NEON ALGORITHM THEORETICAL BASIS DOCUMENT (ATBD) – PHOTOSYNTHETICALLY ACTIVE RADIATION (PAR)

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Change Record

REVISION	DATE	ECO #	DESCRIPTION OF CHANGE
A	08/02/2013	ECO-00797	Initial Release
B	10/23/2015	ECO-03110	Updated document to reflect L1 data product renumbering and revised *Algorithm Implementation* and *Uncertainty* Sections
C	10/15/2018	ECO-05278	Implemented standardized coverage factor of k=2 Moved consistency analyses outline to Future Plans / Modifications Sections Added underwater PAR at buoys and lake inlet/outlet
D	05/07/2020	ECO-006413	Removed mention of de-spiking algorithm. Added a note that the persistence test is only applied during local, daylight hours.
E	04/20/2022	ECO-06809	• Update to reflect change in terminology from relocatable to gradient sites • Added fine print • Added word NEON to document title

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1 DESCRIPTION

Photosynthetically active radiation (PAR) will be continuously monitored by NEON at core and gradient sites. PAR for the top of the tower and the tower profile at terrestrial sites and for the top of the met station and above the water surface at aquatic sites will be measured by Kipp & Zonen's PQS 1 PAR Quantum Sensor. Data products and their associated sensor locations and properties are detailed in **Table 1**. The specific height and location of PAR sensors on the tower will vary between sites. The above water PAR sensors will be located at a standard height of about 3m on the aquatic met station. For detailed information on a specific core or gradient site see the respective site characterization reports.

With a slightly different configuration, PAR above water surface will be measured from a buoy deployment at lake and river sites AD[19].

Underwater PAR will be measured with a submersible Li-Cor 1925A sensor on buoys and at lake inlet/outlets. The inlet/outlet sensors and on-buoy sensors have slightly different configurations which are described in the appropriate command, control, and configuration documents AD[19] and AD[22].

Table 1. PAR data product and sensor details.

Data Product Name	Data Product Number	Instrument PAR is located on	Site Type	Incoming/Outgoing	Sensor Type	Frequency
PAR	NEON.DP1.00024	Tower PAR	Terrestrial	Incoming/ Outgoing	Kipp & Zonen PQS 1	1 Hz
PAR	NEON.DP1.00024	Met Station PAR	Lakes, Rivers, and Streams	Incoming/ Outgoing	Kipp & Zonen PQS 1	1 Hz
PAR at water surface	NEON.DP1.20042	Buoy	Lakes and Rivers	Incoming	Kipp & Zonen PQS 1	1/30 Hz
PAR below water surface	NEON.DP1.20261	Buoy	Lakes and Rivers	Incoming/ Outgoing	Li-Cor 1925A	1/30 Hz
PAR below water surface	NEON.DP1.20261	Lake Inlet	Lakes	Incoming	Li-Cor 1925A	1 Hz
PAR below water surface	NEON.DP1.20261	Lake Outlet	Lakes	Incoming	Li-Cor 1925A	1 Hz
PAR at water surface	NEON.DP1.20042	Instream Sensor Set	Streams	Incoming	Kipp & Zonen PQS 1	1 Hz

