ALGORITHM THEORETICAL BASIS DOCUMENT: PHOTOSYNTHETICALLY ACTIVE RADIATION (PAR)

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CHANGE RECORD

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1 DESCRIPTION

Photosynthetically active radiation (PAR) will be continuously monitored by NEON at core and relocatable sites. PAR for the top of the tower and the tower profile will be derived from the Kipp & Zonen PQS 1 PAR Quantum Sensor. The specific height and location of PAR sensors on the tower will vary between sites. For detailed information on a specific core or relocatable site see the respective site characterization reports.

1.1 Purpose

This document details the algorithms used for creating the NEON Level 1 data product NEON.DXX.XXX.DP1.00024.001.001.XXX.001 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. 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.DXX.XXX.DP1.00024.001.001.XXX.001 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 AND ACRONYMS

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.005004	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
AD[15]	NEON.DOC.000784	ATBD Profile Development
AD[16]	NEON.DOC.001256	C^3 Photosynthetically Active Radiation
AD[17]	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]	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.

2.3 Acronyms

Acronym	**Explanation**
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 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

Table 1 details the PAR measurements related to the L1 DPs provided by the algorithms in this ATBD.

Table 1: Details the PAR measurements related to the L1 DPs provided by the algorithms in this ATBD.

Data product	Averaging Period	Units	Data stream ID
1-minute Mean PAR (Mean_PAR_1)	1-min	µmol s^{-1} m^{-2}	NEON.DXX.XXX.DP1.00024.001.001.0XX.001
1-minute Minimum PAR (Min_PAR_1)	1-min	µmol s^{-1} m^{-2}	NEON.DXX.XXX.DP1.00024.001.002.0XX.001
1-minute Maximum PAR (Max_PAR_1)	1-min	µmol s^{-1} m^{-2}	NEON.DXX.XXX.DP1.00024.001.003.0XX.001
1-minute PAR Variance (σ^2_PAR_1)	1-min	(µmol s^{-1} $m^{-2})^2$	NEON.DXX.XXX.DP1.00024.001.004.0XX.001
1-minute PAR QA/QC Summary (Qsum_PAR_1)	1-min	N/A	NEON.DXX.XXX.DP1.00024.001.005.0XX.001
1-minute PAR QA/QC Report (Qrpt_PAR_1)	1-min	N/A	NEON.DXX.XXX.DP1.00024.001.006.0XX.001
30-minute Mean PAR (Mean_PAR_{30})	30-min	µmol s^{-1} m^{-2}	NEON.DXX.XXX.DP1.00024.001.001.0XX.002
30-minute Minimum PAR (Min_PAR_{30})	30-min	µmol s^{-1} m^{-2}	NEON.DXX.XXX.DP1.00024.001.002.0XX.002
30-minute Maximum PAR (Max_PAR_{30})	30-min	µmol s^{-1} m^{-2}	NEON.DXX.XXX.DP1.00024.001.003.0XX.002
30-minute PAR Variance (σ^2_PAR_{30})	30-min	(µmol s^{-1} $m^{-2})^2$	NEON.DXX.XXX.DP1.00024.001.004.0XX.002
30-minute PAR QA/QC Summary (Qsum_PAR_{30})	30-min	N/A	NEON.DXX.XXX.DP1.00024.001.005.0XX.002

3.2 Input Dependencies

Table 2 details the PAR related L0 DPs that are transformed into L1DPs in this ATBD.

Table 2: Details the PAR related L0 DPs that are transformed into L1DPs in this ATBD.

Data product	Sample Frequency	Units	Data stream ID
PAR Sensor Output (*I*)	1 Hz	V	NEON.DXX.XXX.DP0.00024.001.001.001.0XX.001

3.3 Product Instances

Multiple PAR sensors will be deployed at each site. PAR sensors will be located on the tower top southeast boom arm assembly and on each level of the tower profile. 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.

3.5 Spatial Resolution and Extent

The spatial resolution will depend on the placement of the PAR sensors on the tower infrastructure. Ultimately, a radiation profile will be developed for each tower site from the array of PARs on the tower (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).

4 SCIENTIFIC CONTEXT

Photosynthetically Active Radiation (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 NEON Observatory sensor output is in microvolts and is converted to µmol s^{-1} m^{-2} by application of a

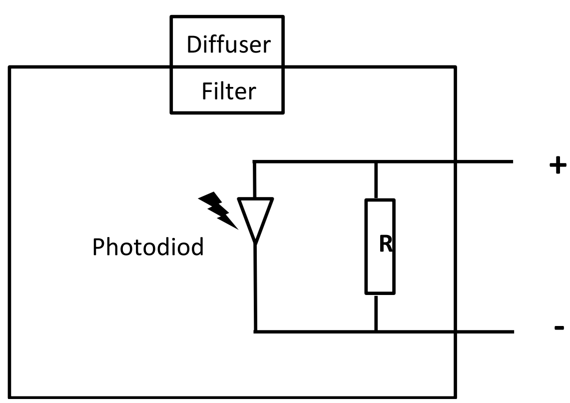

Figure 1. Schematic of typical PAR sensor construction.

calibration factor and algorithm described below.

