NEON ALGORITHM THEORETICAL BASIS DOCUMENT (ATBD): WATER QUALITY

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CHANGE RECORD

REVISION	DATE	ECO#	DESCRIPTION OF CHANGE
A	09/22/2018	ECO-05528	Initial Release

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1 DESCRIPTION

1.1 Description

Contained in this document are details concerning Water Quality measurements made at NEON aquatic sites. Water quality includes specific conductance, dissolved oxygen (concentration and percent saturation), pH, chlorophyll a, turbidity, and, at some stations, fluorescent dissolved organic matter (fDOM). Specifically, the processes necessary to convert "raw" sensor measurements into meaningful scientific units and their associated uncertainties are described.

1.2 Purpose

This document details the algorithms used for creating NEON Level 1 data products for Water Quality from Level 0 data, and ancillary data as defined in this document (such as calibration data) obtained via instrumental measurements made by the YSI EXO2. 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.

1.3 Scope

The theoretical background and entire algorithmic process used to derive Level 1 data from Level 0 data for YSI EXO2 is described in this document. The YSI EXO2 employed is a set of sensor body and probes, which is manufactured by YSI Inc./Xylem Inc.. 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 (NOD) Requirements
AD[02]	NEON.DOC.005003	NEON Scientific Data Products Catalog
AD[03]	NEON.DOC.002652	NEON Level 1, Level 2, and Level 3 Data Products Catalog
AD[04]	NEON.DOC.005005	NEON Level 0 Data Product 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 analysis
AD[08]	NEON.DOC.000746	Evaluating Uncertainty (CVAL)
AD[09]	NEON.DOC.000785	TIS Level 1 Data Products Uncertainty Budget Estimation Plan
AD[10]	NEON.DOC.000751	CVAL Transfer of Standard Procedure
AD[11]	NEON.DOC.000927	NEON Calibration and Sensor Uncertainty Values [1]
AD[12]	NEON.DOC.001113	Quality Flags and Quality Metrics for TIS Data Products
AD[13]	NEON.DOC.005011	NEON Coordinate Systems Specification
AD[14]	NEON.DOC.00xxxx	Water Quality ingest workbook
AD[15]	NEON.DOC.00xxxx	Water Quality publication workbook
AD[16]	NEON.DOC.001152	Aquatic Sampling Strategy
AD[17]	NEON.DOC.001166	NEON Sensor Command, Control and Configuration (c3) Document: Multi-sonde, stream
AD[18]	NEON.DOC.003808	NEON Sensor Command, Control and Configuration (c3) Document: Buoy meteorological station and submerged sensor assembly

2.2 Reference Documents

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

2.3 External References

External references contain information pertinent to this document, but are not NEON configuration-controlled. Examples include manuals, brochures, technical notes, and external websites.

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

ER[01]	EXO User Manual

2.4 Acronyms

Acronym	**Definition**
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
QA/QC	Quality assurance and quality control

2.5 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**
λ	CVALTABLEA1	Calibration table component containing wavelength (independent variable)
$referenceSpectrum$	CVALTABLEB2	Calibration table component containing reference spectrum values (dependent variable)
ρ_{fDOM}	CVALA1	Calibration factor for temperature correction function for fDOM
l_{fDOM}	CVALB1	Calibration factor for absorbance correction function for fDOM
$u_{A1,d}$	U_CVALA1	Combined, standard uncertainty of sensor depth; provided by CVAL
$u_{A1,sCond}$	U_CVALA1	Combined, standard uncertainty of specific conductivity; provided by CVAL
$u_{A1,DOsat}$	U_CVALA1	Combined, standard uncertainty of dissolved oxygen saturation; provided by CVAL
$u_{A1,pH}$	U_CVALA1	Combined, standard uncertainty of pH; provided by CVAL
$u_{A1,chla}$	U_CVALA1	Combined, standard uncertainty of chlorophyll a; provided by CVAL
$u_{A1,turb}$	U_CVALA1	Combined, standard uncertainty of turbidity; provided by CVAL
$u_{A1,fDOM}$	U_CVALA1	Combined, standard uncertainty of fluorescent dissolved organic matter; provided by CVAL
$u_{A1,\rho_{fDOM}}$	U_CVALA4	Combined, standard uncertainty of temperature correction function for fDOM; provided by CVAL
$u_{A1,l_{fDOM}}$	U_CVALA5	Combined, standard uncertainty of absorbance correction function for fDOM; provided by CVAL
$R1_d$	CVALR1	Combined, standard uncertainty of sensor depth; provided by CVAL
$R1_{sCond}$	CVALR1	Combined, standard uncertainty of specific conductivity; provided by CVAL
$R1_{DOsat}$	UCVALR1	Combined, standard uncertainty of dissolved oxygen saturation; provided by CVAL
$R1_{pH}$	CVALR1	Combined, standard uncertainty of pH; provided by CVAL
$R1_{chla}$	CVALR1	Combined, standard uncertainty of chlorophyll a; provided by CVAL
$R1_{turb}$	CVALR1	Combined, standard uncertainty of turbidity; provided by CVAL
$R1_{fDOM}$	CVALR1	Combined, standard uncertainty of fluorescent dissolved organic matter; provided by CVAL

Symbol	Internal Notation	Description
$fDOM$	NA	Raw, calibrated fDOM measurement
$fDOM_{20}$	NA	Temperature corrected, calibrated fDOM measurement
$fDOM_A$	NA	Absorbance corrected, calibrated fDOM measurement
$fDOM_{A,20}$	NA	Absorbance and temperature corrected, calibrated fDOM measurement
T_m	NA	Calibrated temperature reading from the specific conductance probe (surfaceWaterTemperature term)

Table 1: Multisonde L0 inputs for YSI EXO2 measurements

fieldName	**units**	**DPNumber**
specificConductance	microSiemensPerCentimeter	NEON.DOM.SITE.DP0.20005.001.01093.HOR.VER.000
surfaceWaterTemperature	celsius	NEON.DOM.SITE.DP0.20005.001.01378.HOR.VER.000
sensorDepth	meter	NEON.DOM.SITE.DP0.20005.001.01664.HOR.VER.000
dissolvedOxygenSaturation	percent	NEON.DOM.SITE.DP0.20005.001.01360.HOR.VER.000
dissolvedOxygen	milligramsPerLiter	NEON.DOM.SITE.DP0.20005.001.01151.HOR.VER.000
pH	pH	NEON.DOM.SITE.DP0.20005.001.01657.HOR.VER.000
chlorophyll	microgramsPerLiter	NEON.DOM.SITE.DP0.20005.001.01660.HOR.VER.000
turbidity	formazineNephelometricUnit	NEON.DOM.SITE.DP0.20005.001.01662.HOR.VER.000
fDOM	quinineSulfateUnits	NEON.DOM.SITE.DP0.20005.001.01661.HOR.VER.000

Table 2: SUNA L0 inputs for YSI EXO2 measurements

fieldName	**units**	**DPNumber**
rawNitrateSingleCompressedStream	string	NEON.DOM.SITE.DP0.20033.001.02242.HOR.VER.000

3 DATA PRODUCT DESCRIPTION

3.1 Variables Reported

The Water Quality related L1 DPs provided by the algorithms documented in this ATBD are displayed in the accompanying file(s): Water Quality publication workbook, PublicationWorkbook_Water quality_20180709.txt (AD[15]).

3.2 Input Dependencies

Table 1 and Table 2 (above) detail the YSI EXO2 related L0 DPs used to produce L1 YSI EXO2 DPs in this ATBD.

3.3 Product Instances

Two YSI EXO2 will be deployed at each NEON stream site. The upstream sensor, sensor set #1, will not have an fDOM sensor. The downstream sensor, sensor set #2, will have an fDOM sensor in addition to all of the sensors at sensor set #1.