1.1 Purpose

This document details the algorithms used for creating the NEON Level 1 data product NEON.DOM.SITE.DP1.00024.001, NEON.DOM.SITE.DP1.20042.001, and NEON.DOM.SITE.DP1.20261 from Level 0 data, and ancillary data (such as calibration data), obtained via instrumental measurements made by the Kipp & Zonen PQS 1 PAR Quantum Sensor and Li-Cor 1925A. 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 NEON.DOM.SITE.DP1.00024.001, NEON.DOM.SITE.DP1.20042.001, and NEON.DOM.SITE.DP1.20261 from input data. It 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 (NOD) Requirements
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.000782	NEON 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.011000	FIU Technical and Operating Requirements
AD[09]	NEON.DOC.000743	PAR Secondary Calibration Fixture (CVAL)
AD[10]	NEON.DOC.000742	PAR Primary Calibration Fixture (CVAL)
AD[11]	NEON.DOC.002002	Engineering Master Location Sensor Matrix
AD[12]	NEON.DOC.000785	TIS Level 1 Data Products Uncertainty Budget Estimation Plan
AD[13]	NEON.DOC.000746	Evaluating Uncertainty (CVAL)
AD[14]	NEON.DOC.000927	NEON Calibration and Sensor Uncertainty Values[1]
AD[15]	NEON.DOC.000784	ATBD Profile Development
AD[16]	NEON.DOC.001256	C^3 Photosynthetically Available Radiation
AD[17]	NEON.DOC.001113	Quality Flags and Quality Metrics for TIS Data Products
AD[18]	NEON.DOC.001152	Aquatic Sampling Strategy
AD[19]	NEON.DOC.003808	C^3 Buoy meteorological station and submerged sensor assembly
AD[20]	NEON.DOC.004398	Underwater PAR ingest workbook
AD[21]	NEON.DOC.004399	Underwater PAR publication workbook
AD[22]	NEON.DOC.001063	C^3 Underwater PAR
AD[23]	NEON.DOC.002651	NEON Data Product Numbering Convention

2.2 Reference Documents

RD[01]	NEON.DOC.000008 NEON Acronym List
RD[02]	NEON.DOC.000243 NEON Glossary of Terms
RD[03]	Kipp & Zonen (2010) Instruction Sheet for the PQS 1 PAR Quantum Sensor V1008. Kipp & Zonen B.V.P.O. Box 507, 2600 AM Delft. The Netherlands.
RD[04]	Li-Cor Li-1925A Underwater PAR Manual

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

2.3 Acronyms

Acronym	Explanation
AIS	Aquatic Instrument System
AQU	NEON Aquatic Department
ATBD	Algorithm Theoretical Basis Document
CVAL	**NEON Calibration, Validation, and Audit Laboratory**
DP	Data Product
L0	Level 0
L1	Level 1
N/A	Not Applicable
PAR	Photosynthetically Available Radiation

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_1	CVALA1	Calibration coefficient
O_V	U_CVALV4	Offset imposed by the Field DAS for voltage readings (V)
u_{A1}	U_CVALA1	Combined, relative uncertainty of PAR sensor (%)
u_{A3}	U_CVALA3	Combined, relative uncertainty (truth and trueness only) of PAR sensor (%)
u_{V1}	U_CVALV1	Combined, relative uncertainty of Field DAS measurements (%)
u_{V3}	U_CVALV3	Combined, relative uncertainty (truth and trueness only) of Field DAS measurements (%)

2.5 Verb Convention

"Shall" is used whenever a specification expresses a provision that is binding. The verbs "should" and "may" express non-mandatory provisions. "Will" is used to express a declaration of purpose on the part of the design activity.

3 DATA PRODUCT DESCRIPTION

3.1 Variables Reported

Photosynthetically Active Radiation (PAR) related L1 DPs provided by the algorithms documented in this ATBD are displayed in the accompanying par_datapub_NEONDOC002872.txt for NEON.DP1.00024, pws_datapub_NEONDOC000781.txt files for NEON.DP1.20042, and uPAR_datapub_NEONDOC004399.txt for NEON.DP1.20261.

3.2 Input Dependencies

Tables 2, 3, and 4 detail the PAR related L0 DPs that are transformed into L1 DPs in this ATBD.

Table 2. Tower-base PAR L0 DPs that are transformed into L1 DPs in this ATBD (NEON.DP1.00024).

Description	Sample Frequency	Units	Data Product Number
Incoming photosynthetically active radiation (PAR) (irradiance 400-700 nm)	1 Hz	V	NEON.DOM.SITE.DP0.00024.001.01320.HOR.VER.000
Outgoing photosynthetically active radiation (PAR) (irradiance 400-700 nm)	1 Hz	V	NEON.DOM.SITE.DP0.00024.001.01321.HOR.VER.000

Table 3. PAR above water surface, L0 DPs that are transformed into L1DPs in this ATBD (NEON.DP1.20042). For PAR above water surface, frequencies of 1 Hz correspond to the S1 and S2 stream sensors and frequencies of 1 per 30 seconds correspond to buoy sensors. Note that outgoing PAR is not used for the PAR above water surface data product.