4.2 Theory of Algorithm

The Kipp & Zonen PQS 1 PAR Quantum Sensor measures radiation between the wavelengths of 400 nm and 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 coefficients 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 (PAR_1) and thirty-minute (PAR_{30}) averages of PAR will be determined accordingly to create L1 DPs:

$$PAR_1 = \frac{1}{n}\sum_{i=1}^{n} PAR_i \tag{2}$$

where, for each minute average, *n* is the number of measurements in the averaging period T, which is defined as 0 ≤ T < 60 seconds.

Further,

$$PAR_{30} = \frac{1}{n}\sum_{i=1}^{n} PAR_i \tag{3}$$

where, for each thirty-minute average, *n* is the number of measurements in the averaging period T and averaging periods are defined as 0 ≤ T < 1800 seconds.

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 way.

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. Signal de-spiking and time series analysis 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).
5. Descriptive statistics, i.e. minimum, maximum, and variance, will be determined for both one- and thirty-minute averages.
6. QA/QC consistency tests will be applied to one- and thirty-minute averages in accordance with AD[05].
7. QA/QC Summary (Q_{sum}) will be produced for one-and thirty-minute averages according to AD[17].

QA/QC Procedure:

1. **Plausibility Tests** AD[06] – All plausibility tests will be determined for the net radiometer. 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 DP and associated quality flags (QFs) will be generated for each test.

2. **Signal De-spiking and Time Series Analysis** – Time segments and threshold values for the automated despiking QA/QC routine will be specified by FIU and maintained in the CI data store. QFs from the despiking analysis will be applied according to AD[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 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 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 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.

4. **Quality Flags (QFs) and Quality Metrics (QMs)** AD[17] – If a datum has one of the following flags it will not be used to create a L1 DP, $\underline{QF_R}$ and $\underline{QF_D}$. α and β QFs and QMs will be determined for the following flags QF_R, QF_σ, QF_δ, QF_S, QF_N, QF_G, and QF_D. All L1 DPs will have an associated final quality flag, QF_{NEON}, and quality summary, Qsum, as detailed in AD[17]. 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 measurements of PAR.

Tests	Flags
Range	QF_R
Sigma (σ)	QF_σ
Delta (δ)	QF_δ
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_{NEON}

Table 4. Information maintained in the CI data store for PAR.

Tests/Values	CI Data Store Contents
Range	Minimum and maximum values
Sigma (σ)	Time segments and threshold values
Delta (δ)	Time segment and threshold values
Step	Threshold values
Null	Test limit
Signal Despiking and Time Series Analysis	Time segments and threshold values
Calibration	CVAL sensor specific calibration coefficients
Uncertainty	AD[14]
Consistency Analysis	Test limits
Final Quality Flag	AD[17]

6 UNCERTAINTY

Uncertainty of measurement is inevitable (JCGM 2008, 2012; Taylor 1997). It is crucial that uncertainties are identified and quantified to determine statistical interpretations about mean quantity and variance structure; both are important when constructing higher level data products (e.g., L1 DP) and modeled processes. This portion of the document serves to identify, evaluate, and quantify sources of uncertainty relating to 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 PAR assembly is discussed in this section. Sources of uncertainties include those arising from the calibration procedure, PAR sensor, and measurement noise of the DAS (Figure 2).

