NEON ALGORITHM THEORETICAL BASIS DOCUMENT (ATBD):

SURFACE WATER NITRATE

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Change Record

REVISION	DATE	ECO #	DESCRIPTION OF CHANGE
A	09/12/2017	ECO-04874	Initial Release
B	01/03/2019	ECO-05951	Revised averaging window per configuration change
C	10/10/2019	ECO-06279	Revised burst timestamp handling, data regularization, null, and gap flagging to better align with other IS data products.
D	03/16/2022	ECO-06785	Update to reflect change in terminology from relocatable to gradient sites.
E	06/08/2026	ECO-07213	Updated to reflect major changes to data processing pipeline and publication table format.

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LIST OF TABLES AND FIGURES

1 DESCRIPTION

Contained in this document are details concerning the Nitrate in surface water data product (DP1.20033.001). Specifically, the processes used to convert "raw" sensor data into meaningful scientific measurements, and calculate their associated uncertainties are described.

1.1 Purpose

This document details the algorithms used for creating Level 1 Nitrate in surface water data product from Level 0 data. It includes appropriate theoretical background, a detailed discussion of the steps used in data processing including quality assurance and control methods used, and a detailed discussion of how uncertainty estimates for this product are calculated.

1.2 Scope

The theoretical background and entire algorithmic process used by NEON to derive Level 1 data from Level 0 data for Nitrate in surface water is described in this document. While providing background information on the theory of measurement, this document does not provide specific details on the sensor manufacturer's internal algorithms used to estimate nitrate concentrations (as these are proprietary).

2 RELATED DOCUMENTS, ACRONYMS AND VARIABLE NOMENCLATURE

2.1 Applicable Documents

AD[01]	NEON.DOC.000001	NEON OBSERVATORY DESIGN
AD[02]	NEON.DOC.002652	NEON Level 1, Level 2 and Level 3 Data Products Catalog
AD[03]	NEON.DOC.000782	ATBD QA/QC Data Consistency
AD[04]	NEON.DOC.011081	ATBD QA/QC Plausibility Tests
AD[05]	NEON.DOC.000783	ATBD De-spiking and Time Series Analyses
AD[06]	NEON.DOC.000746	Calibration Fixture and Sensor Uncertainty Analysis (CVAL)
AD[07]	NEON.DOC.000785	TIS Level 1 Data Products Uncertainty Budget Estimation Plan
AD[08]	NEON.DOC.000927	NEON Calibration and Sensor Uncertainty Values[1]
AD[09]	NEON.DOC.001113	Quality Flags and Quality Metrics for TIS Data Products
AD[10]	NEON.DOC.001570	NEON Sensor Command, Control and Configuration Document: SUNA Nitrate Analyzer, Wadeable Streams
AD[11]	NEON.DOC.000597	STCDD – 0329950000 – Sensor, Suna Nutrient with Integrated Wiper
AD[12]	NEON.DOC.003808	NEON Sensor Command, Control and Configuration Document: Buoy Meteorological Station and Submerged Sensor Assembly
AD[13]	NEON.DOC.003824	STCDD – 0329950100 – Sensor, Buoy, SUNA Nitrate with Integrated Wiper, Titanium Housing

[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.

2.2 Reference Documents

RD[01]	NEON.DOC.000008	NEON Acronym List
RD[02]	NEON.DOC.000243	NEON Glossary of Terms

2.3 Acronyms

Acronym	Explanation
AIS	Aquatic Instrument System
ATBD	Algorithm Theoretical Basis Document
CI	NEON Cyberinfrastructure
CVAL	NEON Calibration, Validation, and Audit Laboratory
DAS	Data Acquisition System
DP	Data Product
FDAS	Field Data Acquisition System
GRAPE	Grouped Remote Analog Peripheral Equipment
Hz	Hertz

L0	Level 0
L1	Level 1
PRT	Platinum resistance thermometer
QA/QC	Quality assurance and quality control