Description	Sample Frequency	Units	Data Product Number
Incoming photosynthetically active radiation (PAR) (irradiance 400-700 nm)	1 Hz or ~1/30 Hz	V	NEON.DOM.SITE.DP0.20042.001.01320.HOR.VER.000
Outgoing photosynthetically active radiation (PAR) (irradiance 400-700 nm)	1 Hz or ~1/30 Hz	V	NEON.DOM.SITE.DP0.20042.001.01321.HOR.VER.000

Table 4. PAR below water surface L0 DPs that are transformed into L1 DPs in this ATBD (NEON.DP1.20261). For PAR below water surface, frequencies of 1 Hz correspond to the lake inlet and outlet sensors while frequencies of 1 per 30 seconds correspond to buoy sensors.

Description	Sample Frequency	Units	Data Product Number
Incoming photosynthetically active radiation (PAR) (irradiance 400-700 nm)	1 Hz or ~1/30 Hz	V	NEON.DOM.SITE.DP0.20261.001.01320.HOR.VER.000
Outgoing photosynthetically active radiation (PAR) (irradiance 400-700 nm)	1 Hz or ~1/30 Hz	V	NEON.DOM.SITE.DP0.20261.001.01321.HOR.VER.000

3.3 Product Instances

PAR sensors will be located on the tower top, southeast, boom arm assembly and on each level of the tower profile at terrestrial sites, on the south boom of the aquatic met station, atop the in-stream infrastructure above the surface of the water at both sensor sets at stream sites, and located on the buoy platform at lake sites. Underwater PAR sensors will be located at the lake inlet sensor set, lake outlet sensor set, and buoys (located at both lake and river sites). For the exact number of PARs per site see AD[11].

3.4 Temporal Resolution and Extent

One- and thirty-minute averages of PAR will be calculated to form L1 DPs for all land-based measurements and underwater PAR. One, five, and thirty minute averages of PAR will be calculated to form L1 DPs for PAR measurements at the water surface.

3.5 Spatial Resolution and Extent

The spatial resolution will depend on the placement of the PAR sensors on the tower infrastructure. Ultimately, an incoming radiation profile will be developed for each tower site from the array of PARs on the tower. At the tower-top, both incoming and outgoing PAR will be observed (see AD[11] for detail on sensor placement for a specific core site, and AD[15] for description of the algorithms used for deriving this profile). Only incoming radiation will be measured at aquatic met stations, buoy met stations, stream sensor sets, and lake, inlet/outlet, sensor sets and the PAR sensors will represent the point at which the measurement is taken. Note that for PAR at water surface data products only incoming PAR will be used. Outgoing PAR will not be used for PAR at water surface. On buoys, *underwater* PAR will monitor both incoming and outgoing radiation.

4 SCIENTIFIC CONTEXT

PAR is defined as radiation within the range of 400 nm to 700 nm. Radiation within this range drives photosynthesis, the process by which autotrophs (e.g., plants and algae) convert carbon dioxide and water into glucose and oxygen. Photosynthesis is critical to aerobic life on earth and many chemical, physical and biological processes, including the global carbon cycle.

4.1 Theory of Measurement/Observation

Photosynthesis is a chemical process driven by the adsorption of light within the range 400 nm to 700 nm. PAR sensors output data in µV or mV which can be transformed to units of number of photons (counted in micro-moles) per second per square meter or µmol s^{-1} m^{-2}. PAR sensors must have near equal sensitivity (i.e., quantum response) for all photons between the wavelengths of 400 nm and 700 nm to function effectively. Throughout the Observatory sensor output is in microvolts and is converted to µmol s^{-1} m^{-2} by application of a calibration factor and algorithm described below.

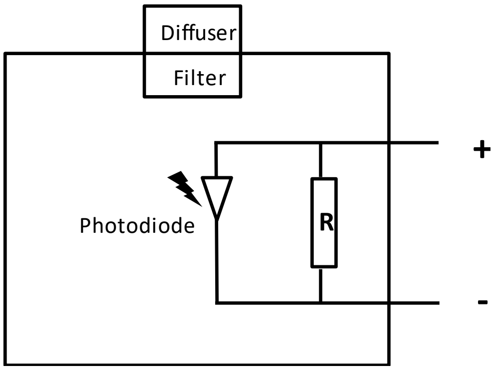

Figure 1. Schematic of typical PAR sensor construction.

