Algorithm Theoretical Basis Document
Quantum Line Sensor

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Change Record

REVISION	DATE	ECO #	DESCRIPTION OF CHANGE
A	Mar 2013		Initial Release
B	Aug 2013		Revised *Algorithm Implementation* and *Uncertainty* Sections
C	Jan 2014		Altered variable nomenclature; Revised *Algorithm Implementation*, *Uncertainty*, and *Future Plans/ Modifications* Sections

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1 DESCRIPTION

The LI-191 Quantum Line Sensor will be deployed in the soil array at NEON TIS sites to measure photosynthetically active radiation (PAR) at the soil surface. Contained in this document are details concerning PAR 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.

1.1 Purpose

This document details the algorithms used for creating NEON Level 1 (L1) data products (DP) from Level 0 data, obtained via instrumental measurements made by Licor LI-191 Quantum Line Sensor [NEON P/N: 0300300000]. It includes a detailed discussion of measurement theory and implementation, theoretical background, data product provenance, quality assurance and control methods used, assumptions, and a detailed estimation of uncertainty resulting in a cumulative uncertainty budget for this product.

1.2 Scope

This document describes the theoretical background and entire algorithmic process for creating L1 DPs from input data (L0). It does not provide computational methodology to implement the details of the approaches presented here, except for cases where they stem directly from algorithmic/mathematical choices explained here.

2 RELATED DOCUMENTS ACRONYMS AND VARIABLE NOMENCLATURE

2.1 Applicable Documents

AD[01]	NEON.DOC.000001	NEON OBSERVATORY
AD[02]	NEON.DOC.005003	NEON Scientific Data Products Catalog
AD[03]	NEON.DOC.005004	NEON Level 1-3 Data Products Catalog
AD[04]	NEON.DOC.005005	NEON Level 0 Data Products Catalog
AD[05]	NEON.DOC.000782	ATBD QA/QC Data Consistency
AD[06]	NEON.DOC.011081	ATBD QA/QC plausibility tests
AD[07]	NEON.DOC.000783	ATBD De-spiking and time series analyses
AD[08]	NEON.DOC.000746	Evaluating Uncertainty (CVAL)
AD[09]	NEON.DOC.000603	NEON Sensor Command, Control, and Configuration - Quantum Line Sensor
AD[10]	NEON.DOC.000785	TIS Level 1 Data Products Uncertainty Budget Estimation Plan
AD[11]	NEON.DOC.000927	NEON Calibration and Sensor Uncertainty Values (CVAL)
AD[12]	NEON.DOC.000752	Line Quanta PAR Calibration Fixture L2R400
AD[13]	NEON.FIU.011071	FIU Site Specific Sensor Location Matrix
AD[14]	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
RD[03]	LI-COR Terrestrial Radiation Sensors Instruction Manual
RD[04]	LI-191SA Line Quantum Sensor Brochure
RD[05]	Comparison of Quantum Sensors with Different Spectral Sensitivities, Technical Note #126

2.3 Acronyms

Acronym	Explanation
ATBD	Algorithm Theoretical Basis Document
CI	NEON Cyberinfrastructure project team
CVAL	NEON Calibration, Validation, and Audit Laboratory
DAS	Data Acquisition System
DP	Data Product
FDAS	Field Data Acquisition System
FIU	Fundamental Instrument Unit
GRAPE	Grouped Remote Analog Peripheral Equipment
L0	Level 0

L1	Level 1
PAR	Photosynthetically Active Radiation
QA/QC	Quality Assurance/Quality Control
TIS	Terrestrial Instrument System

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/Portal Notation	Description
C_1	CVALA1	CVAL calibration coefficient
$\overline{PAR}_1$	meanIncomingPAR_1	One-minute mean Incoming PAR
$\overline{PAR}_{30}$	meanIncomingPAR_30	Thirty-minute mean Incoming PAR
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 voltage measurements (%)
u_{V3}	U_CVALV3	Combined, relative uncertainty (truth and trueness only) of Field DAS voltage measurements (%)
$V_{eff\,A1}$	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)
$V_{eff\,V1}$	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)

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

Level 1 data products that will be produced from this ATBD are shown in Table 1.

