ALGORITHM THEORETICAL BASIS DOCUMENT: PRIMARY PYRANOMETER

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TABLE OF CONTENTS

LIST OF TABLES AND FIGURES

1 DESCRIPTION

1.1 Purpose

This document details the algorithms used for creating NEON L1 DP from L0 DP for tower-based measurements of short wave (SW) radiation, and ancillary data as defined in this document (such as calibration data), obtained via instrumental measurements made by the pyranometer. It includes a detailed discussion of measurement theory and implementation, appropriate theoretical background, data product provenance, quality assurance and control methods used, approximations and/or assumptions made, and a detailed exposition of uncertainty resulting in a cumulative reported uncertainty for this product.

1.2 Scope

The theoretical background and entire algorithmic process used to derive Level 1 data from Level 0 data for the primary pyranometer are described in this document. It is expected that the primary pyranometer employed at all NEON core tower sites to measure SW radiation is the Kipp and Zonen CMP22. In addition, the Kipp and Zonen CV3 ventilation unit will accompany the CMP22 at all NEON sites. This document 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
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 QA/QC Time Series Signal Despiking for TIS Level 1 Data Products
AD[08]	NEON.DOC.000800	CMP22 – Primary Pyranometer Calibration/Validation Procedure
AD[09]	NEON.DOC.000549	C^3 Primary Pyranometer
AD[10]	NEON.DOC.000785	TIS Level 1 Data Products Uncertainty Budget Estimation Plan
AD[11]	NEON.DOC.000746	Evaluating Uncertainty (CVAL)
AD[12]	NEON.DOC.000927	NEON Calibration and Sensor Uncertainty Values
AD[13]	NEON.DOC.002002	Engineering Master Location Sensor 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

2.3 Acronyms

Acronym	Explanation
ATBD	Algorithm Theoretical Basis Document
CVAL	NEON Calibration, Validation, and Audit Laboratory
DAS	Data Acquisition System
DP	Data Product
GRAPE	Grouped Remote Analog Peripheral Equipment
L0	Level 0
L1	Level 1
LW	Longwave (i.e. Far Infra-red Radiation)
PRT	Platinum Resistance Thermometer
SW	Shortwave (i.e. Solar 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 SW radiation-related L1 DPs provided by the algorithms documented in this ATBD.

Table 1. SW radiation-related L1 DPs that are produced in this ATBD.

Data product	Averaging Period	Units	Data Product ID
1-minute Mean Incoming Shortwave Radiation (*Mean_IS*$_1$)	1-min	$W\ m^{-2}$	NEON.DXX.XXX.DP1.00022.001.001.001.001
1-minute Minimum Incoming Shortwave Radiation (*Min_IS*$_1$)	1-min	$W\ m^{-2}$	NEON.DXX.XXX.DP1.00022.001.002.001.001
1-minute Maximum Incoming Shortwave Radiation (*Max_IS*$_1$)	1-min	$W\ m^{-2}$	NEON.DXX.XXX.DP1.00022.001.003.001.001
1-minute Variance Incoming Shortwave Radiation (σ^2_*IS*$_1$)	1-min	$(W\ m^{-2})^2$	NEON.DXX.XXX.DP1.00022.001.004.001.001
1-minute QA/QC Summary Incoming Shortwave Radiation (*Qsum_IS*$_1$)	1-min	Text	NEON.DXX.XXX.DP1.00022.001.005.001.001
1-minute QA/QC Report Incoming Shortwave Radiation (*Qrpt_IS*$_1$)	1-min	Text	NEON.DXX.XXX.DP1.00022.001.006.001.001
30-minute Mean Incoming Shortwave Radiation (*Mean_IS*$_{30}$)	30-min	$W\ m^{-2}$	NEON.DXX.XXX.DP1.00022.001.001.001.002
30-minute Minimum Incoming Shortwave Radiation (*Min_IS*$_{30}$)	30-min	$W\ m^{-2}$	NEON.DXX.XXX.DP1.00022.001.002.001.002
30-minute Maximum Incoming Shortwave Radiation (*Max_IS*$_{30}$)	30-min	$W\ m^{-2}$	NEON.DXX.XXX.DP1.00022.001.003.001.002
30-minute Variance Incoming Shortwave Radiation (σ^2_*IS*$_{30}$)	30-min	$(W\ m^{-2})^2$	NEON.DXX.XXX.DP1.00022.001.004.001.002
30-minute QA/QC Summary Incoming Shortwave Radiation (*Qsum_IS*$_{30}$)	30-min	Text	NEON.DXX.XXX.DP1.00022.001.005.001.002

3.2 Input Dependencies

Table 2 details the SW radiation-related L0 DPs used to produce L1 DPs in this ATBD.