4.2 Theory of Algorithm

The Kipp & Zonen PQS 1 PAR Quantum Sensor measures radiation between the wavelengths of 400 nm and 700 nm. Similarly, the Li-Cor 1925A sensor measures from 400 nm to 700 nm. Within this range the conversion of PAR output from V to µmol s^{-1} m^{-2} can be expressed by the following equation:

$$PAR = I * C_1 \tag{1}$$

Where:

PAR = Photosynthetically active radiation (i.e., 400 – 700 nm) in µmol m^{-2} s^{-1}
C_1 = PAR sensor calibration coefficient provided by CVAL (µmol m^{-2} s^{-1} V^{-1})

I = Sensor output (irradiance) in V

After the L0 DP, I, is converted to PAR, one-minute and thirty-minute averages of incoming and outgoing PAR will be determined according to Eq. (2) and (3) to create the L1 DPs listed in files par_datapub_NEONDOC002872.txt and uPAR_datapub_NEONDOC004399.txt. One-minute, five-minute and 30-minute averages of incoming PAR will be determined according to Eq. (2), (3) and (4) to create the L1 DPs listed in pws_datapub_NEONDOC000781.txt. Individual calibrated measurements, i.e. 1 Hz PAR, will be made available upon request.

$$\overline{PAR}_1 = \frac{1}{n}\sum_{i=1}^{n} PAR_i \tag{2}$$

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

Further,

$$\overline{PAR}_{30} = \frac{1}{n}\sum_{i=1}^{n} PAR_i \tag{3}$$

where, for each 30-minute average, n is the number of measurements during the averaging period and T_i is a 1-Hz PAR measurement taken during the 1800-second averaging period [0, 1800).

The buoy mounted Li-Cor 1925A and PQS-1 return data at about 2 measurements per minute. Because of the communication system at the buoys (AD[19]), it is possible that zero or more than two (probably 3 or 4 maximum) measurements will be returned per minute. Thus, for the buoy Li-Cor 1925A and PQS-1 the number of values that are averaged may not be a consistent count. Usually, 1-minute mean will be just two instantaneous measurements and 30-minute mean will be a mean of 60 measurements. When zero measurements are returned for a given minute, a timestamp and data may not be published to users.

Finally, for PAR measured at the water surface, the five-minute average is included according to the following equation

$$\overline{PAR}_5 = \frac{1}{n}\sum_{i=1}^{n} PAR_i \tag{4}$$

where, for each 5-minute average, n is the number of measurements during the averaging period and T_i is a 1-Hz PAR measurement taken during the 300-second averaging period [0, 300).

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. 1 Hz sensor outputs (I) will be converted to PAR according to Eq. (1) using PAR sensor calibration coefficients provided by CVAL.
2. QA/QC Plausibility tests will be applied to the data stream in accordance with AD[06], details are provided below.
3. One- and thirty-minute PAR averages will be calculated using Eq. (2) and (3).
4. Descriptive statistics, i.e. minimum, maximum, and variance, will be determined for both one- and thirty-minute averages.
5. QA/QC consistency tests will be applied to one- and thirty-minute averages in accordance with AD[05].
   Quality metrics, quality flags, and the final quality flag will be produced for one-, five- and thirty-minute averages according to AD[17].

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

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

2. **Quality Flags (QFs) and Quality Metrics (QMs)** AD[17] – If a datum has failed one of the following tests it will not be used to create a L1 DP, ***range***, ***persistence***, and ***step.*** *The persistence test is only applied during local daylight hours.* α and β QFs and QMs will be determined using the flags listed in **Table 5**. In addition, L1 DPs will have a QA/QC report and quality metrics associated with each flag listed in **Table 5** as well as a final quality flag, as detailed in AD[17]. Ancillary information needed for the algorithm and other information maintained in the CI data store is shown in **Table 6**.

Table 5. Flags associated with PAR measurements.