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
u_{A1}	U_CVALA1	Combined, standard uncertainty of the SUNA nitrate sensor (µM)
u_{A3}	U_CVALA3	Combined, relative uncertainty of the SUNA nitrate sensor (%)
H_i	Parse from L0 string (field 271)	Internal humidity of sensor (%)
$SpAv_L$	Parse from L0 string (field 8)	Spectrum average during light frame
$SpAv_D$	Parse from L0 string (field 9)	Spectrum average during dark frame
NO_3	Parse from L0 string (field 3)	Nitrate Value in micromoles per liter (mM)
T_l	Parse from L0 string (field 269)	Lamp temperature (°C)

3 DATA PRODUCT DESCRIPTION

3.1 Variables Reported

The Surface Water Nitrate-related L1 DPs provided by the algorithms documented in this ATBD are displayed in the accompanying file: swn_datapub_NEONDOC004046.txt.

3.2 Input Dependencies

Table 1 details the Surface Water Nitrate-related L0 DPs used to produce L1 Surface Water Nitrate DPs in this ATBD.

Table 1. List of Surface Water Nitrate-related L0 DPs that are transformed into L1 Surface Water Nitrate DPs in this ATBD.

Description	Sample Frequency	Units	Data Product Number
Nitrate in surface water	burst of 1 dark frame and 20 light frames	NA	NEON.DOM.SITE.DP0.20033.001.02242.HOR.VER.000

3.3 Product Instances

At wadeable stream sites a Submersible Ultraviolet Nitrate Analyzer (SUNA) will be installed in the stream channel at the S2 location and will be mounted onto the in-stream infrastructure that is shared with other submerged aquatic sensors (multisonde, prt and LevelTroll). At lake and river sites, the SUNA will be deployed off the side of the buoy approximately 0.5 m below the surface.

3.4 Temporal Resolution and Extent

L0 data will be collected in burst measurements every 15 minutes, where each burst consists of 1 dark frame and 20 light frames. A portion of the sampling window is averaged and treated as a single instantaneous point measurement every 15 minutes to form L1 DPs.

3.5 Spatial Resolution and Extent

One SUNA will be deployed at a single fixed location at each AQU site.

4 SCIENTIFIC CONTEXT

Nitrate is a bioavailable form of nitrogen. Nitrogen can be a limiting nutrient for primary production in aquatic environments. Runoff of excess nitrogen can lead to eutrophication. Measuring nitrate in aquatic systems is critical to understanding the biogeochemical cycle and mechanisms in the ecosystem. Changes in the concentration of nitrate over time may be an indication of shifts in the trophic structure and community composition of the aquatic ecosystem.

4.1 Theory of Measurement

Nitrate absorbs ultraviolet (UV) light, with peak absorbance occurring over wavelength around 210 nm. The concentration can be estimated from the absorbance using the Beer-Lambert Law. This can be difficult in natural environments, because other common dissolved species also absorb UV light (see **Figure 1**). The most important of these is dissolved organic carbon (DOC). This overlapping absorbance must be accounted for to accurately estimate nitrate.

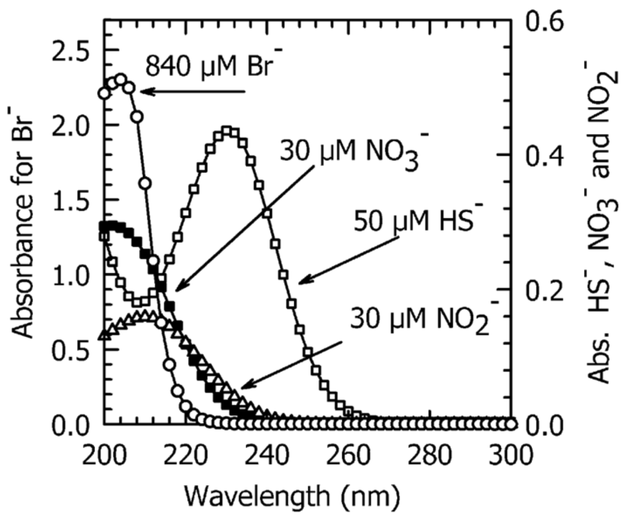

Figure 1. Absorbance spectra for bromide, nitrate, hydrogen sulfide and nitrite in the ultraviolet range.

