. A cross reference table is provided in section 2.4 to convert this notation to that which is used across NEON departments.

3.2 Input Dependencies

Table 3-1 details the biological temperature related L0 DPs used to produced L1 DPs in this ATBD.

Table 3-1: Biological temperature related L0 DPs that are transformed into L1 DPs in this ATBD. Note: The 'VER' in the ninth field of the Data Product ID refers to the vertical location of the sensor. Where numbering beings at the soil surface, i.e., '000' represents sensors at the soil surface, '001' the lowest sensor on the tower infrastructure, and so on and so forth.

Description	Sample Frequency	Units	Data Product Number
Thermopile Output (ρ)	1 Hz	V	NEON.DOM.SITE.DP0.00005.001.01313.HOR.VER.000
Sensor Body Resistance (R_{SB})	1 Hz	Ω	NEON.DOM.SITE.DP0.00005.001.01314.HOR.VER.000

3.3 Product Instances

Biological temperature will be recorded at all tower sites via Apogee SI-111 infrared temperature sensors. All tower sites will have biological temperature sensors located on all tower levels, excluding the tower-top and second highest boom level. In addition to the tower sensors, biological temperature will also be recorded 0.25 m above the soil surface in the middle plot of all soil arrays. Site specific details for the quantity of sensors and their location can be found in AD[10].

3.4 Temporal Resolution and Extent

Biological temperature will be recorded at a rate of 1 Hz for L0 DPs and be used to calculate one- and thirty-minute averages for L1 DPs.

3.5 Spatial Resolution and Extent

Each biological temperature sensor will represent the point in space for the target area of the sensor. This is dependent on the relation of the sensor to its target surface (i.e., angle) as well as its location in the soil array or on the tower infrastructure; site specific details can be found in AD[10].

4 SCIENTIFIC CONTEXT

Ambient air and biological temperatures often vary due to the ability of surface biota to absorb and store ambient radiation. In order to differentiate between ambient air and biological temperatures, NEON will measure both parameters. At tower sites ambient temperature is measured via single and triple redundant aspirated temperature sensors. Biological temperature (i.e., surface temperature) is measured via IR temperature sensors located in the soil array and on the tower infrastructure. Biological temperature can be used in conjunction with other measurements to draw conclusions on topics such as plant respiration, evapotranspiration rates, and stomatal conductance. For example, stomatal closure, estimated by biological temperature, is used as a measure of plant water stress (Jones, 1999). Ultimately, measurements of biological temperature provide ancillary information for NEON's higher level DPs that will inform how climate and land use changes alter ecosystem respiration, energy balance, and fire risk.

4.1 Theory of Measurement

Biological temperature measured via infrared temperature sensors offer a non-contact method of determining surface temperatures. Infrared temperature sensors resolve the amount of infrared radiation emitted by an object through two measurements. 1) A thermopile is used to measure the difference between the target temperature (i.e., biological temperature) and the sensor body. 2) A thermistor measures the temperature of the sensor body, which is used to reference the target temperature. Based on the Stefan-Boltzmann Law, Kalma et al. (1988) proposed a version of the equation where infra-red surface temperatures could be determined by taking into account sensor body temperature:

$$(T_B + 273.15)^4 - T_{SB}^4 = m * \rho + b \tag{1}$$

Where:

T_B = biological Temperature (K)
T_{SB} = Sensor Body Temperature (K)
m = Slope calibration coefficient ($K\ V^{-1}$)
b = Intercept calibration coefficient (K)
ρ = output of the thermopile (V)

Apogee also indicates that an emissivity correction may be necessary when measuring biological temperature. This is a result of the infrared radiometer detecting radiation that includes both radiation emitted by the target surface and background reflected radiation. In addition to Apogee's website, Campbell and Diak (2005) provide supplemental information on the emissivity correction for thermal radiation measurements. As data are gathered, NEON intends to resolve this correction factor and update the algorithm.