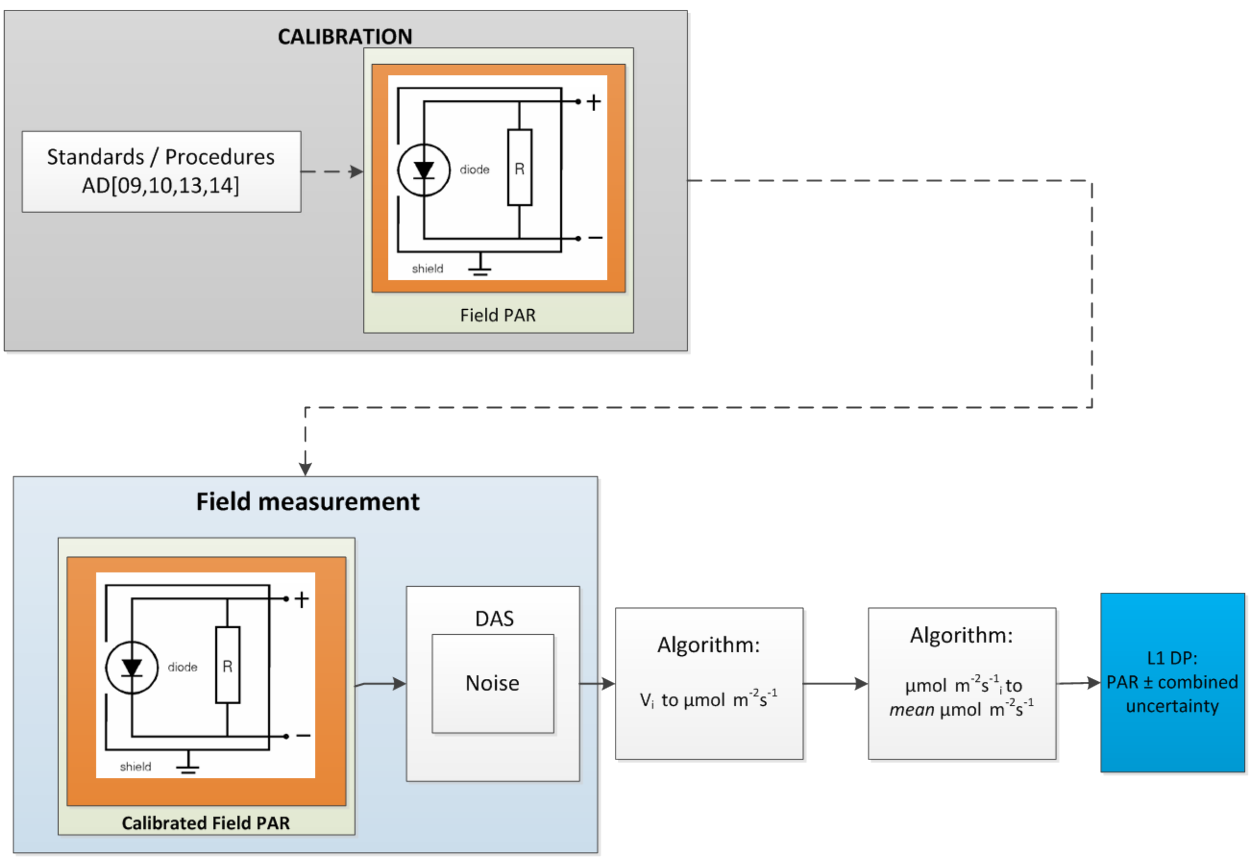

Figure 2: Displays the data flow and associated uncertainties of L1 PAR DPs. Salmon colored boxes represent direct measurement of irradiance based on the theory of PAR (Kipp and Zonen 2004). For more information regarding the methods by which the PAR sensor is calibrated, please refer to AD[09,10,13,14].

6.1.1 Calibration

Uncertainties associated with PAR sensors and their calibration processes are combined into an individual, *relative* uncertainty $u_r(P_{CVAL})$ by CVAL. It represents i) the variation of an individual sensor from the mean of a sensor population, ii) uncertainty of the calibration procedures and iii) uncertainty of coefficients used to convert resistance to calibrated PAR (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 PAR measurements (that is, it does not vary with any specific sensor, DAS component, etc.)

The standard combined uncertainty will be calculated by CI as a function of the *relative* uncertainty and value of the L1 PAR DP for the respective temporal period:

$$u_c\left(P_{CVAL_i}\right) = u_r(P_{CVAL}) * PAR_i \quad [\mu mol\, m^{-2}\, s^{-1}] \tag{4}$$

6.1.2 DAS

To quantify DAS noise, a *relative* uncertainty value, $u_r(\mathrm{V}_{DAS})$ will be provided by CVAL and stored in the CI data store. This value must be converted into a *standard* uncertainty value:

$$u\left(\mathrm{V}_{DAS_i}\right) = (u_r(\mathrm{V}_{DAS}) * I_i) + O_{DAS} \quad [V] \tag{5}$$

Where $u\left(\mathrm{V}_{DAS_i}\right)$ represents the standard uncertainty of an *individual,* raw, voltage measurement, I_i, and O_{DAS} is the offset imposed by the DAS. The offset accounts for readings of 0.00 V; its value will be provided by CVAL and maintained in the CI data store. This individual, standard uncertainty is then multiplied by the absolute value of Eq. (1)'s partial derivative:

$$\frac{\partial PAR_i}{\partial I_i} = C_1 \tag{6}$$

$$u_I(PAR_i) = |C_1| u(I_i) \quad [\mu mol\, m^{-2}\, s^{-1}] \tag{7}$$

Where, $u(I_i) \equiv u\left(\mathrm{V}_{DAS_i}\right)$

6.2 Combined Uncertainty

Deriving a combined uncertainty for our L1 mean PAR DPs can be completed in two steps. Firstly, the combined uncertainty of *individual*, valid (i.e., *those that are not flagged and omitted*) observations made during the averaging period is calculated.