One YSI EXO2 with fDOM will be deployed at each NEON lake or river buoy, which will start a profile through the water column every 4 hours provided that there are at least 2 m of water depth present at the site. The duration of the profile depends on the water depth and number of profile steps. In lakes that are shallow the profiler will remain at the parked depth recording measuremetns every 5 minutes. A profile will take no longer than 4 hours, but often takes less than a half hour at the shallow lakes.

At the Flint River, Georgia (FLNT) there are two mltisondes on one buoy. One is deployed at a fixed depth of 0.5 m below the water surface and another is fixed to the top of the buoy platform with a pump that deliveres water from a deeper depth. This alternate deployment is due to higher velocity water at FLNT that would cause the profiler to be swept up in the current.

3.4 Temporal Resolution and Extent

Measurement of water quality at stream sites will occur *1 per minute (0.01667 Hz)*.

Measurement of water quality will occur at lake and river buoys at *1 per 5 minutes (0.003333 Hz)*.

3.5 Spatial Resolution and Extent

At stream sites the water quality sensors will be deployed about 30 to 45 minutes apart based on water velocity during baseflow conditions.

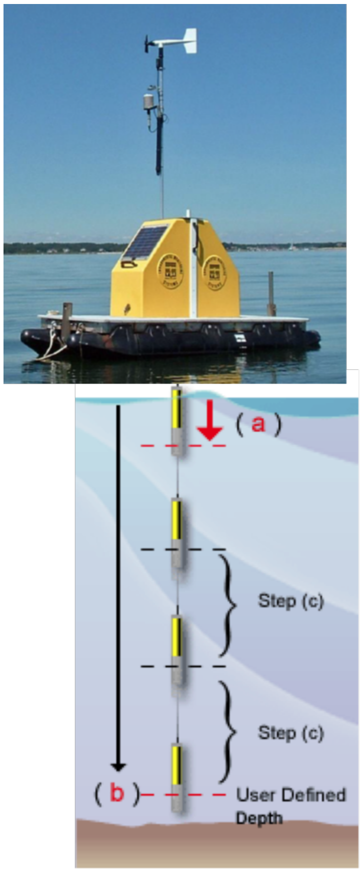
A YSI EXO2 will be part of the submerged sensors on the buoy at lake and river NEON sites, which will be deployed at a deep area of the main basin in lakes and at a deep area outside of the navigation channel in rivers.

4 SCIENTIFIC CONTEXT

Water quality parameters cover a suite of values that range over the course of a day and throughout seasons. These measurements can be useful as a context for intepreting other results or to base metabolism model estimates on. These core parameters are related to a variety of biogeochemical processes important to surface water ecosystems. At lake and river sites, the water quality sonde is mounted to collected information from multiple depths if the water body is at least 2 m deep in order to understand the changes in water quality through the vertical water column (Figure 1). In small streams, however, there are two water quality multisondes deployed longitudinally to capture tha variation in water quality from upstream to downstream (Figure 2).

4.1 Theory of Measurement

All sensors used as part of this data product are part of the YSI EXO2 water quality system. Individual, interchangeable probes are plugged into a body that is configured for deployment. The body remains at a site for its funtional life. The removable probes are field calibrated on a bi-weekly basis and returned to the NEON calibration and validation laboratory on an annual basis, or earlier if field calibration fails, for laboratory calibration.



Buoy (HOR 103) profile description:

- Every 4 hours the buoy uses a depth sounder to check the water depth below the buoy
- If there is at least 2 m of water it will start a profile sequence
- The number of profile steps and distance between them is dictated by the measured water depth
- After the winch moves the water quality mutlisonde to the step depth it equilibrates for 5 minutes
- After the 5 minute equilibration time it takes measurements
- After completing the profile the sonde returns to its parked depth (0.5 m) to collect data every 5 minutes for the remainder of the 4 hour timeframe

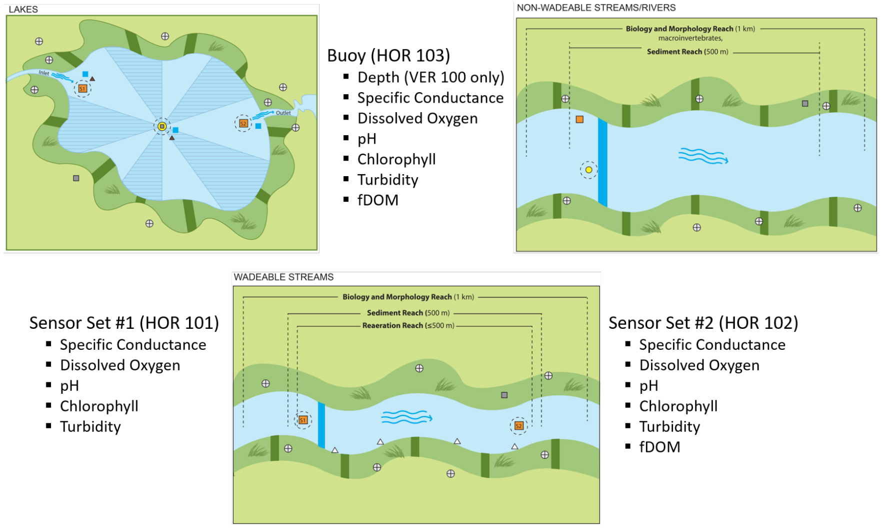
Figure 1: Overview diagrm of the buoy profiling system.

4.1.1 Depth

A non-vented pressure sensor is located in the body of the multisonde. At lake and river sites, where the system is installed on a profiling buoy, the pressure/depth sensor in the body is field calibrated to local barometric pressure initially and bi-weekly. At stream sites, the depth sensor in the body is not calibrated and data is not reported as part of this data product. Pressure measurements collected using a vented level TROLL sensor are used to determine water level at stream sites and are published as part of the Elevation of Surface Water data product (DP1.20016.001).

4.1.2 Specific Conductance

The probe records temperature using a digital thermistor and conductivity using a 4-electrode nickel cell. Specific conductance is calculated based on the temperature corrected conductivity.



Buoy (HOR 103)
- Depth (VER 100 only)
- Specific Conductance
- Dissolved Oxygen
- pH
- Chlorophyll
- Turbidity
- fDOM

Sensor Set #1 (HOR 101)
- Specific Conductance
- Dissolved Oxygen
- pH
- Chlorophyll
- Turbidity

Sensor Set #2 (HOR 102)
- Specific Conductance
- Dissolved Oxygen
- pH
- Chlorophyll
- Turbidity
- fDOM

Figure 2: Overview diagrm of the three types of sites and the multisonde data streams present at each.

4.1.3 Dissolved Oxygen

The EXO utilizes an optical dissolved oxygen sensor that emits a blue light on a luminescent dye embedded in a matrix which is quenched by the presence of oxygen.

4.1.4 pH

The EXO pH sensor uses a standard glass electrode.

4.1.5 Chlorophyll

The EXO total algae sensor is a dual-channel fluorometer that uses a 470nm excitation beam that excites chlorophyll a and a second 590 nm excitation beam that excites the phycocyanin accessory pigment found in blue-green algae (cyanobacteria). Chlorophyll concentration is a biogeochemically relavant parameter that is readily available by remote sensing and can be can serve as a proxy for phytoplankton biomass and light attenuation (Oestreich et al., 2016, Ganju et al., 2014, Jaud et al., 2012).

4.1.6 Turbidity

The EXO turbidity sensor employs a near-IR light source (~780 - 900 nm) and detects scattering at 90 degrees of the incident beam.

4.1.7 fDOM

The EXO fDOM sensor is a fluorometer with a single excitation/emission pair (365nm/480nm) used to detect the fluorescent fraction of the chromophoric DOM when exposed to near-UV light. Because of the impacts of temperature and water column absorbance (from a combination of dissolved and particulate compounds) on these readings corrections must be applied to the calibrated data.