4.2 Theory of Algorithm

The first step in quantifying biological temperature (T_B) is to resolve the sensor body temperature, i.e., the thermistor measurement. However, in order to ensure compatibility between the thermistor and NEON's DAS, it was necessary that the thermistor circuit be *scaled* using a high precision 604 Ω shunt resistor. Therefore, to the following relationship is used to determine the thermistor resistance (R_T) of the sensor body (R_{SB}) (AD[12]):

$$R_{T_i} = \left(\frac{-x * R_{SB_i}}{R_{SB_i} - x}\right) \quad (2)$$

Where:

R_{T_i} = Individual (1 Hz) thermistor resistance (Ω)
R_{SB_i} = Individual sensor body resistance (Ω)
x = 604 (Ω)

As recommend by the manufacturer, Apogee, sensor body temperature is then determined from thermistor resistance via the Steinhart – Hart equation:

$$T_{SB_i} = \frac{1}{A + B * ln(R_{T_i}) + C\left(ln^3(R_{T_i})\right)} \quad (3)$$

Where:

T_{SB_i} = Individual (1 Hz) sensor body temperature (K)
R_{T_i} = Individual thermistor resistance (Ω)
A = $1.129241*10^{-3}$
B = $2.341077*10^{-4}$
C = $8.775468*10^{-8}$

Once individual sensor body temperature (T_{SB_i}) is computed, the slope (m) and intercept (b) calibration coefficients are determined as follows:

$$m_i = C_{M_2} * T_{SB_i}^2 + C_{M_1} * T_{SB_i} + C_{M_0} \quad (4)$$

Where:

m_i = Individual (1 Hz) Slope calibration coefficient (K V^{-1})
C_{M_0} = Calibration coefficient (sensor specific and provided by CVAL) (K V^{-1})
C_{M_1} = Calibration coefficient (sensor specific and provided by CVAL) (V^{-1})
C_{M_2} = Calibration coefficient (sensor specific and provided by CVAL) (K^{-1} V^{-1})
T_{SB_i} = Individual sensor body temperature (K)

Likewise *b* is as follows:

$$b_i = C_{B_2} * T_{SB_i}^2 + C_{B_1} * T_{SB_i} + C_{B_0} \tag{5}$$

Where:

b_i = Individual (1 Hz) Intercept calibration coefficient (K)
C_{B_0} = Calibration coefficient (sensor specific and provided by CVAL) (K V^{-1})
C_{B_1} = Calibration coefficient (sensor specific and provided by CVAL) (V^{-1})
C_{B_2} = Calibration coefficient (sensor specific and provided by CVAL) (K^{-1} V^{-1})
T_{SB_i} = Individual sensor body temperature (K)

Biological temperature (T_{B_i}) is then determined by rearranging Eq. (1) :

$$T_{B_i} = \left(T_{SB_i}^4 + m_i * \rho_i + b_i\right)^{\frac{1}{4}} - 273.15 \quad [^0\mathrm{C}] \tag{6}$$

Where:

T_{B_i} = Individual (1 Hz) biological Temperature (^{0}C)
T_{SB_i} = Individual sensor Body Temperature (K)
m_i = Individual slope calibration coefficient (K V^{-1})
b_i = Individual intercept calibration coefficient (K)
ρ_i = Individual output of the thermopile (V)

Note: Due to potential differences in sample "pairing" of thermistor and thermopile sensor measurements with respect to their individual timestamps, "pairing" will be defined by the two measurements that occur within a one second period where time ∈ [0.000000, 1.000000) seconds.

Once TB has been determined one-minute ($\overline{T_{B}}_1$) and thirty-minute ($\overline{T_{B}}_{30}$) averages of biological temperature will be determined according to Eq. (7) and (8) to create the L1 DPs listed in file irb_datapub_NEONDOC002853.txt. However, individual calibrated measurements, i.e. 1 Hz biological temperature, will be made available upon request.

$$\overline{T_{B}}_1 = \frac{1}{n}\sum_{i=1}^{n} T_{B_i} \quad [^0\mathrm{C}] \tag{7}$$

where, for each 1-minute average, n is the number of measurements during the averaging period and T_{B_i} is a 1-Hz biological temperature measurement taken during the 60-second averaging period [0, 60). For a 1-minute average, n = 60 if all data points are included.

Similarly,

$$\overline{T_{B}}_{30} = \frac{1}{n}\sum_{i=1}^{n} T_{B_i} \quad [^0\mathrm{C}] \tag{8}$$

where, for each 30-minute average, n is the number of measurements during the averaging period and T_{B_i} is a 1-Hz biological temperature measurement taken during the 1800-second averaging period [0, 1800).

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. T_{SB}, m, and b will be determined from L0 DPs according to Eqns. (2)-(5).
2. The sensor test described under Section 1 of the QA/QC procedure will be applied to the data stream.
3. L0 DPs will be converted to biological temperature in degrees Celsius by applying Eq. (6).
4. QA/QC Plausibility tests will be applied to the data stream in accordance with AD[08]. The details are provided below.
5. Signal de-spiking will be applied to the data stream in accordance with AD[09].
6. One- and thirty-minute biological temperature averages will be calculated using Eq. (7) and (8) and descriptive statistics, i.e. minimum, maximum, and variance, will be determined for both averaging periods.
7. Quality metrics, quality flags, and the final quality flag will be produced for one- and thirty-minute averages according to AD[13].