Flags
Range
Persistence
Step
Null
Gap
Alpha
Beta
Final Quality Flag
Valid Calibration

Table 6. Information maintained in the CI data store for PAR.

Tests/Values	**CI Data Store Contents**
Range	Minimum and maximum values
Persistence	Window size, threshold values and maximum time length. Only applicable during daylight hours.
Step	Threshold values
Null	Test limit
Gap	Test limit
Calibration	CVAL sensor specific calibration coefficients
Uncertainty	AD[14]
Final Quality Flag	AD[17]
Valid Calibration	CVAL sensor specific valid calibration date range

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 PAR measurements as well as L1 mean PAR data products. It is a reflection of the information described in AD[12], and is explicitly described for the radiation assembly in the following sections.

6.1 Uncertainty of PAR Measurements

Uncertainty of the PAR 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**. Uncertainty calculations for the LiCor 1925A will use different values, but the same equations as shown for the Kipp & Zonen's PQS 1 PAR Quantum Sensor.

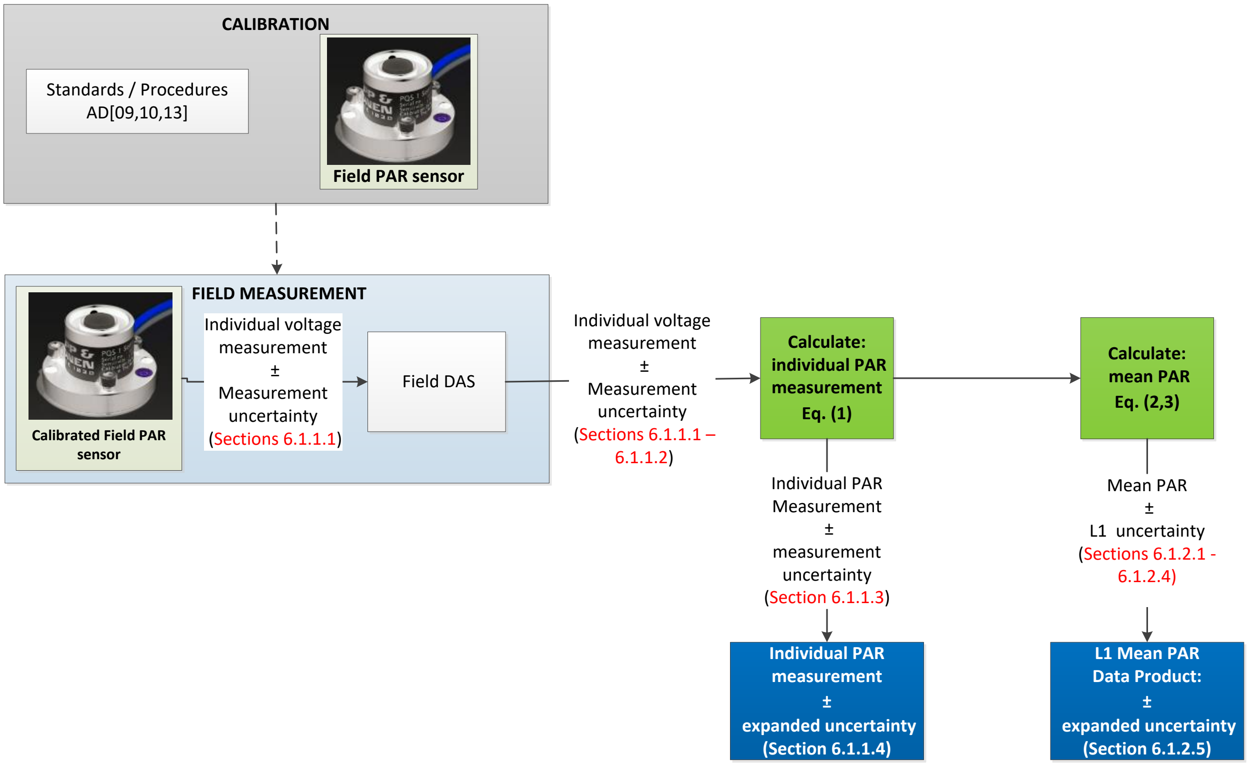

Figure 2. Displays the data flow and associated uncertainties of individual PAR measurements and L1 PAR DPs. For more information regarding the methods by which the PAR sensor is calibrated, please refer to AD[09,10,13].