4.2 Theory of Algorithm

1. One-minute or five-minute instantaneous measurements of will be published along with uncertainty and quality flags. Values outside of the specified ranges in the thresholds file should be flaged and not published.
2. Depth (calibrated and published for buoy sites only), specific conductance, DO (mg/L), DO (%), pH, and turbidity measurements will have calibration factors applied in the field by the sensor body prior to data output. Therefore, calibration coefficients will not need to be applied to these data streams as part of the ATBD workflow.
3. fDOM and chlorophyll sensors use fluorescence to make measurements and this is influenced by light absorbing and scattering compounds in the water column. Due to a shorter pathlength and longer wavelengths light, the chlorophyll readings will include additional uncertainty inputs from CVAL, but will not be corrected. However, fDOM data will be corrected using the absorbance data from the SUNA nitrate analyzer and temperature from the conductivity probe. fDOM measurements will be corrected for the influence of temperature, turbidity, and absorbance similar to Downing et al. (2012).

4.3 Removing buoy data streams with NaN values

Currently, water quality data coming off of the buoy (HOR index 103) are parsed into columns in the order they come in from the sensor. In the case of a sensor returning a NaN value, that is not parsed or stored in the data table. Thus, when an individual probe is malfunctioning and returning NaN values, the data returned from other sensors can be shifted to the wrong column and come in to the database in the wrong stream. Thus, anytime there is a NaN value returned by any of the 20 L0 data stream for a time stamp. All data streams should be converted to NaN or null, the **buoyNAFlag** should be set to 1, the **finalQF** should be set to 1, and all other QFs should be set to -1. If data is coming in without any NaN values the **buoyNAFlag** should be set to 0. The **buoyNAFlag** should only be populated for buoy locations (P/N HB07530100, HOR index 103).

This does not apply to stream locations (HOR index 101 and 102) as a different data logger is used there.

Currently, the only time that a null of gap flag would be set to 1 for buoy data would be if there is no data returned for any of the 20 data streams for a buoy. which would mean the whole sonde wasn't returning data rather than just a probe.

4.4 fDOM correction procedure

Fluorescence is an optical property of water tied to a variety of ecological parameters. Temperature and other, non-fluorescent but optically active, components of surface water can have an impact on fDOM readings that limit the ability to compare fDOM accross sites and over time. For this reason fDOM will be published as temperature and absorbance corrected (**fDOM**) and uncorrected (**rawCalibratedfDOM**) for users interested in both types of data (Downing, 2012; Watras et al. 2011).

4.4.1 Absorbance Corrections

4.4.1.1 Converting SUNA response data to absorbance

There is one SUNA optical nitrate sensor that produces absorbance data at each NEON aquatic site. This one sensor will be used to correct all water quality chlorophyll and fDOM data. The SUNA sensor will be located at HOR 102 at stream sites and 103 at buoy sites. The HOR 102 SUNA data at stream sites will be used to correct both HOR 101 and 102 water quality data. At the FLNT buoy the SUNA at VER 100 will be used to correct the water quality data for VER 100 and VER 110, all other buoys have only one SUNA and one water quality sonde (both at HOR 103 and VER 100).

When SUNA absorbance data is not available for the time range that covers the multisonde data processing, set the **chlorophyllAbsQF** and/or **fDOMAbsQF** to 1 to indicate that the absorbance corrections could not be applied. Skip the algorithms outlined here and proceed with applying the temperature corrections (see section 4.3.2).

In full ASCII mode, streams 11-266 are the spectrum channels returned by the SUNA nitrate analyzer (sunaResponse). These responses can be converted to decadic absorbance values by taking the base 10 log (http://docs.oracle.com/javase/7/docs/api/java/lang/Math.html) of the ratio of the reference spectrum for index i and response for index i. The reference spectrum of 256 values (referenceSpectrum), which is the same number of SUNA response values, will be provided by CVAL as a calibration table (new feature).

Absorbance values will be baseline corrected when the absorbance at the longest wavelength (channel 266) is less than 0. The value of the baseline correction for each frame will be the absorbance at channel 266 subtracted from 0. For instance, if the absorbance at the longest wavelength is -0.02, a value of 0.02 will be added to all light channels for that frame prior to calculating the mean or removing any frames.

Any light frames that have an absorbance value of 0 or less (log10(referenceSpectrum[i]/sunaResponse[i]) <= 0) between wavelengths of 205 and 380 (x[i] > 205 && x[i] < 380) should be removed before calculating the average as they will be problematic when fitting a linear regression for calculating the emission absorbance. The 50 (or fewer following cleaning 0 or negative values) light frame readings collected every 15 minutes should be averaged (using a mean) for each wavelength/channel to create the sunaResponse values. If no frames are left to calculate the average from, the data should be treated like there was no absorbance data and the **chlorophyllAbsQF** and/or **fDOMAbsQF** should be set to 1 to indicate that the absorbance corrections could not be applied. The number of frames that were used to calculate the mean absorbance spectrum should be published for each fDOM reading in the **spectrumCount** field. 0 should be populated if no frames were available.

A for-loop example of the math:

```
for(i = 0; i < referenceSpectrum.length; ++i){
```

```
    y[i] = log10(referenceSpectrum[i]/sunaResponse[i]);
}
```

where

referenceSpectrum[i] and sunaResponse[i] are floating point decimals.

4.4.1.2 Calculate the mean and standard deviation of absorbance (A_{ex}) over the excitation range of the fDOM probe (351 to 361 nm)

x is the wavelength (λ) provided by CVAL in the calibration table as the independent variable with the same length as the referenceSpectrum and streams 13-268 of the SUNA spectrum data. The calculated mean absorbance cannot be negative, if the calculations result in a negative value set A_{ex} to 0 and set $fDOM_A$ equal to $fDOM_m$ and move on to applying temperature corrections (see section 4.3.2).

A for-loop example of the math:

```
abs_sum = 0;
abs_count = 0;
for(i = 0; i < x.length; ++i){
    if(x[i]>351 && x[i]<361){
        abs_sum = abs_sum + y[i];
        abs_count = abs_count + 1;
    }
}
if(abs_sum > 0){
    $A_{ex}$ = abs_sum/abs_count;
}else{
    $A_{ex}$ = 0;
}
```

where abs_sum and A_{ex} are floating point decimals.

When A_{ex} is greater than 0.6, set the **chlorophyllAbsQF** and/or **fDOMAbsQF** to 2 to indicate that the absorbance corrections were applied, but that the absorbance values were high enough to be outside of the linear range of corrections.

The standard deviation of the absorbance range can be calculated with the following equation:

$$u_{A_{ex}} = \sqrt{\frac{\Sigma_{i=1}^{N}(x_i - \overline{x})^2}{N-1}} \tag{1}$$

where

$u_{A_{ex}}$ = uncertainty (standard deviation) of the mean absorbance

N = total number of absorbance values (same as abs_count in the above example)

i = index of the absorbance value

$\overline{x}$ = mean of the absorbance values (same as A_{ex} in the above example)

x_i = absorbance value of index i

A for-loop example of the math:

```
diff_sum = 0; diff_count = 0; for(i = 0; i < x.length; ++i){
    if(x[i]>351 && x[i]<361){
        mean_diff = y[i] - $A_{ex}$;
        sq_diff = mean_diff * mean_diff;
        diff_sum = diff_sum + sq_diff;
        diff_count = diff_count + 1;
    }
}
$u_{A_{ex}}$ = sqrt(diff_sum/(diff_count-1));
```

4.4.1.3 Calculate the mean and standard deviation of the absorbance (A_{em}) over the emission range of the fDOM probe (480 nm)

If the A_{ex} equals 0, set A_{em} to 0 as well. The absorbance correction factor now becomes 1 since 10^0 = 1. Set **chlorophyllAbsQF** and/or **fDOMAbsQF** to 3 to indicate that the calculated absorbance correction factor was 0.