Table 1. List of Level 1 data products that will be produced from this ATBD. Note: The '0XX' in the eighth field of the Data Product ID refers to the horizontal location of the sensor in the soil array. '001' refers to the sensor closest to the tower infrastructure.

Data product	Averaging Period	Units	Data stream ID
1-minute Mean Incoming PAR (meanIncomingPAR_1)	1-min	µmol s^{-1} m^{-2}	NEON.DXX.XXX.DP1.00066.001.001.00X.001
1-minute Minimum Incoming PAR (minIncomingPAR_1)	1-min	µmol s^{-1} m^{-2}	NEON.DXX.XXX.DP1.00066.001.002.00X.001
1-minute Maximum Incoming PAR (maxIncomingPAR_1)	1-min	µmol s^{-1} m^{-2}	NEON.DXX.XXX.DP1.00066.001.003.00X.001
1-minute Incoming PAR Variance (varIncomingPAR_1)	1-min	(µmol s^{-1} $m^{-2})^2$	NEON.DXX.XXX.DP1.00066.001.004.00X.001
1-minute Incoming PAR Skewness (skIncomingPAR_1)	1-min	Unitless	NEON.DXX.XXX.DP1.00066.001.005.00X.001
1-minute Incoming PAR Kurtosis (kuIncomingPAR_1)	1-min	Unitless	NEON.DXX.XXX.DP1.00066.001.006.00X.001
1-minute Incoming PAR QA/QC Summary (QsumIncomingPAR_1)	1-min	N/A	NEON.DXX.XXX.DP1.00066.001.007.00X.001
1-minute Incoming PAR QA/QC Report (QrptIncomingPAR_1)	1-min	N/A	NEON.DXX.XXX.DP1.00066.001.008.00X.001
30-minute Mean Incoming PAR (meanIncomingPAR_30)	30-min	µmol s^{-1} m^{-2}	NEON.DXX.XXX.DP1.00066.001.001.00X.002
30-minute Minimum Incoming PAR (minIncomingPAR_30)	30-min	µmol s^{-1} m^{-2}	NEON.DXX.XXX.DP1.00066.001.002.00X.002
30-minute Maximum Incoming PAR	30-min	µmol s^{-1} m^{-2}	NEON.DXX.XXX.DP1.00066.001.003.00X.002

(maxIncomingPAR_30)			
30-minute Incoming PAR Variance (varIncomingPAR_30)	30-min	$(\mu mol\ s^{-1}\ m^{-2})^2$	NEON.DXX.XXX.DP1.00066.001.004.00X.002
30-minute Incoming PAR Skewness (skIncomingPAR_30)	30-min	Unitless	NEON.DXX.XXX.DP1.00066.001.005.00X.002
30-minute Incoming PAR Kurtosis (kuIncomingPAR_30)	30-min	Unitless	NEON.DXX.XXX.DP1.00066.001.006.00X.002
30-minute Incoming PAR QA/QC Summary (QsumIncomingPAR_30)	30-min	N/A	NEON.DXX.XXX.DP1.00066.001.007.00X.002

3.2 Input Dependencies

A summary of the inputs required to produce the Level 1 data product are shown in Table 2.

Table 2. Level 0 data products that are used to produce the Level 1 data product in this ATBD.

Data product	**Sample Frequency**	**Units**	**Data stream ID NEON.DOM.SIT.DPL.PRN.REV.SPN.HOR.VER.REP**
PAR sensor voltage (E_{out})	1 Hz	V	NEON.DOM.SIT.DP0.00066.001.001.00X.000.001

3.3 Product Instances

Three quantum line sensors will be deployed at each site and shall reside within the soil plots.

3.4 Temporal Resolution and Extent

One- and thirty-minute averages of PAR at the soil surface will be calculated to form L1 DPs.