QA/QC Procedure:

1. **Sensor Test** – If electrical issues or other problems arise from the sensor assembly, they can result in the generation of erroneous input values for the calculation of biological temperature. Therefore, for trouble shooting purposes, prior to the calculation of biological temperature, Eq. (6) will be assessed on whether erroneous inputs were received and a not a number quality flag will be generated accordingly:

$$QF\_NAN = \begin{cases} 1 & \text{if } \left(T_{SB_i}^4 + m_i * \rho_i + b_i\right) \leq 0 \\ 0 & \text{otherwise} \end{cases} \tag{9}$$

   Where:

   T_{SB_i} = Individual sensor Body Temperature (K)
   m_i = Individual slope calibration coefficient (K V^{-1})
   b_i = Individual intercept calibration coefficient (K)
   ρ_i = Individual output of the thermopile (V)

2. **Plausibility Tests** AD[08] – All plausibility tests will be determined for biological temperature. 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.

3. **Signal De-spiking** – The time series de-spiking routine will be run according to AD[09]. Test parameters will be specified by FIU and maintained in the CI data store. Quality flags resulting from the de-spiking analysis will be applied according to AD[13].

4. **Consistency Analysis** – A QA/QC flag for data consistency will be applied according to the consistency analysis outlined in AD[07], and a pass/fail flag will be generated to reflect this activity. For biological temperature consistency analysis, L1 temperature from a given biological temperature sensor will first be compared to the biological temperature sensor above it on the tower infrastructure. If a difference between the two temperature measurements is less than the defined limits, provided by FIU and maintained in the CI data store, then the sensor will have passed the consistency analysis. Alternatively, a temperature difference between the biological temperature sensors outside the defined limits will result in a failed test. A failed test from the above sensor will result in the biological temperature sensor being compared to the biological temperature sensor below it; if this too results in a failed test then the biological temperature sensor will have failed the consistency analysis and be flagged as such. If the biological temperature sensor fails the first test but passes the second then it will have passed the consistency analysis. This structure helps to ensures that non-functional sensors (e.g., sensors that are faulty or down for service) do not bias the test, since a resulting failed test will allow the sensor to be compared to the one below it. Accordingly, the biological temperature sensor on the bottom of the tower will only be compared to the biological temperature sensor above it. Likewise, the uppermost biological temperature sensor will only be compared to the biological temperature sensor below it. Additionally, the consistency analysis will not be run for biological temperature sensor in the soil array.

5. **Quality Flags (QFs) and Quality Metrics (QMs)** AD[13] – If a datum has failed one of the following tests it will not be used to create a L1 DP, ***range***, ***persistence***, ***step*** and ***not a number***. α and β QFs and QMs will be determined for the flags listed in, Table 5-1. In addition, L1 DPs will have a QA/QC report and quality metrics associated with each flag listed in Table 5-1 as well as a final quality flag, as detailed in AD[13]. Ancillary information needed for the algorithm and other information maintained in the CI data store is shown in Table 5-2.

Table 5-1: Flags associated with biological temperature measurements.

Tests
Range
Persistence
Step
Null

Gap
Signal De-spiking
Consistency
Not a number
Alpha
Beta
Final quality flag

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

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 AD[12]
Uncertainty	AD[06]
Consistency Analysis	Test limits
Final Quality Flag	AD[13]

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 L1 mean DPs. It is a reflection of the information described in AD[11], and is explicitly described for the biological temperature assembly in the following sections.

6.1 Uncertainty of Biological Temperature Measurements

Uncertainty of the net radiation assembly is discussed in this section. Discussion is broken down into two topics informing the discrepancy between the two types of uncertainty presented within this document. The first subsection details the sources of *measurement* uncertainty, i.e., those associated with *individual measurements*. The second discusses uncertainties associated with temporally averaged data products. A diagram detailing the data flow and known sources of uncertainty are displayed in Figure 2.