First calculate a slope and intercept of the least-squares fit of a line to the natural log of the calculated absorbance versus wavelength so that an extrapolation to longer wavelengths than collected by the SUNA can be used for the calculations. Use only wavelengths above 205 nm since the spectrometer readings are not accurate below that region for this purpose. Then use the slope and intercept to estimate the absorbance at 480 nm.

The slope can be fit using the following equation:

$$m = \frac{n\Sigma_{i=1}^{n} x_i ln(y_i) - (\Sigma_{i=1}^{n} x_i)(\Sigma_{i=1}^{n} ln(y_i))}{n\Sigma_{i=1}^{n} x_i^2 - (\Sigma_{n=1}^{n} x_i)^2} \tag{2}$$

where

m = slope for least-squares linear fit to log(abs) v. λ

n = index of the spectrum channel, 1:256

x_i = calculated wavelength of the channel

y_i = calculated absorbance of the channel

A for-loop example of the math:

```
sum1 = 0;
sum2 = 0;
sum3 = 0;
sum4 = 0;

for(i=0; i < x.lenth; ++i){
        if(x[i] > 205 && x[i] < 380){
                sum1 = sum1 + (x[i] * log(y[i]));
                sum2 = sum2 + x[i];
                sum3 = sum3 + log(y[i]);
                sum4 = sum4 + x[i] * x[i];
        }
}

m = (x.length * sum1 - sum2 * sum3)/(x.length * sum4 - sum2 * sum2)
```

The intercept can be fit using the following equation:

$$b = \frac{\Sigma_{i=1}^{n} ln(y_i) - m\Sigma_{i=1}^{n} x_i}{n} \tag{3}$$

where

b = intercept for least-squares linear fit to log(abs) v. λ

n = index of the spectrum channel, 1:256

x_i = calculated wavelength of the channel

y_i = calculated absorbance of the channel

m = slope for least-squares linear fit to log(abs) v. λ

A for-loop example of the math:

```
sum1 = 0;
sum2 = 0;

for(i=0; i < x.lenth; ++i){

        if(x[i] > 205 && x[i] < 380){

                sum1 = sum1 + log(y[i]);
                sum2 = sum2 + x[i];

        }

}
```

```
b = (sum1 - m * sum2)/x.length
```

The absorbance at 480 nm can be estimated using the following equation:

$$A_{em} = exp(m \cdot \lambda + b) \tag{4}$$

where

λ = 480 (nm)

m = slope for least-squares linear fit to ln(abs) v. λ

b = intercept for least-squares linear fit to ln(abs) v. λ

The standard deviation of the extrapolation $u_{A_{em}}$ can be estimated with the following equation:

$$u_{A_{em}} = \sqrt{\left(\frac{1}{n-2}\right)\Sigma_{i=1}^{n}(y_i - \hat{y})^2} \tag{5}$$

where

$u_{A_{em}}$ = uncertainty (standard deviation) of y(x)

n = total number of absorbance values (256 for this dataset)

i = index of the absorbance value

$\hat{y}$ = y calculated from the regression equation

y_i = absorbance value of index i

A for-loop example of the math:

```
diff_sum = 0;
diff_count = 0;
for(i = 0; i < x.length; ++i){
    if(x[i] > 205 && x[i] < 380){
        mean_diff = y[i] - (m * x[i] + b);
        sq_diff = mean_diff * mean_diff;
        diff_sum = diff_sum + sq_diff;
        diff_count = diff_count + 1;
    }
}
```

$u_{A_{em}}$ = sqrt(diff_sum/(diff_count-2));

4.4.1.4 Applying absorbance corrections

Since the water quality multisonde data comes in every minute or every 5 minutes, usually, there will be multiple water quality readings per every SUNA absorbance spectrum. The same SUNA absorbance correction values should be applied to all water quality measurements collected within a 15 minute SUNA data window that starts at the time of the collection of the first SUNA light frame.

$$fDOM_A = fDOM_m \cdot 10^{[(A_{ex}+A_{em})\cdot l_{fDOM}]} \tag{6}$$

where

$fDOM_A$ = absorbance corrected fDOM measurement

$fDOM_m$ = raw, calibrated fDOM measurement (QSU)

A_{ex} = mean absorbance for 351 - 361 nm, derived from SUNA data (see section 4.3.1.2)

A_{em} = extrapolated absorbance at 480 nm, derived from SUNA data (see section 4.3.1.3)

$textandl_{fDOM}$ = probe specific effective pathlength, CVAL will provide this value and its corresponding uncertainty

Set **fDOMAbsQF** to 0 to indicate that the absorbance corrections were applied.

4.4.2 Temperature Corrections

Fluorescence data will be reported out corrected to a reference temperature of 20 °C. When temperature data is not available for the time range that covers the multisonde data processing, **fDOMTempQF** to 1 to indicate that the temperature corrections could not be applied. Otherwise, set **fDOMTempQF** to 0 to indicate that the temperature corrections were applied.

$$fDOM_{20} = \frac{fDOM}{1 - \rho_{fDOM}(T_m - 20)} \tag{7}$$

where

$fDOM_{20}$ = fDOM measurement corrected to 20 °C

$fDOM$ = raw, calibrated fDOM measurement taken at temperature m

ρ_{fDOM} = temperature-specific fluorescence coefficient (Watras et al. 2011) derived for NEON probes. CVAL will provide this value and its corresponding uncertainty.

T_m = temperature of the water when the fDOM reading was collected. This is from the **surfaceWaterTemperature** stream of the sonde.

4.4.3 Final Equation for fDOM corrections

The final equations for absorbance and temperature corrected fDOM values are:

$$fDOM_{A,20} = \frac{fDOM_m \cdot 10^{[(A_{ex}+A_{em})\cdot l_{fDOM}]}}{1 - \rho_{fDOM}(T_m - 20)} \tag{8}$$

4.5 Publishing buoy depth data streams

The depth measurements made by the water quality multisonde are calibrated only for buoy sites (P/N HB07530100, HOR index 103, VER index 100). A single buoy at FLNT has a non-profiling multisonde attached to a pump (VER 110) in addition to a sonde in a standpipe (VER 100). The sonde with the pump system should not have data populated for the depth stream since the sonde is not in the water measuring the pressure of the water column. The following fields should only be populated in the pub WB for profiling buoys: - sensorDepth - sensorDepthExpUncert - sensorDepthValidCalQF - sensorDepthSuspectCalQF

4.6 Publishing fDOM data streams

There is not an fDOM sensor installed at sensor set #1 in streams (P/N HB07530010, HOR index 101). The following fields should only be populated for lake/river or sensor set #2 locations (P/N HB07530100, HOR index 103; P/N HB07530000 HOR index 102): - fDOM - fDOMExpUncert - fDOMRangeQF - fDOMStepQF - fDOMNullQF - fDOMGapQF - fDOMConsistQF - fDOMSpikeQF - fDOMValidCalQF - fDOMSuspectCalQF - fDOMPersistenceQF - fDOMalphaQF - fDOMbetaQF - fDOMTempQF - fDOMAbsQF - fDOMSciRvwQF

4.7 Special Considerations

Buoys will be deployed at 7 lake sites and 3 large river sites within NEON. These buoys are comprised of sensor sets which measure meteorological parameters over a water surface along with submerged sensors that measure physical and chemical parameters of the water body. The water quality multisonde profiles every 4 hours. Depending on the depth of the water the water quality *buoy data may come in more or less frequently than once every 5 minutes*. For instance, in deeper lakes it make take a few minutes to travel meters between profile steps causing the data to come in every 8 or 9 minutes rather than every 5 minutes. *This is not always predictable because the depth of the lakes can fluctuate and the distance between the profile steps could vary.*

5 ALGORITHM IMPLEMENTATION

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

1. Data streams will be evaluted for any NaN values and data will be cleaned and flagged.
2. fDOM will be corrected for absorbance and temperature.
3. QA/QC Plausibility tests will be applied to the data stream in accordance with AD[06]. The details are provided below.
4. Signal de-spiking will be applied to the data stream in accordance with AD[07].
5. Quality flags will be produced for instantaneous measurements according to AD[12].