Table 2. SW radiation-related L0 DPs that are used to produce L1 DPs via this ATBD.

Data product	Sample Frequency	Units	Data Product ID
Pyranometer (*P*)	1 Hz	*V*	NEON.DXX.XXX.DP0.00022.001.001.001.001.001
Sensor Body Temperature	1 Hz	*Ω*	NEON.DXX.XXX.DP0.00022.001.002.001.001.001
Fan Tachometer Speed	1 Hz	*rpm*	NEON.DXX.XXX.DP0.00022.001.003.001.001.001
Heater Flag (QF_H)	State Change	*NA*	NEON.DXX.XXX.DP0.00022.001.004.001.001.001
Heater Flag (QF_H)	State Change	*NA*	NEON.DXX.XXX.DP0.00022.001.005.001.001.001

3.3 Product Instances

One primary pyranometer will be deployed at core tower sites only, see AD[13] for specific details.

3.4 Temporal Resolution and Extent

One- and thirty-minute averages of incoming SW radiation will be calculated to form L1 DPs.

3.5 Spatial Resolution and Extent

The primary pyranometer will be located at the top level at all core tower sites. Thus, observations reflect the point in space where pyranometer is affixed to the tower infrastructure, see AD[13] for specific details.

4 SCIENTIFIC CONTEXT

The sun's energy is emitted to the earth mainly in the form of incoming short wave (SW) radiation, with a small portion it falling LW radiation wavelengths. Pyranometers serve to quantify SW radiation and in turn provide a foundation for investigations of the Earth's climate. Incoming SW radiation, which is composed primarily of ultraviolet, visible, and a portion of infra-red wavelengths, is the primary driver for the Earth's climate. As such, the observations of incoming shortwave radiation are of great interest to the scientific and broader community in assessing the Earth's energy budget.

4.1 Theory of Measurement

The Kipp and Zonen CMP22 pyranometer is a passive sensor that uses a thermopile to detect incoming SW radiation flux (λ 200 to 3600 nm). The Kipp and Zonen CV3 ventilation unit will also be installed on each pyranometer, and includes both a fan and two five watt heaters. The ventilation unit will help to prevent temperature differentials and the buildup of precipitation (i.e. dew, frost, ice, etc.). The fan will always be operational, while the heaters will be activated based on the sensor body temperature according to AD[09].

The thermopile's surface is coated with a non-spectrally selective black paint that absorbs SW radiation. The sensing element for the thermopile is composed of numerous thermocouple junction pairs that are connected electrically in series. As the sensor absorbs SW radiation, active or 'hot' thermocouple junctions increase in temperature. The temperature differential between an active junction and a reference or 'cold' junction (i.e. kept at a fixed temperature) produces an electromotive force. This electromotive force is directly proportional to the temperature differential; known as a thermoelectric effect. Thus, the temperature difference across the thermal resistance of the detector (i.e. thermopile) is converted into a voltage that is a linear function of the absorbed solar irradiance. Since the physical properties of each thermopile and sensor will vary slightly, so will the sensitivity of each pyranometer. Therefore, for each pyranometer, even for the same model, it is necessary to determine unique sensor specific sensitivity calibration factors. Details on how these sensitivity calibration factors were determined can be found in AD[08].