3.5 Spatial Resolution and Extent

The spatial resolution will depend on the placement of the quantum line sensor in the soil array. To maximize spatial coverage, quantum line sensors will be deployed in three (i.e., one sensor per plot) out of five soil plots that comprise the soil array at each TIS site. Their measurements will be representative of the point in space where they are located. A description of how the sensors are located within plots is described in AD[13].

4 SCIENTIFIC CONTEXT

Radiation in the 400 nm to 700 nm waveband represents most of the visible solar radiation. This waveband is utilized directly by plant biochemical processes in photosynthesis to convert light energy into chemical energy, which can be stored in the molecular bonds of organic molecules (e.g., sugars). This specific waveband is defined as Photosynthetically Active Radiation (PAR). PAR is also often referred to as Photosynthetic Photon Flux Density (PPFD), and estimated in quanta per unit area and per unit time, or µmol m^{-2} s^{-1}.

PAR measured via the quantum line sensor will provide information on the light availability at the ground level. This has significant ecophysiological applications as the light at the ground is patchy due to sunflecks, i.e., spots on the ground where direct (or near direct) solar radiation is incident. Many understory plants take advantage of these sunflecks through adaptation of their activation energy to charge the photosystems I and II (Jones, 1992; Salsbury and Ross 1978). While this ATBD describes the conversion of L0 to L1 data products, the data from the quantum line sensors is used in conjunction with the vertical profile of PAR sensors from the top to bottom of the tower structure. Ultimately, quantum line sensor data will inform higher-level data products and contribute to our understanding of energy balance and radiation transfer into and within the canopy. This will help to foster energy balance research by helping to answer various questions, such as how much radiation is attenuated or absorbed by the plant canopy and how much remains for biochemical processes.

4.1 Theory of Measurement/Observation

LI-COR191 Quantum Sensor is designed for measuring PAR in applications where the solar radiation to be measured is spatially inhomogeneous, e.g., below plant canopies. Rather than using multiple detectors, the LI-191 uses a one meter long quartz rod under a diffuser to conduct light to a single high quantum sensor (RD[03]). The integrated horizontal measurement of PAR at the ground portrays a more representative measure than a single 'point' sensor.

The dashed black line in Figure 1 shows the ideal relative response of a quantum sensor in terms of sensitivity to photons: the sensor has no sensitivity (clear cutoffs) to light below 400 nm and above 700 nm, and a constant sensitivity to all photons across the 400 to 700 nm wavelength ranges. The sensitivity of the LI-191 (the solid blue line in Figure 1) oscillates around the ideal quantum responses and has sharp cutoffs below 400 and above 700 nm (RD[05]). Output of the LI-191 is not biased significantly at either the blue or red ends of the spectrum. The actual area under each deviation from ideal is small and errors tend to cancel (RD[05]).

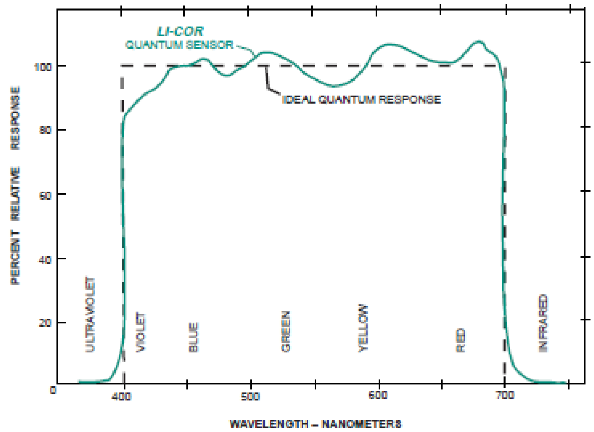

Figure 1. Relative spectral response of LI-191 quantum sensor (solid blue line) and ideal quantum sensor (dashed black line). Source: RD[04].