The Submersible Ultraviolet Nitrate Analyzer (SUNA) is a UV spectrophotometer manufactured by SeaBird Coastal. The SUNA measures absorbance at 256 discrete wavelengths from 190-370 nm. The SUNA compares the absorbance in the sample to the absorbance in a deionized water reference sample to calculate the additional absorbance due to the UV absorbing species in the sample. The SUNA uses the absorbance over longer wavelengths to correct for the effects of overlapping absorbance by other species such as DOC in the nitrate absorption range (216.5–240 nm). For each sample, the SUNA internally converts absorbance measurements across multiple wavelengths into a single nitrate estimate.

4.2 Theory of Algorithm

The SUNA nitrate sensor produces an ASCII file that contains 286 data fields (**Table 2**). To accommodate this large number of fields, the streamed data are concatenated such that each measurement is reported as a single string of characters, where the data stream field positions and associated data fields are seperated by colons.

Table 2. Positions of data fields that are captured with the SUNA and placed into the concatenated string, L0 data stream, identified in **Table 1** above.

L0 Data Stream Field Position	Full ASCII Data Fields
0	Light/Dark Frame
1	Date field (numeric)
2	Time field (numeric)
3	Nitrate concentration in micromolar
4	Nitrogen as nitrate in mg/L
5	Absorbance at 254 nm
6	Absorbance at 350 nm
7	Bromide trace
8	Spec Average or SW Average(Dark Correction Method)
9	Dark Signal Average (average dark intensity)
10	Integration Time Factor
11-266	Spectrometer intensity at wavelengths 1-256
267	Temperature of sensor in ºC
268	Spectrometer temperature in ºC
269	Lamp temperature in ºC
270	Cumulative lamp time in seconds
271	Relative humidity in %
272	Main voltage in Volts
273	Lamp voltage in Volts
274	Internal voltage in Volts
275	Main current in milliAmps
276	Fit aux 1
277	Fit aux 2
278	Fit base 1
279	Fit base 2
280	Fit RMSE
281	CTD Time
282	CTD Salinity
283	CTD Temperature
284	CTD Pressure
285	Check sum of data stream

Under normal operations, the SUNA is configured in periodic mode to take a burst of measurements every 15-minutes. The first measurement of each burst is a dark measurement in which the SUNA lamp is turned off. The purpose of the dark measurement is to account for any stray ambient light reaching the detector of the spectrophotometer. Dark measurements are indicated by a value of 0 in data field 0. A dark measurement will be used to find the beginning of each burst since all bursts should start with one dark frame and should be followed by multiple light measurements.

Following the dark measurement is a sequence of 20 light measurements, where the SUNA lamp is turned on. Light measurements are indicated by a value of 1 in data field 0. The first nine light measurements after the lamp turns on are intentionally omitted. Nine was the number of measurements required for the SUNA lamp output to stabilize as determined by the NEON CVAL lab. Thus, under normal operations, 11 light measurements (numbers 10-20 in the burst) will be used to calculate the L1 Data Product statistics (mean, max, min, variance and expanded uncertainty). For example, the formula used to calculate ***surfWaterNitrateMean*** is shown Equation 1.

$$\overline{NO_3} = \frac{1}{n-9} \sum_{i=10}^{i=n} NO_{3,i} \qquad \text{Equation 1}$$

Where:

$i =$ light measurement position within the burst.

$n =$ total number of unflagged light measurements within the burst.

$NO_{3,i}$ = individual nitrate measurements in µM.

$\overline{NO_3}$ = average nitrate per 15-minute burst in µM.

There may be situations where the number of light measurements used in calculating the statistics is less than 11. Measurements which receive a QA/QC plausibility or sensor-specific quality flag are not used in the average. These tests are described in detail in Algorithm Implementation section. Similarly, there may be situations where the number of light measurements used in calculating the statistics is more than 11. Prior to 2019, the SUNA was configured to collect 50 light measurements per burst rather than 20. At buoy sites there were periods with poor radio connection when the SUNA was configured to collect 25 light measurements to allow for potentially "dropped" measurements. While the first 9 light measurements of each burst are dropped, any additional unflagged measurements beyond the expected 20 are also included in the statistics. The number of measurements used in calculating the L1 statistics is indicated in the ***surfWaterNitrateNumPts*** field in the L1 data table.