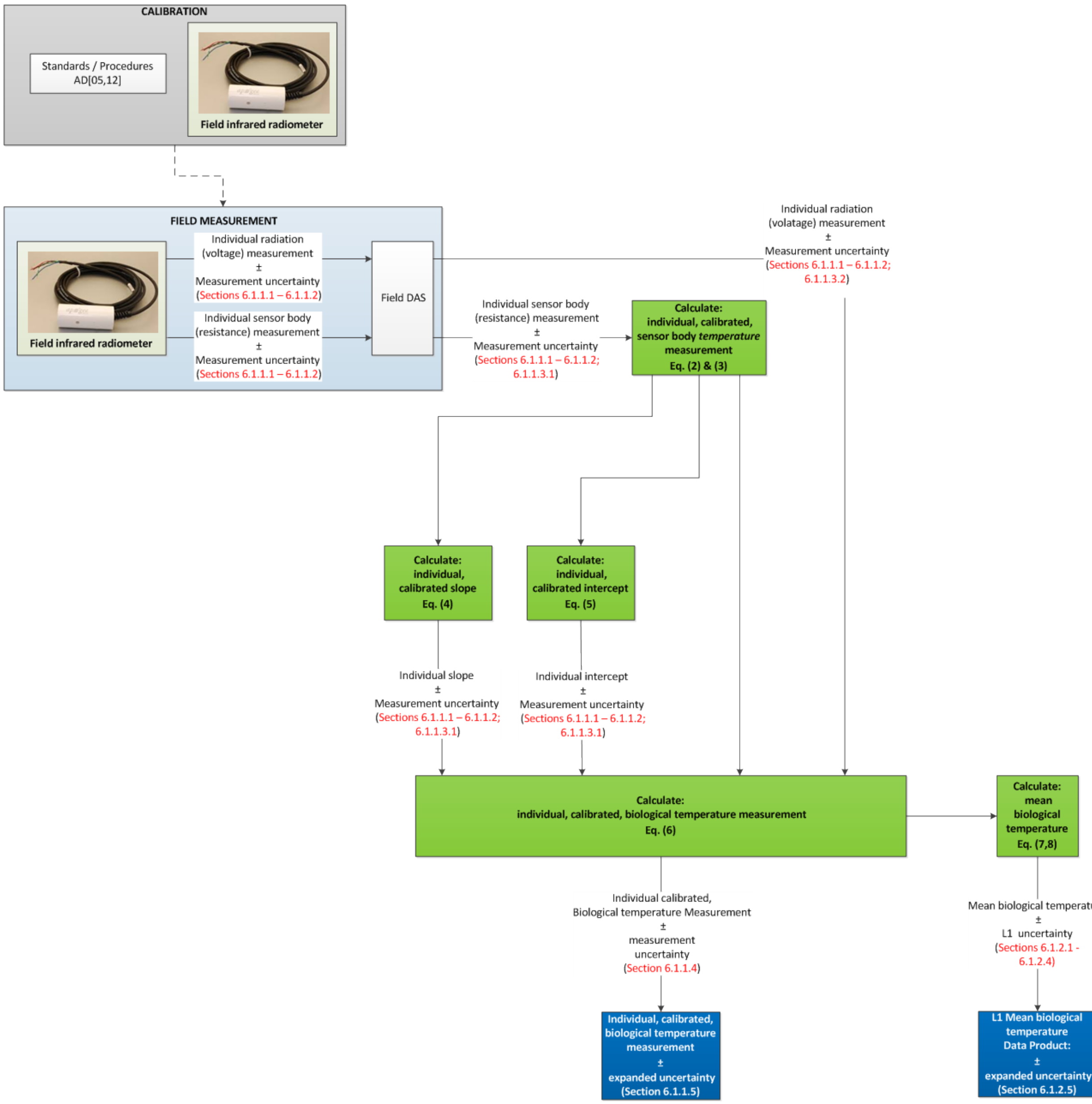

Figure 1: Displays the data flow and sources of uncertainty for individual biological temperature measurements and L1 mean biological temperature DPs. For a detailed explanation of the biological temperature sensor calibration procedures please refer to AD[05,12].

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[11] for further details concerning the discrepancies between quantification of measurement uncertainties and temporally averaged data product 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:

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

where

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

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

Thus, the uncertainty of the measurand can be found be summing the input uncertainties in quadrature. For biological temperature measurements, the sources of uncertainty are depicted in Figure 1. The calculation of these input uncertainties is discussed below.

6.1.1.1 Calibration

Uncertainties associated with the calibration process propagate into a combined, standard, measurement uncertainty. This 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 Eqns. (4),(5) and (6)). It is a constant value that will be provided by CVAL (AD[06]), stored in the CI data store, and applied to all *individual biological temperature measurements* (that is, it does not vary with any specific sensor, DAS component, etc.). A detailed summary of the calibration procedures and corresponding uncertainty estimates can be found in AD[05,12].