4.2 Theory of Algorithm

The LI-191 sensor is a current output device. However, the current will be converted to voltage through a fixed resistor (1250 ohms, provided by ENG) in the sensor which will require an independent calibration coefficient for each sensor. The calibration coefficient for each sensor will be determined by CVAL according to AD[12]. Using the sensor calibration coefficient and voltage output from the sensor, PAR is obtained in the required SI units (µmol m^{-2} s^{-1}) by:

$$PAR_i = C_1 * I_i \tag{1}$$

Where:

PAR_i = Individual (1 Hz) PAR at the soil surface (µmol m^{-2} s^{-1})

I_i = Individual Li-191 sensor output (V)

C_1 = LI-191 sensor calibration coefficient (µmol m^{-2} s^{-1} V^{-1}, provided by CVAL and sensor specific)

After PAR is determined, one-minute ($\overline{PAR_1}$) and thirty-minute ($\overline{PAR_{30}}$) averages of PAR will be determined according to Eq. (2) and (3) to create L1 DPs. 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 PAR_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.

and

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

where, for each 30-minute average, n is the number of measurements during the averaging period and PAR_i is a 1-Hz PAR 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.

The third and fourth standardized moments of a random variable are known as the skewness and kurtosis of the random variable, respectively. The skewness is used as a measure of the asymmetry of the distribution and the kurtosis as a measure of the peakedness of the distribution. Together, sample estimates of these measures are often used to assess the normality of a distribution.

Both the skewness and the kurtosis will be estimated for one-minute and thirty-minute averaging periods of PAR as follows (NIST/SEMATECH, 2013):

Skewness:

$$\text{skew(PAR)} = \frac{1}{(n-1)} \cdot \frac{\sum_{i=1}^{n}(PAR_i - \overline{PAR})^3}{s^3(PAR)} \qquad (4)$$

Kurtosis:

$$\text{kurt(PAR)} = \frac{1}{(n-1)} \cdot \frac{\sum_{i=1}^{n}(PAR_i - \overline{PAR})^4}{s^4(PAR)} \qquad (5)$$

Where:

$$s(\text{PAR}) = \left(\frac{1}{(n-1)} \cdot \sum_{i=1}^{n}(PAR_i - \overline{PAR})^2\right)^{1/2} \qquad (5)$$

is the standard deviation of PAR for either a one or thirty minute averaging period (µmol m^{-2} s^{-1}) and

skew(PAR)	= PAR skewness for a given one- or thirty-minute average (unitless)
kurt(PAR)	= PAR kurtosis for a given one- or thirty-minute average (unitless)
$\overline{PAR}$	= One-minute or thirty-minute PAR average
n	= Number of measurements for a given one- or thirty-minute average

5 ALGORITHM IMPLEMENTATION

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

1. 1 Hz data will be converted to PAR (µmol m^{-2} s^{-1}) using to Eq. (1) as described in section 4.2.
2. QA/QC Plausibility tests will be applied to the data stream in accordance with AD[06]. The details are provided below.
3. Signal de-spiking will be applied to the data stream in accordance with AD[07].
4. One- and thirty-minute PAR averages will be calculated using Eq. (2) and (3) and descriptive statistics (i.e. minimum, maximum, variance, skewness, and kurtosis) will be determined for both averaging periods.
5. QA/QC consistency tests will be applied to one- and thirty-minute average in accordance with AD[05].
6. QA/QC Summary (Qsum) will be produced for one- and thirty-minute averages according to AD[14].

<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 CI data store. 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**– The time series despiking routine will be run according to AD[07]. Test parameters will be specified by FIU and maintained in the CI data store. Quality flags resulting from the despiking analysis will be applied according to AD[07].

3. **Consistency Analysis** – A QA/QC flag for data consistency will be applied according to the redundancy analysis outlined in AD[05], and a pass/fail flag will be generated to reflect this analysis. Assume soil type and ground cover are the same among soil plots at a given site and assume that the position of sensors are located within the soil array as shown in the Figure 2(a). To evaluate PAR at the soil surface for consistency, L1 PAR from a given LI-191 quantum line sensor (a quantum line sensor at position 2) will first be compared to the LI-191 sensor at position 1. 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 its consistency analysis. Alternatively, a PAR difference between the LI-191 sensors outside the defined limits will result in a failed test. A failed test between the sensors in position 1 and 2, will result in the g LI-191 sensor at position 2 being compared to the sensor at position 3. If this too results in a failed test, then the LI-191 sensor will have failed the consistency test and be flagged as such (Figure 2(b)). If the LI-191 sensor fails the first test but passes the second then it will have passed the consistency test. This test structure helps to ensure that non-functional sensors (e.g., sensors that are faulty or due for service) do not bias the test, since a resulting