5 ALGORITHM IMPLEMENTATION

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

1. For data that were streamed in real-time to NEON HQ, extract L0 values from the appropriate fields of the concatenated data string for each measurement.
2. Ingest CSV files of logged data that are downloaded from the SUNA at quarterly intervals.
3. Streamed and logged data are merged. When both are present, logged data are prioritized over streamed data because they are less likely to be incomplete or corrupt due to data transmission issues. When logged data are used, the ***nitrateLogData*** quality flag is set to 1. If logged data are missing, the streamed data are used (if available) and the ***nitrateLogData*** quality flag is set to 0. This convention is a bit different than other NEON data products where the preference is to use streamed data over logged data. For the Nitrate in surface water data product, a logged data flag of 1 indicates the preferred data source (logged data) was available and used. This quality flag is informational, and does not cause a measurement to be excluded from use in the subsequent stats calculation.
4. If there is not a valid calibration record on file, the ***nitrateValidCal*** quality flag is set to 1. If there is a valid calibration of file, but the values are outside the expected range, the ***nitrateSuspectCal*** quality flag is set to 1. These quality flags are informational, and do not cause a measurement to be excluded from use in the subsequent stats calculation.
5. QA/QC Plausibility tests will be performed on the nitrate concentration (data field 3) according to AD[04]. Values which fail a QA/QC Plausibility test will have the quality flag for the respective test set to 1. Additional details are provided below. Measurements which fail a QA/QC Plausibility test are not included in the subsequent stats calculation.
6. Sensor-specific QA/QC test will be performed on the respective data stream values. Values which fail a Sensor-specific QA/QC test will have the quality flag for the respective test set to 1. Additional details are provided below. Measurements which fail a Sensor-specific QA/QC test are not included in the subsequent stats calculation.
7. The dark measurements and first 9 light measurements of each burst are identified and removed.
8. Descriptive statistics including mean, min, max, and variance are calculated for the nitrate concentration within each 15-minute burst. Only measurements which did not receive a QAQC Plausibility or Sensor-specific QAQC quality flag are used in the stats calculation. The number of unflagged measurements used to calculate the stats is also reported.
9. The expanded uncertainty for each 15-minute burst are calculated. Additional details are provided below.
10. Quality metrics, which aggregate individual quality flags, are calculated for each 15-minute burst according to AD[09].
11. The ***insufficientDataQF*** is set to 1 for any 15-minute burst where less than the required number of unflagged measurements where available to calculate the stats and the expanded uncertainty. For this data product, 5 was chosen as the minimum required number of measurements based on convergence of the expanded uncertainty on a stable value.
12. The ***nitrateConfigQF*** is set to 1 for any 15-minute burst where the SUNA was incorrectly configured in continuous mode. The main reason for the SUNA to be in continuous mode is for

field calibration. Sometimes, the SUNA may accidentally be redeployed in continuous mode, and this data may sometimes still be usable. Therefore, it is advised that users evaluate data with the ***nitrateConfigQF*** on a case by case basis.

13. Prior to each annual release, the data are manually reviewed, and the ***ScRvwQF*** is set to 1 for any 15-minute burst determined to be erroneous or suspect.
14. For any 15-minute burst, the ***finalQF*** is set to 1 if the ***insufficientDataQF***, ***nitrateConfigQF*** or ***SciRvwQF*** are set to 1.

6 QA/QC PROCEEDURES

6.1 QA/QC Plausibility Testing:

The following QA/QC plausibility tests will be determined for the nitrate in surface water data product: range, step, persistence and spike. See AD[04] for more detailed information on QAQC Plausibility tests. For the nitrate in surface water data product, QA/QC Plausibility tests will only be run within bursts, and not across 15-minute bursts. For example, if the difference between the last measurement of one burst and the first measurement of the subsequent burst is greater than the step test threshold, the step quality flag will not be triggered because in truth, these are not actually "sequential" measurements.