4.2 Theory of Algorithm

4.2.1 Kipp and Zonen CMP22 Pyranometer and CV3 ventilation unit

An internal PRT 100 in the CMP22 will be used to control of the heater in the CV3 ventilation unit as described in AD[09]. The PRT signal must be converted from resistance to degrees Celsius prior to being used for heater control. The PRT signal will be converted to degrees Celsius according to Kipp and Zonen's specifications (Kipp and Zonen, 2010):

$$T = \frac{-\alpha\sqrt{\alpha^2 - 4\beta * \left(\frac{-R}{100} + 1\right)}}{2\beta} \tag{1}$$

Where:

T	= PRT 100 temperature (°C)
α	= $3.9083*10^{-3}$
β	= $-5.8019*10^{-7}$
R	= PRT 100 resistance (Ω)

4.2.2 Short-wave Radiation Measurement

The thermopile output from the pyranometer is converted into from V to W m^{-2} as a function of sensor specific sensitivities; these will determined by CVAL according to AD[08]. Using the sensor specific sensitivity and the output from the thermopile, incoming SW radiation is determined:

$$S_{I_i} = P_i * C_1 \tag{2}$$

Where:

S_{I_i} = Individual (1 Hz) incoming Short Wave Radiation (W m^{-2})
P_i = Individual pyranometer output (V)
C_1 = Pyranometer sensor specific sensitivity (W m^{-2} V^{-1}) Provided by CVAL

After incoming SW radiation is determined and the QA/QC procedures explained in Section 5 have been implemented, one-minute ($S_{I\text{-}1min}$) and thirty-minute ($S_{I\text{-}30min}$) averages will be determined to create L1 DPs:

$$\overline{S}_{I_1} = \frac{1}{n}\sum_{i=x}^{n} S_{I_i} \tag{3}$$

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

Similarly;

$$\overline{S}_{I_{30}} = \frac{1}{n}\sum_{i=x}^{n} S_{I_i} \tag{4}$$

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 order.

1. SW radiation will be determined from the L0 DPs through Eq. (2).
2. QA/QC Plausibility tests will be applied to the data stream in accordance with AD[06], details are provided below.
3. Signal despiking and time series analysis will be applied to the data stream in accordance with AD[07].
4. One- and thirty-minute incoming shortwave radiation averages will be calculated using Eq. (3) and (4) and descriptive statistics, i.e. minimum, maximum, and variance, will be determined for both averaging periods.
5. QA/QC consistency tests will be applied to one- and thirty-minute averages in accordance with AD[05].
6. QA/QC summaries (e.g. $Qsum\_IS_1$ and $Qsum\_IS_{30}$) will be created (flags are defined below).

QA/QC Procedure:

1. **Plausibility Tests** AD[08] - All plausibility tests will be determined for the primary pyranometer. 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. **Sensor Test** – The two five watt heaters in the CV3 venation unit are operated according to the C^3 document, AD[09]. When the heaters are operational, flags will be set and applied to the L0 DPs. Due to the nature of SW radiation, the heaters will only induce minimal variability in measurements, which will be discussed in Section 6.1.3. Flags from the heaters will be used to determine uncertainty estimates and to provide ancillary information that may be useful for troubleshooting. Thus, heater flags will be combined with the other quality flags to form the L1 QA/QC summary.

3. **Signal Despiking and Time Series Analysis** – 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].

4. **Consistency Analysis** – Currently, there is no plan to run consistency analysis on the L1 DP for the pyranometer. However, time series consistency analysis may be explored in the future.

   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, $\underline{QF_R}$ 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[14]. Flags that may be associated with SW radiation measurements, as well as information maintained in the CI data store can be found below in Tables 3 and 4.

Table 3. Flags associated with SW radiation measurements.

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
Sensor Test (Heater Flag)	QF_H
Final quality flag	QF_{NEON}

Table 4. Information maintained in the CI data store for the primary pyranometer.

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	AD[08]
Uncertainty	AD[12]
Sensor Test	AD[09]
Final Quality Flag	AD[14]

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 L1 mean DPs. It is a reflection of the information described in AD[10], and is explicitly described for the primary pyranometer assembly in the following sections.

6.1 Uncertainty of Insolation Measurements

Uncertainty of the primary pyranometer assembly is discussed in this section. Sources of uncertainties include those arising from the sensor, calibration procedure, ventilation unit (two heaters and a fan), and noise introduced by the DAS (Figure 1).