$$u_c(PAR_i) = \left(u_c{}^2\left(P_{CVAL_i}\right) + u_I{}^2(PAR_i)\right)^{\frac{1}{2}} \quad [\mu mol\, m^{-2}\, s^{-1}] \tag{8}$$

The resulting value is multiplied by the partial derivative of the L1 DP. Since the DP is a temporal average, the partial derivative is simply:

$$\frac{\partial \overline{PAR}}{\partial PAR_i} = \frac{1}{n} \tag{9}$$

Where n represents the number of valid observations made during the averaging period. The absolute value of Eq. (9) is then multiplied by Eq. (8):

$$u_{PAR_i}(\overline{PAR}) = \left|\frac{1}{n}\right| u_c(PAR_i) \quad [\mu mol\, m^{-2}\, s^{-1}] \tag{10}$$

Finally, the uncertainty of the L1 mean DP is calculated by calculating the sum of squares. In this case, the resulting values of Eq. (10) are squared:

$$u_c(\overline{PAR}) = \left(\sum_{i=1}^{n} u_{PAR_i}{}^2(\overline{PAR})\right)^{\frac{1}{2}} \quad [\mu mol\, m^{-2}\, s^{-1}] \tag{11}$$

<u>Note</u>: In some applications the environmental (natural) variation of PAR may be of equal or greater interest than the measurement uncertainty (i.e., combined uncertainty derived in Eq. (11)). Because of this, the natural variation of the mean is presented:

$$u(\overline{PAR}) = \left(\frac{s^2(PAR_i)}{n}\right)^{\frac{1}{2}} \quad [\mu mol\, m^{-2}\, s^{-1}] \tag{12}$$

Where, $s^2(PAR_i)$ is the variance DP (NEON.DXX.XXX.DP1.00024.001.004.0XX.00X) and n are the number of observations used to generate the DP. It should be noted that such an equation *assumes* the data are normally distributed.

6.3 Expanded Uncertainty

The expanded uncertainty for L1 PAR DPs can be derived with the following equations:

$$V_{eff\,PAR_i} = \frac{u_c{}^4(PAR_i)}{\frac{u_c{}^4\left(P_{CVAL_i}\right)}{Veff_{P_{CVAL}}} + \frac{u_I{}^4(PAR_i)}{Veff_{V_{DAS}}}} \tag{13}$$

Where $Veff_{P_{CVAL}}$ and $Veff_{V_{DAS}}$ are functions of the number of tests conducted by CVAL during calibration – their values will be stored in the CI data store.

Second, the effective degrees of freedom must be calculated for our L1 mean PAR DP:

$$V_{eff_{\overline{PAR}}} = \frac{u_c{}^4(\overline{PAR})}{\sum_{i=1}^{n}\left(\frac{(u_c(PAR_i)/n)^4}{V_{eff_{PAR_i}}}\right)} \tag{14}$$

Finally, the expanded uncertainty is calculated:

$$U_{95}(\overline{PAR}) = k_{95} * u_c(\overline{PAR}) \quad [\mu mol\, m^{-2}\, s^{-1}] \tag{15}$$

Where k_{95} is the coverage factor obtained with the aid of:

- Table 5 from AD[12]
- $V_{eff}(\overline{PAR})$

6.4 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. Individual uncertainty values denoted in this budget are either provided here (within this document) or will be provided by other NEON teams (e.g., CVAL) and stored in the CI data store.

Table 5: Uncertainty budget for L1 PAR DPs. Shaded rows denote propagation (from lightest to darkest) of uncertainties.

Source of uncertainty	**Standard uncertainty component u(X_i)**	**Type of eval.**	**Value of standard uncertainty** $[\mu mol\, m^{-2}\, s^{-1}]$	$c_i \equiv \frac{\partial f}{\partial x_i}$	$u_i(Y) \equiv \lvert c_i \rvert u(x_i)$ $[\mu mol\, m^{-2}\, s^{-1}]$	**Degrees of Freedom**
L1 PAR DP	$u_c(\overline{PAR})$	A	Eq. (11)	N/A	N/A	Eq. (14)
1 Hz PAR	$u_c(PAR_i)$	A	Eq. (8)	Eq. (9)	Eq. (10)	Eq. (13)
Sensor/calibration	$u_c(P_{CVAL_i})$	AD[14]	Eq. (4)	1	Eq. (4)	AD[14]
Noise (DAS)	$u(I_i)$	AD[14]	Eq. (5) [V]	Eq. (6)	Eq. (7)	AD[14]
						k_{95}: $V_{eff_{\overline{PAR}}}$ & Table 5 of AD[12] $U_{95}(\overline{PAR})$: Eq. (15)

7 FUTURE PLANS AND MODIFICATIONS

This document will be amended to include radiation measurements used in the soil arrays and on the tower top.

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

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