6.1.1.2 Emissivity

We acknowledge that uncertainty may exist as a result of emissivity, yet it is unquantifiable at this time. As NEON data are collected and analyzed, it may be possible to quantify this uncertainty.

6.1.1.3 Field DAS

Because CVAL will calibrate biological temperature sensors, uncertainties attributable to the sensors are essentially quantified during the calibration process. However, uncertainty is also introduced by the Field DAS through the collection of the raw sensor body resistance and thermopile output, R_{SB_i} and ρ_i, respectively. Since biological temperature is ultimately a function of these two variables, the partial derivatives of Eq. (6) with respect to R_{SB_i} and ρ_i must be quantified to allow for proper quantification of the field DAS uncertainty.

The partial derivative of Eq. (6) with respect to R_{SB_i} is derived first. The absolute value of this derivative is then multiplied by the uncertainty of the raw measurement due to the field DAS, i.e. $u_c\left(R_{FDAS_i}\right)$. Analogous computations are made with respect to the thermopile measurements. These two uncertainty terms, along with the term provided by CVAL (Section 6.1.1.1) are then added in quadrature to obtain the overall estimate of measurement uncertainty. This is a direct application of Eqn. (10).

6.1.1.3.1 Sensor body resistance

The combined, standard uncertainty introduced by the Field DAS through the sensor body resistance measurement is:

$$u_{FDAS}\left(R_{SB_i}\right) = \left(u_{R1} * R_{SB\,i}\right) + O_R \tag{11}$$

Where:

$u_{FDAS}\left(R_{SB_i}\right)$ = combined, standard uncertainty introduced by the Field DAS through the sensor body resistance (Ω)

$R_{SB\,i}$ = sensor body output (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 Eq. (6) with respect to the sensor body resistance, R_{SB_i}, can be partitioned as follows:

$$\frac{\partial T_{B_i}}{\partial R_{SB_i}} = \frac{\partial T_{B_i}}{\partial T_{SB_i}} * \frac{dT_{SB_i}}{dR_{SB_i}} \tag{12}$$

where:

$\frac{\partial T_{B_i}}{\partial R_{SB_i}}$ = partial derivative of Eq. (6) with respect to $R_{SB\,i}$ (^{0}C Ω^{-1})

$\frac{\partial T_{B_i}}{\partial T_{SB_i}}$ = partial derivative of Eq. (6) with respect to $T_{SB\,i}$ (^{0}C K^{-1})

$\frac{dT_{SB_i}}{dR_{SB_i}}$ = derivative of Eq. (3), substituting Eq. (2) for $R_{T\,i}$, with respect to $R_{SB\,i}$ (K Ω^{-1}).

To calculate the partial derivative of biological temperature with respect to sensor body temperature, first note that m_i and b_i are both functions of sensor body temperature, i.e., combining Eqns. (4), (5) and (6) and rearranging terms:

$$T_{B_i} = \left[T_{SB_i}^4 + T_{SB_i}^2\left(C_{M_2} * \rho_i + C_{B_2}\right) + T_{SB_i}\left(C_{M_1} * \rho_i + C_{B_1}\right) + C_{M_0} * \rho_i + C_{B_0}\right]^{1/4} - 273.15 \tag{13}$$

Thus,

$$\frac{\partial T_{B_i}}{\partial T_{SB_i}} = \frac{1}{4}\left(T_{B_i} + 273.15\right)^{-3} * \left[4T_{SB_i}^3 + 2T_{SB_i} * \left(C_{M_2} * \rho_i + C_{B_2}\right) + C_{M_1} * \rho_i + C_{B_1}\right] \tag{14}$$

It remains to calculate the derivative of sensor body temperature with respect to sensor body resistance:

$$\frac{dT_{SB_i}}{dR_{SB_i}} = \frac{T_{SB_i}^2 * x\left(B + 3 * C * ln^2\left(\frac{-x * R_{SB_i}}{R_{SB_i} - x}\right)\right)}{R_{SB_i}\left(R_{SB_i} - x\right)} \tag{15}$$

where:

A	= 1.129241*10 $^{-3}$
B	= 2.341077*10 $^{-4}$
C	= 8.775468*10 $^{-8}$

It follows from Eqns. (12), (14) and (15) that

$$\frac{\partial T_{B_i}}{\partial R_{SB_i}} = \frac{1}{4}\left(T_{B_i} + 273.15\right)^{-3} * \left[4T_{SB_i}^3 + 2T_{SB_i} * \left(C_{M_2} * \rho_i + C_{B_2}\right) + C_{M_1} * \rho_i + C_{B_1}\right] * \left[\frac{T_{SB_i}^2 * x\left(B + 3 * C * ln^2\left(\frac{-x * R_{SB_i}}{R_{SB_i} - x}\right)\right)}{R_{SB_i}\left(R_{SB_i} - x\right)}\right] \tag{16}$$

The standard uncertainty of an individual biological temperature measurement due to the field DAS with respect to the raw sensor body resistance measurement is then:

$$u_{FDAS_{SB_i}}(T_{B_i}) = \left|\frac{\partial T_{B_i}}{\partial R_{SB_i}}\right| u_{FDAS}(R_{SB_i}) \quad (17)$$

6.1.1.3.2 Thermopile measurement

The combined, standard uncertainty introduced by the Field DAS through the thermopile measurement is:

$$u_{FDAS}(\rho_i) = (u_{V1} * \rho_i) + O_V \quad (18)$$

Where:

$u_{FDAS}(\rho_i)$ = combined, standard uncertainty of the thermopile output introduced by the Field DAS (V)

ρ = thermopile output (V)

u_{V1} = combined, relative Field DAS uncertainty for voltage measurements provided by CVAL (unitless)

O_V = offset imposed by the FDAS provided by CVAL (V)

The partial derivative of Eq. (6) with respect to the thermopile measurement, ρ_i, is:

$$\frac{\partial T_{B_i}}{\partial \rho_i} = \frac{1}{4}\left(T_{B_i} + 273.15\right)^{-3} * m_i \quad (19)$$

The standard uncertainty of biological temperature due to the field DAS with respect to the raw thermopile measurement is then:

$$u_{FDAS_{\rho_i}}(T_{B_i}) = \left|\frac{\partial T_{B_i}}{\partial \rho_i}\right| u_{FDAS}(\rho_i) \quad (20)$$

Where:

$u_{FDAS_{\rho_i}}(T_{B_i})$ = converted, combined, standard uncertainty introduced by the Field DAS through the thermopile output (^{0}C)

6.1.1.4 Combined Measurement Uncertainty

The combined, standard, measurement uncertainty for an individual measurement, $u_c(TB_i)$, is computed by summing the individual uncertainties in quadrature:

$$u_c(T_{B_i}) = \left(u_{A1}^2 + u_{FDAS_{SB_i}}^2(T_{B_i}) + u_{FDAS_{\rho_i}}^2(T_{B_i})\right)^{\frac{1}{2}} \quad [°C] \tag{21}$$

This is a direct application of Eqn. (2).

6.1.1.5 Expanded Measurement Uncertainty

To derive an expanded measurement uncertainty, the effective degrees of freedom of for the individual measurement must be computed:

$$V_{eff_{T_{B_i}}} = \frac{u_c^4(T_{B_i})}{\frac{u_{A1}^4}{V_{eff_{A1}}} + \frac{u_{FDAS_{SB_i}}^4(T_{B_i})}{V_{eff_{R1}}} + \frac{u_{FDAS_{\rho_i}}^4(T_{B_i})}{V_{eff_{V1}}}} \tag{22}$$

Where,

$V_{eff_{T_{B_i}}}$ = effective degrees of freedom relating to quantification of the combined, standard, measurement uncertainty (unitless)

$V_{eff_{A1}}$ = effective degrees of freedom relating to quantification of sensor uncertainty; provided by CVAL (unitless)

$V_{eff_{R1}}$ = effective degrees of freedom relating to quantification of field DAS uncertainty for resistance measurements; provided by CVAL (unitless)

$V_{eff_{V1}}$ = effective degrees of freedom relating to quantification of field DAS uncertainty for voltage measurements; provided by CVAL (unitless)

Next, the expanded measurement uncertainty is calculated:

$$U_{95}(T_{B_i}) = k_{95,V_{eff_{TB_i}}} * u_c(T_{B_{i_i}}) \tag{23}$$

Where:

$U_{95}(T_{B_i})$ = expanded measurement uncertainty at 95% confidence (℃)

$k_{95,V_{eff_{T_{B_i}}}}$ = coverage factor obtained with the aid of Table 4 in AD[11] (unitless)

6.1.2 Uncertainty of L1 Mean Data Product

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 insolation measurements for a specified time period:

$$u_{NAT}(\overline{T_B}) = \frac{s(T_B)}{\sqrt{n}} \quad (24)$$

Where,

$u_{NAT}(\overline{T_B})$ = standard error of the mean (natural variation) (^oC)

$s(T_B)$ = experimental standard deviation of individual observations for the defined time period (^oC)

n = number of observations made during the defined time period. (unitless)

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, this uncertainty, u_{A3}, does not account for i) individual sensor repeatability, or ii) the variation of sensors' responses over a population (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 [6]) and stored in the CI data store. Please refer to AD[11] for further justification regarding evaluation and quantification of this combined uncertainty.