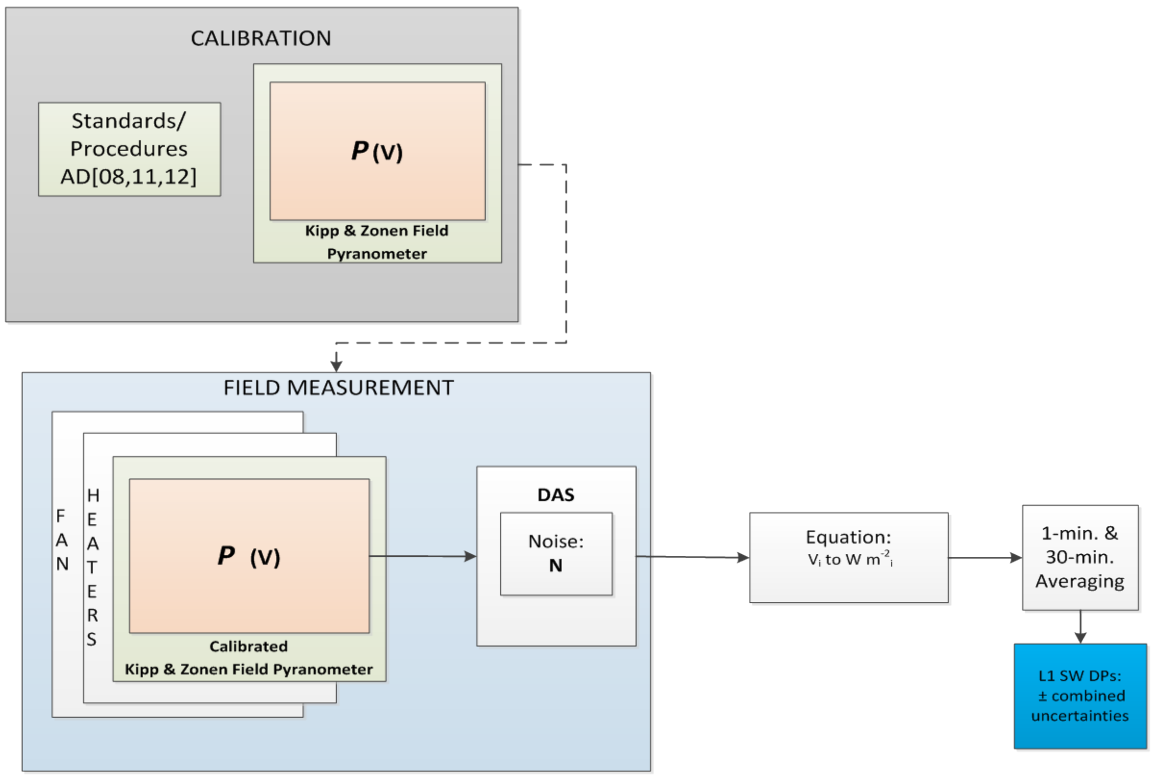

Figure 1: Displays the data flow and associated uncertainties of L1 incoming SW radiation DPs. Salmon colored boxes represent direct measurement of incoming SW radiation based on the theory of passive radiation sensor resistance. For a detailed explanation of pyranometer calibration procedures, please refer to AD[08,11,12].

6.1.1 Calibration

Uncertainties associated with pyranometers and their calibration processes are combined into a standard uncertainty $u_c(S_{I_{CVAL}})$ by CVAL. This combined uncertainty 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 raw signals to calibrated radiation. It is a constant value that will be provided by CVAL (AD[12]), stored in the CI data store, and applied to all radiation measurements (that is, it does not vary with any specific sensor, DAS component, etc.).