6.2 Sensor-specific QA/QC Testing:

Several QA/QC tests specific to the SUNA will be performed. The first is for the internal relative humidity of the SUNA (data field 271). High internal humidity can affect sensor performance and potentially damage the sensor. The ***internalHumidityQF*** is set to 1 if the internal humidity is greater than 35°C.

$$\text{internalHumidityQF=} \left| \begin{array}{l} 1 \text{ if } T_l \geq 35°\text{C} \\ \\ 0 \text{ otherwise} \end{array} \right. \qquad \text{Equation 2}$$

The second sensor-specific QA/QC test is for the SUNA lamp temperature (data field 269). High internal humidity can affect sensor performance, and will also cause the SUNA lamp to shut off and only collect dark measurments to prevent damage to the sensor. The ***lampTemperatureQF*** is set to 1 if the internal humidity is greater than 40%.

$$\text{lampTemperatureQF=} \left| \begin{array}{l} 1 \text{ if } H_i \geq 40\% \\ \\ \end{array} \right. \qquad \text{Equation 3}$$

0 otherwise

The third sensor-specific QA/QC test is the ratio of the light measurement intensity averaged across all 256 wavelength channels of the 190-370 nm UV spectrum (data field 8) to the dark measurement intensity averaged across all wavelength channels of the spectrum (data field 9). A low spectral ratio indicates that the SUNA lamp is not putting out enough light to accurately measure the fraction being absorbed, or the SUNA's optical window is being obstructed. If the average intensity of the light measurement is not greater than at least twice the intensity of the dark measurement for the respective burst, the ***lightdarkSpectralRatioQF*** is set to 1. The SUNA also internally checks that the absorbance over the 35 wavelength channels in the nitrate absorbance range of 217-240nm is less than 1.3 and omits these from the internal data processing. If less than 10 channels within this range have an absorbance less than 1.3 the SUNA does not predict a concentration and instead reports a "-1" error code. If nitrate in µM (data field 3) and nitrate in mg/L (data field 4) are both exactly -1.00 it indicates an error code. These measurements should also fail the standard spectral ratio test described above, but as a precaution the ***lightDarkSpectralRatioQF*** is manually set to 1.

$$\text{lightDarkSpectralRatioQF=}\left|\begin{array}{l} 1 \text{ if } SpAv_L \leq 2 \times SpAv_D \\ 1 \text{ if } NO_{3(\mu M)} = NO_{3(mg/L)} = "-1" \\ 0 \text{ otherwise} \end{array}\right. \qquad \text{Equation 4}$$

Measurements which have received a QA/QC Plausibility or Sensor-specific QA/QC quality flag are not used for calculating statistics or uncertainty for the 15-minute bursts. Measurements which have received a ***nitrateLogData***, ***nitrateValidCal*** or ***nitrateSuspectCal*** are still included as these flags are informational only.

7 UNCERTAINTY

Uncertainty of the SUNA nitrate analyzer assembly is discussed in this section. The section is broken down into two topics. The first discusses the sources of *measurement* uncertainty, i.e., those associated with *individual nitrate measurements*. The second discusses uncertainties associated with temporally averaged data products. A more detailed discussion of uncertainty associated with NEON data products is provided in detail in AD[07] and AD[08].

7.1 Uncertainty of Individual Measurements

The following subsections present the measurement uncertainties associated with *individual* measurements. These uncertainties should not be confused with the uncertainties associated with the *mean* of a group of measurements presented in the subsequent section. We urge the reader to refer to AD[07] for further details concerning the differences between the different types of uncertainty.

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:

$$\boldsymbol{u_c(y)} = \left(\sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i}\right)^2 \boldsymbol{u^2(x_i)}\right)^{\frac{1}{2}} \qquad \text{Equation 5}$$

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. For surface water nitrate measurements, the sources of uncertainty are discussed below.

7.1.1 Digital to Analog Conversion

The SUNA V2 nitrate sensor has an internal Analog to Digital (A/D) converter and outputs data in digital form. Therefore, no data conversions occur within the DAS, and uncertainty introduced by the DAS can be considered negligible.