failed test will allow the sensor to be compared to the other one. Accordingly, the sensors at position 1 and 3 will be first compared to the nearby sensor (sensor at position 2) and then to each other. L1 DPs that fail the Consistency Analysis will continue to be reported, but will have an associated failed flag that will be included in the QA/QC summary. Note that the evaluation procedures of PAR at the soil surface for consistency may not be applied if soil type and ground cover are not consistent amongst the soil plots.

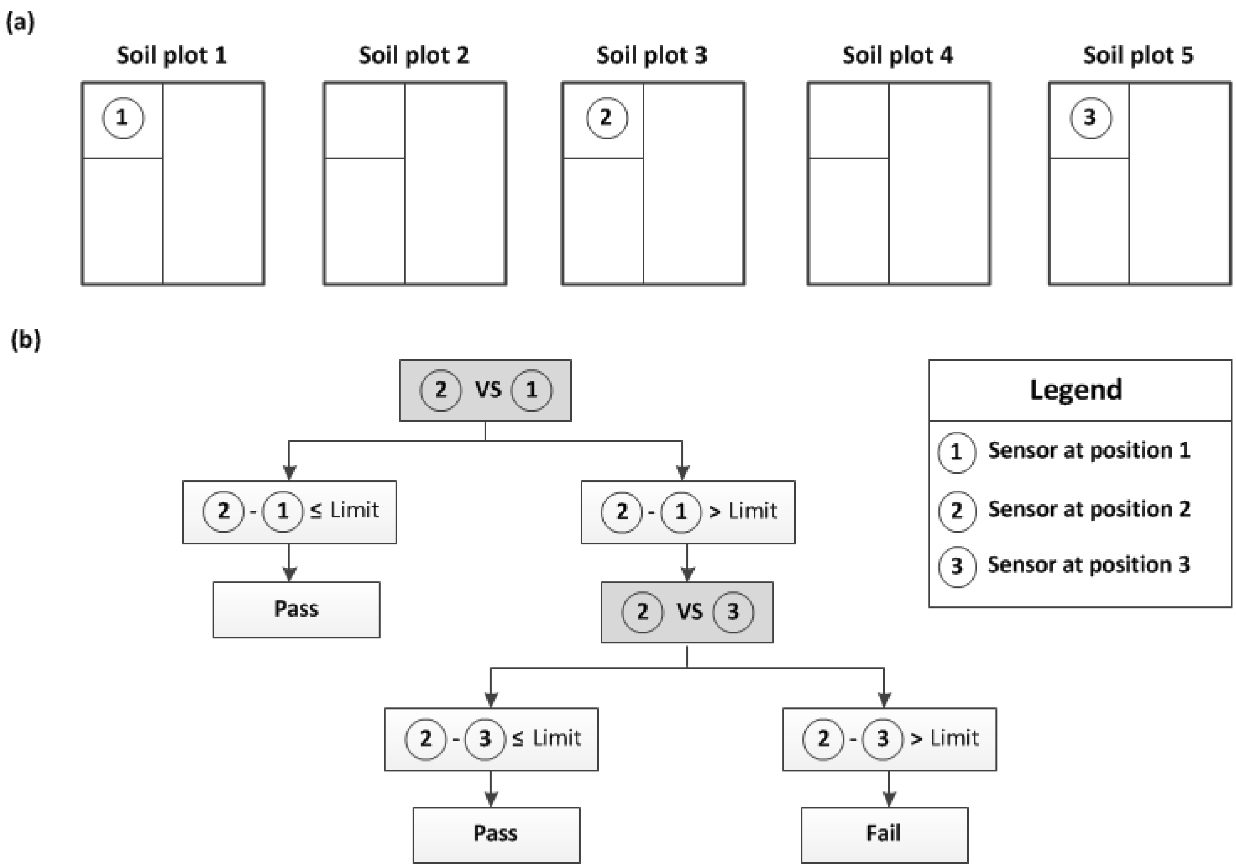

Figure 2. (a) Diagram of the position of the LI-191 sensors within the soil array and (b) consistency test flow diagram for the LI-191 sensor deployed at position 2.