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[12] 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 measured *y* is a function of *n* input quantities

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

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

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.

Thus, the uncertainty of the measurand can be found by summing the input uncertainties in quadrature. The calculation of these input uncertainties is discussed below.

6.1.1.1 Calibration

Uncertainties associated with the calibration process propagate into a combined, relative, 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 Eq. (1)). It is a relative value [%] that will be provided by CVAL (AD[14]) and stored in the CI data store. After converting from [%] to measurement units, it will be applied to all individual PAR 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[09,10,13].

The combined, standard, measurement uncertainty due to the calibration process, $u_{CVAL}(PAR_i)$, is calculated as follows:

$$u_{CVAL}(PAR_i) = u_{A1} * PAR_i \tag{5}$$

6.1.1.2 Field DAS

Uncertainty calculations for the Campbell CR1000 will use the same equations as those for the Grape data loggers. To quantify the uncertainty introduced by the Field DAS (FDAS), the following equations are computed.

$$u_{FDAS}(I_i) = (u_{V1} * I_i) + O_V \tag{6}$$

Where:

$u_{FDAS}(I_i)$ = combined, standard uncertainty introduced by the Field DAS through the irradiance reading (V)

I_i = Sensor output (irradiance; V)

u_{V1} = combined, relative Field DAS uncertainty for voltage readings provided by CVAL (unitless)
O_V = offset imposed by the FDAS for voltage readings provided by CVAL (V)

The partial derivative of a PAR measurement with respect to the irradiance reading is:

$$\frac{\partial PAR_i}{\partial I_i} = C_1; \tag{7}$$

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

$$u_{FDAS}(PAR_i) = \left|\frac{\partial PAR_i}{\partial I_i}\right| u_{FDAS}(I_i) \tag{8}$$

where:

$\frac{\partial PAR_i}{\partial I_i}$ = partial derivative of Eq. (1) with respect to I_i (µmol m^{-2} s^{-1} V^{-1})
C_1 = calibration coefficient provided by CVAL (µmol m^{-2} s^{-1} V^{-1})
$u_{FDAS}(PAR_i)$ = converted, combined, standard uncertainty of PAR_i introduced by the Field DAS (µmol m^{-2} s^{-1})

6.1.1.3 Combined Measurement Uncertainty

The combined, standard, measurement uncertainty for an individual PAR measurement, $u_c(PAR_i)$, is given in units of µmol m^{-2} s^{-1} and computed by summing the individual uncertainties in quadrature:

$$u_c(PAR_i) = \left(u_{CVAL}^2(PAR_i) + u_{FDAS}^2(PAR_i)\right)^{\frac{1}{2}} \tag{9}$$

6.1.1.4 Expanded Measurement Uncertainty

The expanded measurement uncertainty is calculated as:

$$U_{95}(PAR_i) = k_{95} * u_c(PAR_i) \tag{10}$$

Where:

$U_{95}(PAR_i)$ = expanded measurement uncertainty at 95% confidence (µmol m^{-2} s^{-1})

k_{95} = 2; coverage factor for 95% confidence (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 determine the validity of the L1 mean PAR DP, its uncertainty must be calculated. The distribution of the individual measurements is used as metric to quantify this uncertainty. 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:

$$u_{NAT}(\overline{PAR}) = \frac{s(PAR_i)}{\sqrt{n}} \tag{11}$$

Where,

$u_{NAT}(\overline{PAR})$ = standard error of the mean (natural variation) (µmol m^{-2} s^{-1})

$s(PAR_i)$ = experimental standard deviation of individual observations for the defined time period (µmol m^{-2} s^{-1})

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

6.1.2.2 Calibration

The uncertainty detailed here is similar to that described in Section 6.1.1.1. However, this combined, relative 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 relative value [%] that will be provided by CVAL (AD[14]) and stored in the CI data store. After converting to measurement units, the uncertainty will be applied to the *maximum* PAR value observed over the averaging period.