5.2 QA/QC Procedure:

1. **Plausibility Tests** - All plausibility tests will be determined for each measurement type (AD[06]). Test parameters will be provided by AQU and maintained in the CI data store. All plausibility tests will be applied to the sensor's L0 DP and an associated quality flags (QFs) will be generated for each test.
2. **Signal De-spiking and Time Series Analysis** - The time series de-spiking routine will be run according to AD[07]. Test parameters will be specified by AQU and maintained in the CI data store. Quality flags resulting from the de-spiking analysis will be applied according to AD[07].
3. Placeholder for Consistency Analysis (see section 7 for future implementation).
4. **Quality Flags (QFs) and Quality Metrics (QMs) AD[12]** - The following tests will be used to create the alpha and beta quality flags: fDOMTempQF, fDOMAbsQF, range, step (except for depth), spike, suspectCal, validCal, and persistence. QFs and QMs will be determined using the flags in Table 3. In addition, L1 DPs will have alpha and beta quality flags as well as a final quality flag, as detailed below. Ancillary information needed for the algorithm and other information maintained in the CI data store is shown in Table 4. Since the profiling buoy multisondes will collect data at varying frequencies, the null test time range will vary from site to site. See the attached ATBD-specific thresholds file "CLdata_thresholds_WQ_nullFrequencies.csv" in the CI data store for specific frequencies for each site, column "Null Test Frequency (1/min)".

$$QF_\alpha = \begin{cases} \text{0 if all QF = 0} \\ \text{1 if any QF = 1} \end{cases}$$

$$QF_\beta = \begin{cases} \text{0 if all QF = 0} \\ \text{1 if any QF = -1} \end{cases}$$

$$QF_{final} = \begin{cases} \text{0 if } QF_\alpha = 0 \\ \text{1 if } QF_\alpha = 1 \\ \text{1 if range test cannot be run, i.e. is -1} \end{cases}$$

Table 3: Flags associated with YSI EXO2 measurements at S1 (HOR 101), S2 (HOR 102), and buoy (HOR 103)

Tests	**Apply at S1**	**Apply at S2**	**Apply at buoy**
buoyNAFlag			X
fDOMTempQF		X	X
fDOMAbsQF		X	X
Range	X	X	X
Persistence	X	X	X
Step	X	X	X (except for depth)
Null	X	X	X
Gap	X	X	X
Valid Calibration	X	X	X
Suspect Calibration	X	X	X
Signal Despiking	X	X	X (except for depth)
Alpha Quality Flag (QF_α)	X	X	X
Beta Quality Flag (QF_β)	X	X	X
Final Quality Flag (QF_{final})	X	X	X

Note: For the dissolvedOxygen and dissolvedOxygenSaturation data streams, the calibration file for dissolvedOxygenSaturation will be used to determine whether or not there is a valid calibration file and if the calibration factors are suspect. Calibrating dissolvedOxygenSaturation simultaneously calibrates dissolvedOxygen for a probe and a separate calibration file is not produced.

Note: The persistence test should be applied to L0 fDOM data streams prior to any temperature or absorbance corrections in order to detect stuck values that may be obscured by changes in temperature or absorbance when those corrections are applied.

Table 4: Information maintained in the CI data store for YSI EXO2

Tests/Values	**CI Data Store Contents**
Range	Minimum and maximum values
Persistence	Window size, threshold values and maximum time length
Step	Threshold values
Null	ATBD-specific thresholds file
Gap	Test limit
Valid Calibration	CVAL sensor specific valid calibration date range
Suspect Calibration	CVAL sensor specific calibration pass or fail result
Signal Despiking	Time segments and threshold values
Calibration	CVAL sensor specific calibration coefficients
Uncertainty	AD[11]
Final Quality Flag	Section 5.2, step 4 of ATBD

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 AIS measurements will provide a measure of the reliability and applicability of individual measurements and AIS data products. This portion of the document serves to identify, evaluate, and quantify sources of uncertainty relating to individual, calibrated water quality measurements. It is a reflection of the information described in AD[11], and is explicitly described for the water quality assembly in the following sections. Uncertainty of the YSI EXO2 assembly is discussed in this section that informs the sources of *measurement* uncertainty, i.e., those associated with *individual measurements*. Diagrams detailing the data flow and known sources of uncertainty are displayed in Figure 3, Figure 4, and Figure 5.

6.1 Measurement Uncertainty

The following subsections present the uncertainties associated with *individual water quality observations*. It is important to note that the uncertainties presented in the following subsections are *measurement uncertainties*, that is, they reflect the uncertainty of an *individual* measurement. These uncertainties should not be confused with those presented in Section 6.1.2. We urge the reader to refer to AD[11] for further details concerning the discrepancies between quantification of measurement uncertainties and L1 uncertainties.

NEON calculates measurement uncertainties according to recommendations of the Joint Committee for Guides in Metrology (JCGM) 2008. In essence, if a measurand y is a function of n input quantities $x_i (i = 1, ..., n)$, i.e.,

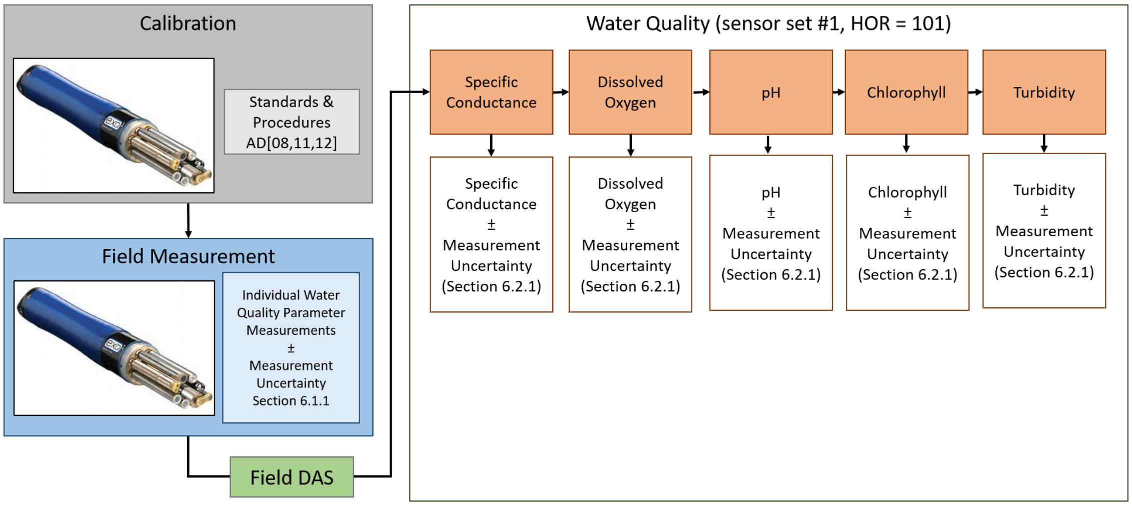


Figure 3: Data flow and associated uncertainties of individual measurements for Water Quality at sensor set 1 and associated L1 DPs.

$y = f(x_1, x_2, ..., x_n)$, the combined measurement uncertainty of y, assuming the inputs are independent, can be calculated as follows:

$$u_c(y) = \left(\sum_{i=1}^{N} \left(\frac{\partial f}{\partial x_i} \right)^2 u^2 \left(x_i \right) \right)^{\frac{1}{2}} \tag{9}$$

where

$\frac{\partial f}{\partial x_i}$ = partial derivative of y with respect to x_i

$u\left(x_i\right)$ = Combined uncertainty of x_i

Thus, the uncertainty of the measurand can be found be summing the input uncertainties in quadrature. For water quality measurements, the sources of uncertainty are depicted in **??** and the calcualtions of these input uncertainties is discussed below.