4. **Quality Flags (QFs) and Quality Metrics (QMs)** AD[14] – If a datum has one of the following flags it will not be used to create a L1 DP, ***QF_RH*** and ***QF_D***. α and β QFs and QMs will be determined for the following flags QF_RH, QF_RS, QF_P, QF_S, QF_N, QF_G, and QF_D. All L1 DPs will have an associated final quality flag, QF_FINAL, and quality summary, Qsum, as detailed in AD[14]. Flags that may be associated with measurements of PAR, as well as information maintained in the CI data store can be found below in Tables 3 and 4.

Table 3. Flags associated with the quantum line sensor.

Tests	Flags

Range (hard and soft)	QF_RH QF_RS
Persistence	QF_P
Step	QF_S
Null	QF_N
Gap	QF_G
Signal Despiking and Time Series Analysis	QF_D QF_O QF_I
Consistency Analysis	QF_V
Final quality flag	QF_FINAL

Table 4. Information maintained in the CI data store for the quantum line sensor.

Tests/Values	CI Data Store Contents
Range (hard and soft)	Minimum and maximum values
Persistence	Window size, threshold values and maximum time length
Step	Threshold values
Null	Test limit
Gap	Test limit
Signal Despiking and Time Series Analysis	Time segments and threshold values
Calibration	CVAL sensor specific calibration coefficients
Uncertainty	AD[11]
Consistency Analysis	Test limits
Final Quality Flag	AD[14]

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 measurments as well as the L1 mean PAR DPs. 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 quantum line assembly is discussed in this section. The section is broken down into two topics. The first informs the sources of *measurement* uncertainty, i.e., those associated with *individual measurements*. The second details uncertainties associated with temporally averaged data products. A diagram detailing the data flow and known sources of uncertainty are displayed in Figure 3.