6.1.2.3 Field DAS

Since the L1 mean biological temperature DP is a function of the individual biological temperature measurements, any measurement bias introduced by the Field DAS will be reflected in the L1 mean data product. Here, the raw measurements that maximize the combined uncertainty of an individual measurement (Eq.(21)) are 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[11].

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 uncertainties associated with a raw resistance and a raw voltage propagate through to the uncertainties of the measurement attributable to the Field DAS resistance and voltage readings (Eqs. (11)-(20)).

6.1.2.3.1 Resistance output (sensor body):

$$u_{FDAS(TT)}\left(R_{SB_{MAX}}\right) = \left(u_{R3} * R_{SB_{MAX}}\right) + O_R \quad [\Omega] \tag{25}$$

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

$$MAX = \{i: u_c(T_{B_i}) = \max[u_c(T_{B_1}), \dots, u_c(T_{B_n})]\}. \tag{26}$$

And,

$u_{FDAS(TT)}\left(R_{SB_{MAX}}\right)$	= combined, standard, Field DAS *Truth* and *Trueness* uncertainty due to the sensor body resistance (Ω)
$R_{SB_{MAX}}$	= sensor body resistance reading corresponding to the MAX index (Ω)
u_{R3}	= relative, combined, Field DAS *Truth* and *Trueness* uncertainty for resistance measurements, provided by CVAL (unitless)
O_R	= offset imposed by the FDAS for resistance measurements, provided by CVAL (Ω)

Thus, from Eq. (17)

$$u_{FDAS(TT)_{SB}}(\overline{T_B}) = \left|\frac{\partial T_B}{\partial R_{SB}}\right|_{R_{SB_{MAX}}} u_{FDAS(TT)}\left(R_{SB_{MAX}}\right). \quad [^0\mathrm{C}] \tag{27}$$

where

$\left|\frac{\partial T_B}{\partial R_{SB}}\right|_{R_{SB_{MAX}}}$ = partial derivative of T_B with respect to R_{SB} (Eq. (16)) evaluated at $R_{SB_{MAX}}$ (^{o}C Ω^{-1})

6.1.2.3.2 Thermopile output (voltage):

$$u_{FDAS(TT)}(\rho_{MAX}) = (u_{V3} * \rho_{MAX}) + O_V \quad [\mathrm{V}] \tag{28}$$

Where:

$u_{FDAS(TT)}(\rho_{MAX})$ = combined, standard, Field DAS *Truth* and *Trueness* uncertainty due to the thermopile measurement (V)

ρ_{MAX} = thermopile voltage output corresponding to the MAX index (V)

u_{V3} = relative, combined, Field DAS *Truth* and *Trueness* uncertainty for voltage measurments, provided by CVAL (unitless)

O_V = offset imposed by the FDAS for voltage readings, provided by CVAL (V)

Thus, from Eq. (20)

$$u_{FDAS(TT)_\rho}(\overline{T_B}) = \left|\frac{\partial T_B}{\partial \rho}\right|_{\rho_{MAX}} u_{FDAS(TT)}(\rho_{MAX}) \quad [^{0}\mathrm{C}] \tag{29}$$

where

$\left|\frac{\partial T_B}{\partial \rho}\right|_{\rho_{MAX}}$ = partial derivative of T_B with respect to ρ (Eq. (19)) evaluated at ρ_{MAX} (^{o}C V^{-1})

6.1.2.4 Combined Uncertainty

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

$$u_c(\overline{T_B}) = \left(u_{NAT}^2(\overline{T_B}) + u_{A3}^2 + u_{FDAS(TT)_{SB}}^2(\overline{T_B}) + u_{FDAS(TT)_\rho}^2(\overline{T_B})\right)^{\frac{1}{2}} \tag{30}$$