$$u_{CVAL(TT)}\left(\overline{PAR}\right) = u_{A3} * PAR_{MAX} \qquad (12)$$

Where, the subscript "MAX" represents the maximum PAR value observed over a set (averaging period) of observations. Mathematically, this can be defined as:

$$MAX = \{i: u_c(PAR_i) = \max[u_c(PAR_1), \dots, u_c(PAR_n)]\}. \qquad (13)$$

And,

$u_{CVAL(TT)}\left(\overline{PAR}\right)$	= combined, standard, Field DAS truth and trueness uncertainty due to the PAR measurement (µmol m^{-2} s^{-1})
PAR_{MAX}	= PAR measurement corresponding to the maximum, combined, standard measurement uncertainty of PAR during the averaging period (µmol m^{-2} s^{-1})
u_{A3}	= Combined, relative uncertainty (truth and trueness only) of PAR sensor (%)

Please refer to AD[12] for further justification regarding evaluation and quantification of using the maximum index for quantification of these L1 mean data product uncertainties.

6.1.2.3 Field DAS

Since the L1 mean DP is a function of the individual measurements, any measurement bias introduced by the Field DAS will be reflected in the L1 mean data product. Here, the raw measurement that maximizes the combined uncertainty of an individual measurement (Eq. (13)) 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[12].

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 voltage propagates through to the uncertainty of the measurement attributable to the Field DAS (Eqs. (6)-(8)).

$$u_{FDAS(TT)}(I_{MAX}) = (u_{V3} * I_{MAX}) + O_V \tag{14}$$

Where,

$u_{FDAS(TT)}(I_{MAX})$ = Field DAS *Truth* and *Trueness* uncertainty of I_{MAX} (V)
I_{MAX} = individual, *maximum,* irradiance measurement observed during the averaging period (V)
u_{V3} = combined, relative, Field DAS uncertainty (truth and trueness only) provided by CVAL (%)
O_V = offset imposed by the FDAS for voltage readings provided by CVAL (V)

Thus, analogous to Eq. (8):

$$u_{FDAS(TT)}(\overline{PAR}) = \left|\frac{\partial PAR_i}{\partial I_i}\right|_{I_{MAX}} u_{FDAS(TT)}(I_{MAX}) \tag{15}$$

Where,

$\left|\frac{\partial PAR_i}{\partial I_i}\right|_{I_{MAX}}$ = partial derivative of PAR_i with respect to I_i (Eq.(7)) evaluated at I_{MAX} (µmol m^{-2} s^{-1} V^{-1})
C_1 = calibration coefficient provided by CVAL (µmol m^{-2} s^{-1} V^{-1})
$u_{FDAS(TT)}(\overline{PAR})$ = *Truth* and *Trueness* uncertainty of the mean DP introduced by the Field DAS (µmol m^{-2} s^{-1})

6.1.2.4 Combined Uncertainty

The combined uncertainty for our L1 mean PAR data product, $u_c(\overline{\mathrm{PAR}})$, given in units of µmol m^{-2} s^{-1}, is computed by summing the uncertainties from Sections 6.1.2.1 through 6.1.2.3 in quadrature:

$$u_c(\overline{\mathrm{PAR}}) = \left(u_{NAT}^2(\overline{PAR}) + u_{CVAL(TT)}^2(\overline{PAR}) + u_{FDAS(TT)}^2(\overline{PAR})\right)^{\frac{1}{2}} \tag{16}$$

6.1.2.5 Expanded Uncertainty

The expanded uncertainty is calculated as:

$$U_{95}(\overline{\mathrm{PAR}}) = k_{95} * u_c(\overline{\mathrm{PAR}}) \tag{17}$$

Where:

$U_{95}(\overline{\mathrm{PAR}})$ = expanded L1 mean data product uncertainty at 95% confidence (µmol m^{-2} s^{-1})

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

6.1.2.6 Communicated Precision

L1 mean PAR data products will be reported to 0.01 µmol m^{-2} s^{-1}. The FDAS is capable of measuring voltage at a resolution of 0.5 µV. Assuming a 10 µV (µmol m^{-2} s^{-1})$^{-1}$ maximum calibration sensitivity of the PAR sensor, the resultant resolution of an individual PAR measurement is 0.05 µmol m^{-2} s^{-1}. Lab-measured PAR sensor repeatability is on the order of 0.02%. The Campbell Scientific logger on the buoys has a resolution of 3.33 µV for a range of +/-25 mV differential on the multiplexer. Assuming a 10 µV (µmol m^{-2} s^{-1})$^{-1}$ maximum calibration sensitivity of the PAR sensor, the resultant resolution of an individual PAR measurement is 0.33 µmol m^{-2} s^{-1} for the buoy deployments.