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:

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

Where $u\left(\mathrm{V}_{DAS_i}\right)$ represents the standard uncertainty of an *individual,* raw, voltage measurement, V_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 (AD[12]) and maintained in the CI data store. This individual, standard uncertainty is then multiplied by the absolute value of Eq. (2)'s partial derivative with respect to I_i:

$$\frac{\partial S_{I_i}}{\partial P_i} = C_1 \tag{6}$$

$$u_P\left(S_{I_i}\right) = \left|\frac{\partial S_{I_i}}{\partial P_i}\right| u(P_i) \quad [W\ m^{-2}\ ] \tag{7}$$

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

6.1.3 Ventilation Unit

Pyranometer performance can be improved by using a well-designed ventilation unit (i.e., a fan and two heaters), as it helps prevent temperature differentials and buildup of moisture (Kipp and Zonen 1999). Although use of the Kipp and Zonen ventilation unit improves measurement accuracy, it affects the variability of the measurement, thus adding uncertainty to the measurement. At this time we cannot quantify the extent of this variability and thus, we cannot quantify related uncertainties. However, with sufficient operational experience, such uncertainties may be better estimated.

6.2 Combined Uncertainty

Deriving a combined uncertainty for our L1 mean incoming shortwave 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.

$$u_c\left(S_{I_i}\right) = \left(u_c{}^2\left(P_{I\,CVAL}\right) + u_P{}^2\left(S_{I_i}\right)\right)^{\frac{1}{2}} \quad [W\ m^{-2}] \tag{8}$$

The resulting value is multiplied by the partial derivative of the L1 DP. Since the DP is a temporal average, the partial derivative with respect to an individual measurement is simply:

$$\frac{\partial \overline{S_I}}{\partial S_{I_i}} = \frac{1}{n} \tag{9}$$

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):

$$u_{S_{I_i}}(\overline{S_I}) = \left|\frac{\partial \overline{S_I}}{\partial S_{I_i}}\right| u_c(S_{I_i}) \quad [W\ m^{-2}] \tag{10}$$

Finally, the combined uncertainty of the L1 mean DP is calculated via quadrature:

$$u_c(S_I) = \left(\sum_{i=1}^{n} u_{S_{I_i}}{}^2(\overline{S_I})\right)^{\frac{1}{2}} \quad [W\ m^{-2}] \tag{11}$$

6.3 Expanded Uncertainty

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

$$V_{eff\,S_{I_i}} = \frac{u_c{}^4(S_{I_i})}{\frac{u_c{}^4(S_{I_{CVAL}})}{Veff_{S_{I_{CVAL}}}} + \frac{u_P{}^4(S_{I_i})}{Veff_{V_{DAS}}}} \tag{12}$$

Where $Veff_{S_{I_{CVAL}}}$ 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 DP:

$$V_{eff_{\overline{S_I}}} = \frac{u_c{}^4(\overline{S_I})}{\sum_{i=1}^{n}\left(\frac{(u_c(S_{I_i})/n)^4}{V_{eff\,S_{I_i}}}\right)} \tag{13}$$

Finally, the expanded uncertainty is calculated:

$$U_{95}(\overline{S_I}) = k_{95} * u_c(\overline{S_I}) \quad [W\ m^{-2}] \tag{14}$$

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

- Table 5 from AD[10]
- $V_{eff_{\overline{S_I}}}$

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 incoming SW radiation DPs. Shaded rows denote the order of uncertainty propagation (from lightest to darkest).

Source of uncertainty	**Standard uncertainty component $u(x_i)$**	**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 Inc. SW DP	$u_c(\overline{S_I})$	Eq. (11)	--	--	Eq. (13)
1 Hz Inc. SW	$u_c(S_{I_i})$	Eq. (8)	Eq. (9)	Eq. (10)	Eq. (12)
Sensor/calibration	$u_c(S_{I_{CVAL_i}})$	AD[12]	1	AD[12]	AD[12]
Noise (DAS)	$u(P_i)$	Eq. (5) [V]	Eq. (6)	Eq. (7)	AD[12]
					k_{95}: $V_{eff_{\overline{S_I}}}$ & Table 5 of AD[10]
					$U_{95}(\overline{S_I})$: Eq. (14)

7 FUTURE PLANS AND MODIFICATIONS

Future system flags may be incorporated into the data stream and included in the QA/QC summary DP (*$Qsum_{1min}$* and *$Qsum_{30min}$*) that summarizes any flagged data that went into the computation of the L1 DP.

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