6.1.1 DAS

The YSI EXO2 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.

6.1.2 Calibration

Uncertainties associated with the YSI EXO2 calibration process will be provided by CVAL as individual standard combined uncertainty values. These uncertainties $u_{A1,x}$ (see Section 2.5) represent i) the repeatability and reproducibility of the sensor and the lab DAS and ii) uncertainty of the calibration procedures and coefficients including

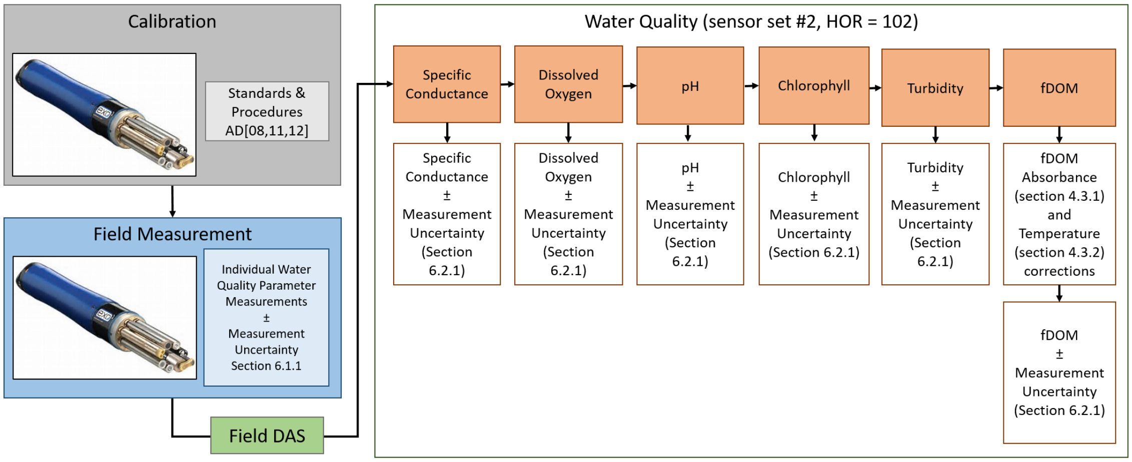


Figure 4: Data flow and associated uncertainties of individual measurements for Water Quality at sensor set 2 and associated L1 DPs.

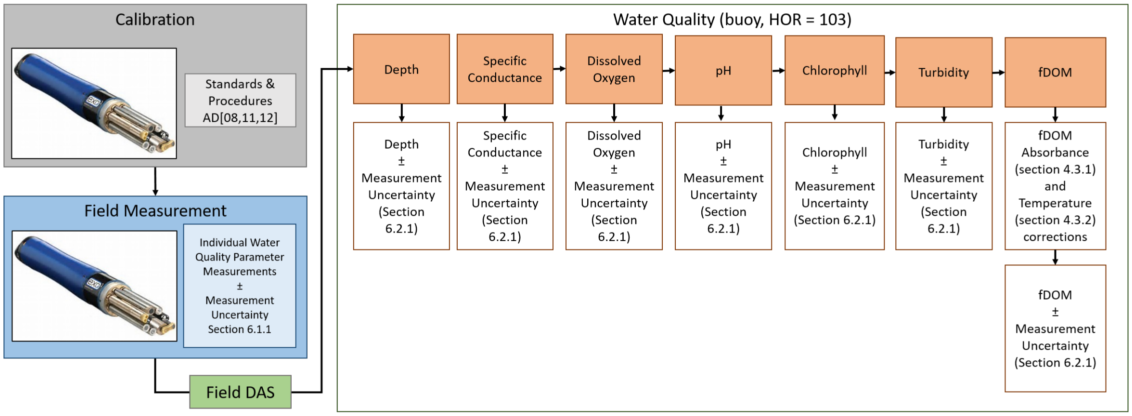


Figure 5: Data flow and associated uncertainties of individual measurements for Water Quality at the buoy locations and associated L1 DPs.

uncertainty in the standard (truth). Both are constant values that will be provided by CVAL, stored in the CI data store, and applied to all *individual measurements* (that is, the uncertainty values do 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[10] and AD[11].

6.1.3 Combined Measurement Uncertainties

6.1.3.1 Depth measurement uncertainty:

Because the only known quantifiable uncertainties are those provided by CVAL, the combined uncertainty is simply equal to the standard uncertainty values provided by CVAL, $u_{A1,d}$, multiplied by the L1 value.

$$u_{c_{depth}} = \sqrt{(u_{A1,d} \cdot sensorDepth)^2} \tag{10}$$

6.1.3.2 specific conductance measurement uncertainty:

Because the only known quantifiable uncertainties are those provided by CVAL, the combined uncertainty is simply equal to the standard uncertainty values provided by CVAL, $u_{A1,sCond}$, multiplied by the L1 value.

$$u_{c_{sCond}} = \sqrt{(u_{A1,sCond} \cdot specificConductance)^2} \tag{11}$$

6.1.3.3 DO (mg/L) measurement uncertainty:

Dissolved oxygen in mg/L is calculated internally by the probe using the DO percent saturation value, the measured temperature, and the barometric pressure at the time of the last calibration. According to manufacturer specifications, the accuracy of the measurements is $\pm$ 1% of reading between 0 - 20 mg/L and $\pm$ 5% of reading between 20 - 50 mg/L. So, the uncertainty can be calculated

$$u_{c_{DO}} = \sqrt{(u_{A1,DO} \cdot dissolvedOxygen)^2} \tag{12}$$

where

$$u_{A1,DO} = \begin{cases} 0.01 \text{ if } \textbf{dissolvedOxygen} \text{ is} > 0 \text{ and} <= 20 \text{ mg/L} \\ 0.05 \text{ if } \textbf{dissolvedOxygen} \text{ is} > 20 \text{ and} < 50 \text{ mg/L} \end{cases}$$

6.1.3.4 DO (%) measurement uncertainty:

Because the only known quantifiable uncertainties are those provided by CVAL, the combined uncertainty is simply equal to the standard uncertainty values provided by CVAL, $u_{A1,DOsat}$, multiplied by the L1 value.

$$u_{c_{DOsat}} = \sqrt{(u_{A1,DOsat} \cdot dissolvedOxygenSaturation)^2} \tag{13}$$

6.1.3.5 pH measurement uncertainty:

Because the only known quantifiable uncertainties are those provided by CVAL, the combined uncertainty is simply equal to the standard uncertainty values provided by CVAL, $u_{A1,pH}$, multiplied by the L1 value.

$$u_{c_{pH}} = \sqrt{(u_{A1,pH} \cdot pH)^2} \tag{14}$$

6.1.3.6 turbidity measurement uncertainty:

Because the only known quantifiable uncertainties are those provided by CVAL, the combined uncertainty is simply equal to the standard uncertainty values provided by CVAL, $u_{A1,turb}$, multiplied by the L1 value.

$$u_{c_{turb}} = \sqrt{(u_{A1,turb} \cdot turbidity)^2} \tag{15}$$

.

6.1.3.7 chlorophyll measurement uncertainty:

Because the only known quantifiable uncertainties are those provided by CVAL, the combined uncertainty is simply equal to the standard uncertainty values provided by CVAL, $u_{A1,chla}$, multiplied by the L1 value. The uncertainty provided by CVAL will include estimates of uncertainty related to the impacts of turbidity, which can both increase and decrease the chla readings due to light scattering towards or away from the sensor's detector. The temperature dependence of chla fluorescence is not captured in these uncertainty estimates.

$$u_{c_{chla}} = \sqrt{(u_{A1,chla} \cdot chlorophyll)^2} \tag{16}$$

.