6.1.3 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. Uncertainty budget calculations for the LiCor 1925A will use different values, but the same equations as shown for the Kipp & Zonen's PQS 1 PAR Quantum Sensor.

Table 7. Uncertainty budget for an individual PAR measurement. Shaded rows denote the order of uncertainty propagation (from lightest to darkest).

Source of measurement uncertainty	**Measurement uncertainty component** $\boldsymbol{u(x_i)}$	**Measurement uncertainty value**	$\frac{\partial f}{\partial x_i}$	$u_{x_i}(Y) \equiv \left\lvert\frac{\partial f}{\partial x_i}\right\rvert u(x_i)$ [$\mu mol\ m^{-2}\ s^{-1}$]
1 Hz PAR	$u_c(PAR_i)$	Eq. (9) [$\mu mol\ m^{-2}\ s^{-1}$]	n/a	n/a
Sensor/calibration	$u_{CVAL}(PAR_i)$	Eq. (5) [$\mu mol\ m^{-2}\ s^{-1}$]	1	Eq. (5)
Field DAS	$u_{FDAS}(PAR_i)$	Eq. (6) [V]	Eq. (7)	Eq. (8)

Table 8. Uncertainty budget for L1 mean PAR measurements. Shaded rows denote the order of uncertainty propagation (from lightest to darkest).

Source of uncertainty	**Uncertainty component** $\boldsymbol{u(x_i)}$	**Uncertainty value**	$\frac{\partial f}{\partial x_i}$	$u_{x_i}(Y) \equiv \left\lvert\frac{\partial f}{\partial x_i}\right\rvert u(x_i)$ [$\mu mol\ m^{-2}\ s^{-1}$]
L1 mean PAR	$u_c(\overline{PAR})$	Eq. (16) [$\mu mol\ m^{-2}\ s^{-1}$]	n/a	n/a
Natural variation	$u_{NAT}(\overline{PAR})$	Eq. (11) [$\mu mol\ m^{-2}\ s^{-1}$]	1	Eq. (11)
Sensor/calibration	$u_{CVAL(TT)}(\overline{PAR})$	Eq. (12) [$\mu mol\ m^{-2}\ s^{-1}$]	1	Eq. (12)
Field DAS	$u_{FDAS(TT)}(\overline{PAR})$	Eq. (14) [V]	Eq. (7)	Eq. (15)

7 FUTURE PLANS AND MODIFICATIONS

Individual calibrated and QA/QCD measurements with their respective uncertainties may become a common data output. Likewise, future system flags may be incorporated into the data stream and included in the QA/QC summary. 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. A QA/QC flag for data consistency will be applied data streams from terrestrial sites according to the redundancy analysis outlined in AD[05], and a pass/fail flag will be generated to reflect this activity. To evaluate PAR for consistency, L1 PAR from a given sensor will first be compared to the sensor above it on the tower infrastructure. If a difference between the two PAR 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 PAR difference between the sensors outside the defined limits will result in a failed test. A failed test from the above sensor will result in the sensor being compared to the sensor below it; if this too results in a failed test then the sensor will have failed the consistency analysis and be flagged as such. If the sensor fails the first test but passes the second then it will have passed the consistency analysis. This structure helps to ensure 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 sensor on the bottom of the tower will only be compared to the sensor above it and the uppermost sensor will only be compared to the sensor below it.

QA/QC tests may be expanded to include a flag for when above water PAR sensor on buoys are not within +/- 5 degrees south of sensor infrastructure. This can be accomplished using compass orientation data.

Ideally, future updates to the buoy Campbell CR1000 data logger will allow for PAR data to stream at the same frequency as the tower and inlet/outlet sensors of 1 Hz.

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