6.1.2.5 Expanded Uncertainty

To derive an expanded measurement uncertainty for our L1 mean temperature DP, the effective degrees of freedom of the data product must first be computed:

$$V_{eff_{\overline{T_B}}} = \frac{u_c^4(\overline{T_B})}{\frac{u_{NAT}^4(\overline{T_B})}{n-1} + \frac{u_{A3}^4}{V_{eff_{A3}}} + \frac{u_{FDAS(TT)_{SB}}^4(\overline{T_B})}{V_{eff_{R3}}} + \frac{u_{FDAS(TT)_\rho}^4(\overline{T_B})}{V_{eff_{V3}}}} \tag{31}$$

Where,

$V_{eff_{\overline{T_B}}}$ = effective degrees of freedom relating to quantification of the combined, standard, measurement uncertainty (unitless)

$n-1$ = effective degrees of freedom relating to quantification of the natural variation (standard error) of the L1 mean data product; n= number of temperature measurements used to calculate $\overline{T_B}$ (unitless)

$V_{eff_{A3}}$ = effective degrees of freedom relating to quantification of sensor calibration uncertainty (not including repeatability or sensor variation amongst a population of sensors); provided by CVAL (unitless)

$V_{eff_{R3}}$ =effective degrees of freedom relating to quantification of field DAS uncertainty for resistance measurements (not including repeatability or variation amongst a population of DASs); provided by CVAL (unitless)

$V_{eff_{V3}}$ = effective degrees of freedom relating to quantification of field DAS uncertainty for voltage measurements (not including repeatability or variation amongst a population of DASs); provided by CVAL (unitless)

Next, the expanded uncertainty is calculated:

$$U_{95}(\overline{T_B}) = k_{95,V_{eff_{\overline{T_B}}}} * u_c(\overline{T_B}) \quad [{}^0\text{C}] \tag{32}$$

Where:

$U_{95}(\overline{T_B})$ = expanded L1 mean data product uncertainty at 95% confidence (°C)

$k_{95,V_{eff_{\overline{T_B}}}}$ = coverage factor obtained with the aid of Table 5 in AD[11] (unitless)

6.2 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. Uncertainties denoted in this budget are either derived within this document or will be provided by other NEON teams (e.g., CVAL) and stored in the CI data store.

Table 6-1: Uncertainty budget for an individual biological temperature measurement. 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	$\frac{\partial f}{\partial x_i}$	$u_{x_i}(Y) \equiv \left\|\frac{\partial f}{\partial x_i}\right\| u(x_i)$[°C]	Degrees of Freedom
1 Hz Bio Temp	$u_c(T_B)$	Eq. (21) [°C]	n/a	n/a	Eq. (22)
Sensor/calibration	u_{A1}	AD[06] [°C]	1	u_{A1}	AD[06]
FDAS (Sensor Body Resistance)	$u_{FDAS}(R_{SB_i})$	Eq. (11) [Ω]	Eq. (16) [°C Ω^{-1}]	Eq.(17)	AD[06]
FDAS (Thermopile)	$u_{FDAS}(V_{\rho_i})$	Eq. (18) [V]	Eq. (19) [°C V^{-1}]	Eq. (20)	AD[06]

Table 6-2: Uncertainty budget for L1 mean biological temperature measurements. Shaded rows denote the order of uncertainty propagation (from lightest to darkest).

Source of uncertainty	uncertainty component $u(x_i)$	uncertainty value	$\frac{\partial f}{\partial x_i}$	$u_{u_{x_i}}(Y) \equiv \left\|\frac{\partial f}{\partial x_i}\right\| u(x_i)$[°C]	Degrees of Freedom
L1 mean Bio Temp	$u_c(\overline{T_B})$	Eq. (30) [°C]	n/a	n/a	Eq. (31)
Natural variation	$u_{NAT}(\overline{T_B})$	Eq. (24) [°C]	1	Eq. (24)	$n-1$
Sensor/calibration	u_{A3}	AD[06] [°C]	1	u_{A3}	AD[06]
FDAS (Sensor Body Resistance)	$u_{FDAS(TT)}(R_{SB_{MAX}})$	Eq. (25) [Ω]	Eq.(16)	Eq. (27) [°C]	AD[06]
FDAS (thermopile)	$u_{FDAS(TT)}(V_{\rho MAX})$	Eq. (28)[V]	Eq.(19)	Eq. (29) [°C]	AD[06]

7 FUTURE PLANS AND MODIFICATIONS

Future system flags may be incorporated into the data stream. Additionally, individual calibrated and QA/QCD measurements with their respective uncertainties may become a common data output in the future.

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

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