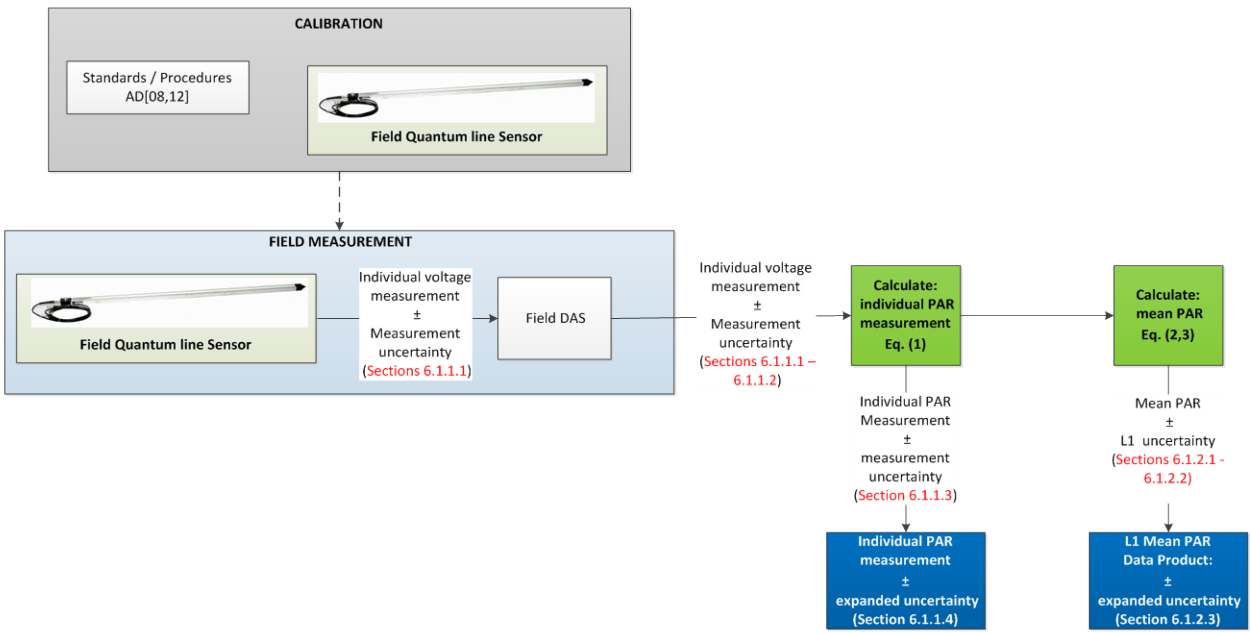

Figure 3. Displays the data flow and associated uncertainties of individual PAR measurements and L1 PAR DPs. For more information regarding the methods by which the PAR sensor is calibrated, please refer to AD[08, 12].

6.1.1 Measurement Uncertainty

The following subsections present the uncertainties associated with *individual PAR 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* PAR measurement. These uncertainties should not be confused with those presented in Section 6.1.2. We urge the reader to refer to AD[10] for further details concerning discrepancies between quantification of measurement uncertainties and L1 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:

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

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.

Thus, the uncertainty of the measurand can be found be summing the input uncertainties in quadrature. For PAR measurements, the sources of uncertainty are depicted in 3. 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 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, $u_{CVAL}(PAR_i)$, is calculated as follows:

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

6.1.1.2 Field DAS

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

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

Where:

$u_{FDAS}(I_i)$ = combined, standard uncertainty of the voltage measurement introduced by the Field Das (V)

I = Sensor output (irradiance; V)

u_{V1} = combined, relative Field DAS uncertainty for voltage measurements 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 measurement 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 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 (Eq. (4)):

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

6.1.1.4 Expanded Measurement Uncertainty

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

$$V_{eff\,PAR_i} = \frac{u_c^4(PAR_i)}{\frac{u_{CVAL}^4(PAR_i)}{V_{eff\,A1}} + \frac{u_{FDAS}^4(PAR_i)}{V_{eff\,V1}}} \tag{10}$$

$V_{eff\,PAR_i}$ = 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 calibration uncertainty; provided by CVAL in AD[14] (unitless)

$V_{eff_{V1}}$ = effective degrees of freedom relating to quantification of field DAS uncertainty; provided by CVAL in AD[14] (unitless)

Next, the expanded measurement uncertainty is calculated:

$$U_{95}(PAR_i) = k_{95,V_{eff_{PAR_i}}} * u_c(PAR_i) \tag{11}$$

Where:

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

$k_{95,V_{eff_{PAR_i}}}$ = coverage factor obtained with the aid of Table 5 in AD[12] (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 *standard deviation of the mean (natural variation),* is computed. This value reflects the repeatability of insolation measurements for a specified time period:

$$u_{NAT}(\overline{PAR}) = \frac{s(PAR_i)}{\sqrt{n}} \tag{12}$$

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.

$$u_{CVAL(TT)}(\overline{PAR}) = u_{A3} * PAR_{MAX} \quad (13)$$

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

$$MAX = \{i: u_c(T_i) = \max[u_c(PAR_1), \dots, u_c(PAR_n)]\}. \quad (14)$$

And,

$u_{CVAL(TT)}(\overline{PAR})$	= 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.(9)) 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 resistance propagates through to the uncertainty of the measurement attributable to the Field DAS (Eqs. (6)-(8)).

$$u_{FDAS(TT)}(I_{MAX}) = (u_{V3} * I_{MAX}) + O_V \tag{15}$$

Where:

$u_{FDAS(TT)}(I_{MAX})$ = Field DAS *Truth* and *Trueness* uncertainty of I_{MAX} (V)

I_{MAX} = individual irradiance measurement observed at MAX index (V)

u_{V3} = combined, relative, Field DAS uncertainty (truth and trueness only) for voltage measurements; provided by CVAL (%)