7.1.2 Calibration Uncertainty

The SUNA reference (blank) is calibrated in the field using deionized water as a single-point calibration. According to the manufacturer (SeaBird 2018), if the sensor is properly field-calibrated, the nitrate concentration should have an accuracy as follows:

$$\text{Measurement Accuracy} = \begin{cases} 2\ \mu M \quad \text{if} \quad \overline{NO_3} \leq 20\ \mu M \\ \overline{NO_3} \times 10\% \quad \text{if} \quad 20\ \mu M < NO_{3,i} \leq 1000\ \mu M \end{cases} \qquad \text{Equation 6}$$

The values 0-1000 µM represent the expected environmental range across the NEON Aquatic Sites. The uncertainty is assumed to be the manufactures reported accuracy divided by 3. Therefore, the uncertainty will be 0.666 µM (u_{A1}) or 3.33% (u_{A3}) of the measurement, depending on the concentration of the individual measurements. These values will be given by CVAL as $\{u_{A1}\}$ and $\{u_{A3}\}$ (see Section 2.4) representing i) the repeatability and reproducibility of the sensor and ii) uncertainty of the calibration procedures and coefficients including uncertainty in the standard (truth). This will be provided by CVAL, stored in the CI data store, and applied to all *individual nitrate measurements.* CI will need to use the appropriate uncertainty value for individual measurements based on the concentration as follows:

$$\text{Individual measurement uncertainty } \{u_{An}\} = \begin{cases} u_{A1} \text{ if } \overline{NO_3} \leq 20\ \mu M \\ u_{A3}, \text{ if } 20\ \mu M < \overline{NO_3} \leq 1000\ \mu M \end{cases} \qquad \text{Equation 7}$$

7.1.3 Combined Uncertainty

Because the only known quantifiable uncertainties are those provided by the manufacturer, the combined uncertainty of nitrate is simply a product to the standard uncertainty value given by the manufacturer and provided by CVAL, u_{A1}, (See Sections 2.4 and 7.1.2).

$$\boldsymbol{u_{CAL}}(\overline{NO_3}) = \begin{cases} u_{An} \text{ if } \overline{NO_3} \leq 20\ \mu M \\ u_{An} \times \overline{NO_3} \text{ if } 20\ \mu M < \overline{NO_3} \leq 1000\ \mu M \end{cases} \qquad \text{Equation 8}$$

Where,

$u_{CAL}(\overline{NO_3})$ = standard calibration uncertainty of an individual measurement (µM)

u_{An} = u_{A1} or u_{A3}, depending on concentration range as identified in 7.1.2, calibration uncertainty provided by CVAL (%, from manufacturer)

$\overline{NO_3}$ = averaged nitrate measurements (µM)

7.2 Uncertainty of temporally averaged L1 DPs

The following subsections discuss uncertainties associated with temporally averaged Level 1 data products. As stated previously, it is important to note the differences between the individual measurement uncertainties presented in the previous section 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.

7.2.1 Repeatability (Natural Variation)

To quantify the uncertainty attributable to random effects, the distribution of the individual measurements is used. Specifically, the *estimated standard error of the mean (natural variation)* is computed. This value reflects the repeatability of measurements for a specified time period:

$$\boldsymbol{u_{NAT}(\overline{NO_3}) = \sqrt{\frac{\sigma^2}{n}}} \qquad \text{Equation 9}$$

Where

$\overline{NO_3}$ = averaged nitrate measurements (µM)

$u_{NAT}(\overline{NO_3})$ = standard error of the mean (natural variation)

σ = standard deviation of individual within the averaging window (of the burst)

n = number of observations made within the averaging window (of the burst)

7.2.2 Calibration

The calibration uncertainty for a L1 mean DP is similar to that described in Section 7.1.2. However, the uncertainties provided by CVAL (see Section 2.4) do not account for i) individual sensor repeatability, or ii) the variation of sensors' responses over a population (reproducibility). These components estimate the uncertainties due to the accuracy of the instrumentation in the form of *Truth* and *Trueness*, a quantity that is not captured by the standard error of the mean. This is a constant value that will be provided by CVAL and stored in the CI data store. Please refer to AD[07] for further justification regarding evaluation and quantification of this combined uncertainty.