6.1.3.8 fDOM measurement uncertainty when absorbance and temperature corrections are applied:

6.1.3.8.1 fDOM measurement uncertainty associated with fDOM measurements:

The partial derivatives of Equation 8 with respect to fDOM measured values must be calculated in order to identify the sensitivity coefficient of fDOM.

$$\frac{\partial fDOM_{A,20}}{\partial fDOM} = \frac{10^{[l_{fDOM}(A_{ex}+A_{em})]}}{1-\rho_{fDOM}(T_m-20)} \tag{17}$$

To derive the partial uncertainty of corrected fDOM as a function of the measured fDOM, the absolute value of this sensitivity coefficient is multiplied by the uncertainty of the measured fDOM.

$$u_{fDOM}(fDOM_{A,20}) = \left|\frac{\partial fDOM_{A,20}}{\partial fDOM}\right| \cdot u_{A1,fDOM} \cdot fDOM \tag{18}$$

6.1.3.8.2 fDOM measurement uncertainty associated with temperature:

The partial derivatives of Equation 8 with respect to measured temperature values must be calculated in order to identify the sensitivity coefficient of fDOM.

$$\frac{\partial fDOM_{A,20}}{\partial T_m} = \frac{fDOM \cdot \rho_{fDOM} \cdot 10^{[l_{fDOM}(A_{ex}+A_{em})]}}{((T_m - 20)\rho_{fDOM} - 1)^2} \tag{19}$$

To derive the partial uncertainty of corrected fDOM as a function of the measured temperature, the absolute value of this sensitivity coefficient is multiplied by the uncertainty of temperature measurement.

$$u_{T_m}(fDOM_{A,20}) = \left| \frac{\partial fDOM_{A,20}}{\partial T_m} \right| \cdot u_{A1,temp} \tag{20}$$

where (according to manufacturer specifications)

$$u_{A1,temp} = \begin{cases} 0.01\ ^{\circ}\text{C if } \textbf{surfaceWaterTemperature} \text{ is > -5 and <= 35 } ^{\circ}\text{C} \\ 0.05\ ^{\circ}\text{C if } \textbf{surfaceWaterTemperature} \text{ is > 35 } ^{\circ}\text{C} \end{cases}$$

6.1.3.8.3 fDOM measurement uncertainty associated with temperature relationship ρ:

The partial derivatives of Equation 8 with respect to the temperature relationship ρ must be calculated in order to identify the sensitivity coefficient of fDOM.

$$\frac{\partial fDOM_{A,20}}{\partial \rho_{fDOM}} = \frac{fDOM(T_m - 20)10^{[l_{fDOM}(A_{ex}+A_{em})]}}{(1 - (T_m - 20)\rho_{fDOM})^2} \tag{21}$$

To derive the partial uncertainty of corrected fDOM as a function of the temperature relationship ρ, the absolute value of this sensitivity coefficient is multiplied by the uncertainty of the temperature relationship ρ.

$$u_{\rho_{fDOM}}(fDOM_{A,20}) = \left| \frac{\partial fDOM_{A,20}}{\partial \rho_{fDOM}} \right| \cdot u_{A1,\rho_{fDOM}} \tag{22}$$

6.1.3.8.4 fDOM measurement uncertainty associated with A_{ex}:

The partial derivatives of Equation 8 with respect to A_{ex} must be calculated in order to identify the sensitivity coefficient of fDOM.

$$\frac{\partial fDOM_{A,20}}{\partial A_{ex}} = -\frac{fDOM \cdot l_{fDOM} log(10)10^{[l_{fDOM}(A_{ex}+A_{em})]}}{\rho_{fDOM}(T_m - 20) - 1} \tag{23}$$

To derive the partial uncertainty of corrected fDOM as a function of A_{ex}, the absolute value of this sensitivity coefficient is multiplied by the uncertainty of A_{ex}.

$$u_{A_{ex}}(fDOM_{A,20}) = \left| \frac{\partial fDOM_{A,20}}{\partial A_{ex}} \right| \cdot u_{A_{ex}} \tag{24}$$

6.1.3.8.5 fDOM measurement uncertainty associated with A_{em}:

The partial derivatives of Equation 8 with respect to A_{em} must be calculated in order to identify the sensitivity coefficient of fDOM.

$$\frac{\partial fDOM_{A,20}}{\partial A_{em}} = -\frac{fDOM l_{fDOM} log(10) 10^{[l_{fDOM}(A_{ex}+A_{em})]}}{\rho_{fDOM}(T_m - 20) - 1} \tag{25}$$

To derive the partial uncertainty of corrected fDOM as a function of A_{em}, the absolute value of this sensitivity coefficient is multiplied by the uncertainty of A_{em}.

$$u_{A_{em}}(fDOM_{A,20}) = \left|\frac{\partial fDOM_{A,20}}{\partial A_{em}}\right| \cdot u_{A1,A_{em}} \tag{26}$$

6.1.3.8.6 fDOM measurement uncertainty associated with l:

The partial derivatives of Equation 8 with respect to l must be calculated in order to identify the sensitivity coefficient of fDOM.

$$\frac{\partial fDOM_{A,20}}{\partial l_{fDOM}} = -\frac{fDOM l_{fDOM} log(10)(A_{ex} + A_{em}) 10^{[l(A_{ex}+A_{em})]}}{\rho_{fDOM}(T_m - 20) - 1} \tag{27}$$

To derive the partial uncertainty of corrected fDOM as a function of l, the absolute value of this sensitivity coefficient is multiplied by the uncertainty of l.

$$u_{l_{fDOM}}(fDOM_{A,20}) = \left|\frac{\partial fDOM_{A,20}}{\partial l_{fDOM}}\right| \cdot u_{A1,l_{fDOM}} \tag{28}$$

6.1.3.8.7 fDOM combined measurement uncertainty when absorbance and temperature corrections are applied:

$$\begin{aligned} u_{c_{fDOM_{A,20}}} = \Big(& u_{fDOM}(fDOM_{A,20})^2 + u_{T_m}(fDOM_{A,20})^2 + u_{\rho_{fDOM}}(fDOM_{A,20})^2 + u_{l_{fDOM}}(fDOM_{A,20})^2 \\ & + u_{A_{ex}}(fDOM_{A,20})^2 + u_{A_{em}}(fDOM_{A,20})^2\Big)^{\frac{1}{2}} \end{aligned} \tag{29}$$

6.1.3.9 fDOM measurement uncertainty when only absorbance corrections are applied:

6.1.3.9.1 fDOM measurement uncertainty associated with fDOM measurements:

The partial derivatives of Equation 6 with respect to fDOM measured values must be calculated in order to identify the sensitivity coefficient of fDOM.

$$\frac{\partial fDOM_{A,20}}{\partial fDOM} = 10^{[l_{fDOM}(A_{ex}+A_{em})]} \tag{30}$$

To derive the partial uncertainty of corrected fDOM as a function of the measured fDOM, the absolute value of this sensitivity coefficient is multiplied by the uncertainty of the measured fDOM.

$$u_{fDOM}(fDOM_{A,20}) = \left|\frac{\partial fDOM_{A,20}}{\partial fDOM}\right| \cdot u_{A1,fDOM} \cdot fDOM \tag{31}$$

6.1.3.9.2 fDOM measurement uncertainty associated with A_{ex}:

The partial derivatives of Equation 6 with respect to A_{ex} must be calculated in order to identify the sensitivity coefficient of fDOM.

$$\frac{\partial fDOM_{A}}{\partial A_{ex}} = l_{fDOM} \cdot fDOM10^{l_{fDOM}(A_{ex}+A_{em})} \tag{32}$$

To derive the partial uncertainty of corrected fDOM as a function of A_{ex}, the absolute value of this sensitivity coefficient is multiplied by the uncertainty of A_{ex}.

$$u_{A_{ex}}(fDOM_{A}) = \left|\frac{\partial fDOM_{A}}{\partial A_{ex}}\right| \cdot u_{A_{ex}} \tag{33}$$

6.1.3.9.3 fDOM measurement uncertainty associated with A_{em}:

The partial derivatives of Equation 6 with respect to A_{em} must be calculated in order to identify the sensitivity coefficient of fDOM.