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

Thus, analogous to Eq. (8),

$$u_{FDAS(TT)}(\overline{PAR}) = \left|\frac{\partial PAR_i}{\partial I_i}\right|_{I_{MAX}} u_{FDAS(TT)}(I_{MAX}) \tag{16}$$

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:

$$u_c(\overline{\mathrm{PAR}}) = \left(u_{NAT}^2(\overline{PAR}) + u_{CVAL(TT)}^2(\overline{PAR}) + u_{FDAS(TT)}^2(\overline{PAR})\right)^{\frac{1}{2}} \tag{17}$$

6.1.2.5 Expanded Uncertainty

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

$$V_{eff_{\overline{\mathrm{PAR}}}} = \frac{u_c{}^4(\overline{\mathrm{PAR}})}{\frac{u_{NAT}^4(\overline{PAR})}{n-1} + \frac{u_{CVAL(TT)}^4(\overline{PAR})}{V_{eff_{A2}}} + \frac{u_{FDAS(TT)}^4(\overline{PAR})}{V_{eff_{V3}}}} \quad (18)$$

Where:

$V_{eff_{\overline{\mathrm{PAR}}}}$ = effective degrees of freedom relating to quantification of the L1, mean, data product uncertainty (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 in AD[14] (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 in AD[14] (unitless)

Next, the expanded uncertainty is calculated:

$$U_{95}(\overline{\mathrm{PAR}}) = k_{95,V_{eff_{\overline{\mathrm{PAR}}}}} * u_c(\overline{\mathrm{PAR}}) \quad (19)$$

Where:

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

$k_{95,V_{eff_{\overline{\mathrm{PAR}}}}}$ = coverage factor obtained with the aid of Table 5 in AD[12] (unitless)

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.

Table 5. 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 $u(x_i)$**	**Measurement uncertainty value**	$\frac{\partial f}{\partial x_i}$	$u_{x_i}(Y) \equiv \left\lvert\frac{\partial f}{\partial x_i}\right\rvert u(x_i)$ $[\mu mol\ m^{-2}\ s^{-1}]$	**Degrees of Freedom**
1 Hz PAR	$u_c(PAR_i)$	Eq. (9) $[\mu mol\ m^{-2}\ s^{-1}]$	n/a	n/a	Eq. (10)
Sensor/calibration	$u_{CVAL}(PAR_i)$	Eq. (5)	1	Eq. (5)	$V_{eff_{A1}}$

Field DAS	$u_{FDAS}(I_i)$	$[\mu mol\ m^{-2}\ s^{-1}]$ Eq. (6) [V]	Eq. (7)	Eq. (8)	$V_{eff}{}_{V1}$

Table 6. Uncertainty budget for L1 mean PAR measurements. Shaded rows denote the order of uncertainty propagation (from lightest to darkest).

Source of uncertainty	**Uncertainty component** $u(x_i)$	**Uncertainty value**	$\frac{\partial f}{\partial x_i}$	$u_{x_i}(Y) \equiv \left\lvert\frac{\partial f}{\partial x_i}\right\rvert u(x_i)$ $[\mu mol\ m^{-2}\ s^{-1}]$	**Degrees of Freedom**
L1 mean PAR	$u_c(\overline{PAR})$	Eq. (17) $[\mu mol\ m^{-2}\ s^{-1}]$	n/a	n/a	Eq. (18)
Natural variation	$u_{NAT}(\overline{PAR})$	Eq. (12) $[\mu mol\ m^{-2}\ s^{-1}]$	1	Eq. (12)	$n-1$
Sensor/calibration	$u_{CVAL(TT)}(\overline{PAR})$	Eq. (13) $[\mu mol\ m^{-2}\ s^{-1}]$	1	Eq. (13)	$V_{eff}{}_{A3}$
Field DAS	$u_{FDAS(TT)}(\overline{PAR})$	Eq. (15)[V]	Eq.	Eq. (16)	$V_{eff}{}_{V3}$

7 FUTURE PLANS AND MODIFICATIONS

Future system flags may be incorporated into the data stream and included in the QA/QC summary. 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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9 CHANGELOG

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