7.2.3 Combined Uncertainty

The combined uncertainty for L1 data products are computed by summing the uncertainties from repeatability/natural variation and the CVAL provided uncertainties in quadrature:

$$\boldsymbol{u_c(\overline{NO_3}) = \left[u_{NAT}^2(\overline{NO_3}) + u_{CAL}^2(\overline{NO_3})\right]^{\frac{1}{2}}} \qquad \text{Equation 10}$$

7.2.4 Communicating Precision

L1 mean surface water nitrate data products will be reported to 0.1 µM. The sensor is capable of measuring nitrate at a precision of 0.3 µM. The resolution of individual nitrate measurements is 0.1 µM, as this maintains the proper significant figures, despite the reported resolution being greater than the 0.3 µM precision and limit of detection.

7.2.5 Expanded Uncertainty

We assume the measurement variability is normally distributed (Gaussian). The combined uncertainty represents plus or minus one standard deviation or a confidence interval of 68%. This confidence level is below the industry standard and is therefore expanded to a 95% confidence interval. This is typically calculated by multiplying the combined uncertainty, $u_{c,r}(y)$, by a coverage factor, k_p.

$$\boldsymbol{U_p = k_p\, u_{c,r}(y)} \qquad \text{Equation 11}$$

Where $k_{95} = 1.96$ for $p = 95$ for a given degrees of freedom. k_p is approximated by a t-distribution with an effective degrees of freedom, v_{eff}, obtained from the Welch-Saterwaite formula:

$$\boldsymbol{v_{eff} = \frac{u_c^4(y)}{\sum_{i=1}^{n} \frac{u_i^4(y)}{v_i}}} \qquad \text{Equation 12}$$

The coverage factor then becomes $k_p = t_p(v_{eff})$, where $t_p(v_{eff})$ is obtained from a table.

However to simplify the calculations further, we can conservatively estimate the expanded uncertainty at a 95% confidence level to be two times the combined uncertainty.

$$\boldsymbol{U_{Expanded} = 2 \times u_c} \qquad \text{Equation 13}$$

This expansion is to be applied to all combined uncertainties for the L1 DP described herein.

7.3 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 3. Uncertainty budget for individual measurements. 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**	$\boldsymbol{\frac{\partial f}{\partial x_i}}$	$\boldsymbol{u_{x_i}(Y) \equiv \left\lvert\frac{\partial f}{\partial x_i}\right\rvert u(x_i)}$
Nitrate	$u_{CAL}(NO_{3,i})$	AD[08]	n/a	Eq. 8

Table 4. Uncertainty budget for means. Shaded rows denote the order of uncertainty propagation (from lightest to darkest).

Source of Uncertainty	Uncertainty Component $u(x)$	Uncertainty Value	$\frac{\partial f}{\partial x_i}$	$u_{u_{x_i}}(Y) \equiv \left\lvert\frac{\partial f}{\partial x_i}\right\rvert u(x_i)$
Nitrate	$u_c(\overline{NO_3})$	Eq. (10)	n/a	Eq. 10
Calibration	$u_{CAL}(NO_{3,i})$	AD[08]	n/a	Eq. 8
Natural variation	$u_{NAT}(\overline{NO_3})$	Eq. 9	n/a	Eq. 9

8 FUTURE PLANS AND MODIFICATIONS

In the future, calibration and maintenance records may be used to generate an additional sensor-specific flag to better indicate when field calibration or cleaning was occurring, and possibly remove the associated measurements from the published data. Currently these data are included, and only flagged by the ***nitrateConfigQF*** (which also triggers the ***finalQF***).

Another possible future enhancement is to develop more comprehensive flags for when a stream is dry and the sensor is reading in the air, or has been intentionally removed because the stream is expected to remain dry. Currently these data are only flagged by the ***SciRewQF*** (which also triggers the finalQF), and an entry is made in the issue log accompanying the download.

9 BIBLIOGRAPHY

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