$$\frac{\partial fDOM_{A}}{\partial A_{em}} = l_{fDOM} \cdot fDOM10^{l_{fDOM}(A_{ex}+A_{em})} \tag{34}$$

To derive the partial uncertainty of corrected fDOM as a function of A_{em}, the absolute value of this sensitivity coefficient is multiplied by the uncertainty of A_{em}.

$$u_{A_{em}}(fDOM_{A}) = \left|\frac{\partial fDOM_{A}}{\partial A_{em}}\right| \cdot u_{A1,A_{em}} \tag{35}$$

6.1.3.9.4 fDOM measurement uncertainty associated with l:

The partial derivatives of Equation 6 with respect to l must be calculated in order to identify the sensitivity coefficient of fDOM.

$$\frac{\partial fDOM_A}{\partial l_{fDOM}} = fDOM(A_{ex} + A_{em})10^{l_{fDOM}(A_{ex}+A_{em})} \tag{36}$$

To derive the partial uncertainty of corrected fDOM as a function of l, the absolute value of this sensitivity coefficient is multiplied by the uncertainty of l.

$$u_{l_{fDOM}}(fDOM_A) = \left|\frac{\partial fDOM_A}{\partial l_{fDOM}}\right| \cdot u_{A1,l_{fDOM}} \tag{37}$$

6.1.3.9.5 fDOM combined measurement uncertainty when only absorbance corrections are applied:

$$u_{c_{fDOM_A}} = \left(u_{fDOM}(fDOM_A)^2 + u_{l_{fDOM}}(fDOM_A)^2 + u_{A_{ex}}(fDOM_A)^2 + u_{A_{em}}(fDOM_A)^2\right)^{\frac{1}{2}} \tag{38}$$

6.1.3.10 fDOM measurement uncertainty when only temperature corrections are applied:

6.1.3.10.1 fDOM measurement uncertainty associated with fDOM measurements:

The partial derivatives of Equation 7 with respect to fDOM measured values must be calculated in order to identify the sensitivity coefficient of fDOM.

$$\frac{\partial fDOM_{20}}{\partial fDOM} = \frac{1}{1 - \rho_{fDOM}(T_m - 20)} \tag{39}$$

To derive the partial uncertainty of corrected fDOM as a function of the measured fDOM, the absolute value of this sensitivity coefficient is multiplied by the uncertainty of the measured fDOM.

$$u_{fDOM}(fDOM_{20}) = \left|\frac{\partial fDOM_{20}}{\partial fDOM}\right| \cdot u_{A1,fDOM} \cdot fDOM \tag{40}$$

6.1.3.10.2 fDOM measurement uncertainty associated with temperature:

The partial derivatives of Equation 7 with respect to measured temperature values must be calculated in order to identify the sensitivity coefficient of fDOM.

$$\frac{\partial fDOM_{20}}{\partial T_m} = \frac{fDOM(T_m - 20)}{(1 - \rho_{fDOM}(T_m - 20))^2} \tag{41}$$

To derive the partial uncertainty of corrected fDOM as a function of the measured temperature, the absolute value of this sensitivity coefficient is multiplied by the uncertainty of temperature measurement.

$$u_{T_m}(fDOM_{20}) = \left|\frac{\partial fDOM_{20}}{\partial T_m}\right| \cdot u_{A1,temp} \tag{42}$$

where (according to manufacturer specifications)

$$u_{A1,temp} = \begin{cases} 0.01\ ^\circ\text{C if } \textbf{surfaceWaterTemperature} \text{ is > -5 and <= 35 } ^\circ\text{C} \\ 0.05\ ^\circ\text{C if } \textbf{surfaceWaterTemperature} \text{ is > 35 } ^\circ\text{C} \end{cases}$$

6.1.3.10.3 fDOM measurement uncertainty associated with temperature relationship ρ:

The partial derivatives of Equation 7 with respect to the temperature relationship ρ must be calculated in order to identify the sensitivity coefficient of fDOM.

$$\frac{\partial fDOM_{20}}{\partial \rho_{fDOM}} = \frac{fDOM\rho_{fDOM}}{(1 - \rho_{fDOM}(T_m - 20))^2} \tag{43}$$

To derive the partial uncertainty of corrected fDOM as a function of the temperature relationship ρ, the absolute value of this sensitivity coefficient is multiplied by the uncertainty of the temperature relationship ρ.

$$u_{\rho_{fDOM}}(fDOM_{20}) = \left|\frac{\partial fDOM_{20}}{\partial \rho_{fDOM}}\right| \cdot u_{A1,\rho_{fDOM}} \tag{44}$$

6.1.3.10.4 fDOM combined measurement uncertainty when only temperature corrections are applied:

$$u_{c_{fDOM_{20}}} = \left(u_{fDOM}(fDOM_{20})^2 + u_{T_m}(fDOM_{20})^2 + u_{\rho_{fDOM}}(fDOM_{20})^2\right)^{\frac{1}{2}} \tag{45}$$

6.1.3.11 fDOM measurement uncertainty when absorbance and temperature corrections are not applied:

The only quantifiable uncertainty associated with raw, calibrated fDOM measurements are those associated with the measurement itself. When temperature and absorbance corrections are not applied the combined measurement uncertainty is defined by the following equations:

$$u_{c_{fDOM}} = \sqrt{(u_{A1,fDOM} \cdot fDOM)^2} \tag{46}$$

Table 5: Uncertainty budget for individual measurements of depth, Specific Conductance, DO ($\frac{mg}{L}$), DO (percent), pH, chlorophyll, turbidity.

Source of Measurement Uncertainty	**Measurement Uncertainty Component** $u(x_i)$	**Measurement Uncertainty Value**	$\frac{\partial f}{\partial x_i}$	$u_{x_i}(Y) \equiv \lvert\frac{\partial f}{\partial x_i}\rvert u(x_i)$
depth	$u_{A1,d}$	$u_{A1,d}$	1	$u_{A1,d}$
specific conductance	$u_{A1,sCond}$	$u_{A1,sCond}$	1	$u_{A1,sCond}$
DO ($\frac{mg}{L}$)	$u_{A1,DO}$	$u_{A1,DO}$	1	$u_{A1,DO}$
DO (percent)	$u_{A1,DOsat}$	$u_{A1,DOsat}$	1	$u_{A1,DOsat}$
pH	$u_{A1,pH}$	$u_{A1,pH}$	1	$u_{A1,pH}$
chlorophyll	$u_{A1,chla}$	$u_{A1,chla}$	1	$u_{A1,chla}$
turbidity	$u_{A1,turb}$	$u_{A1,turb}$	1	$u_{A1,turb}$

6.1.3.12 Expanded Measurement Uncertainty

The expanded measurement uncertainty is calculated as:

$$u_{95}(x) = k_{95} \cdot u_x \tag{47}$$

Where,

$u_{95}(x)$ = expanded uncertainty measurement uncertainty for measurement x at 95% confidence

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

u_x = combines uncertainty for measurement x

6.2 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 (Tables 5 & 6 & 7 & 8 & 9).

7 FUTURE PLANS AND MODIFICATIONS

Details concerning the evaluation and quantification of Sensor drift will be added to the uncertainty section.

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

Table 6: Uncertainty budget for temperature and absorbance corrected individual measurements of fDOM. Shaded rows denate the order of uncertainty propagation (from lightest to darkest).

Source of Measurement Uncertainty	**Measurement Uncertainty Component** $u(x_i)$	**Measurement Uncertainty Value**	$\frac{\partial f}{\partial x_i}$	$u_{x_i}(Y) \equiv \lvert\frac{\partial f}{\partial x_i}\rvert u(x_i)$
fDOM	$u_{A1,fDOM}$	$u_{A1,fDOM}$	Equation 18	Equation 17
temperature	$u_{A1,temp}$	$u_{A1,temp}$	Equation 40	Equation 19
A_{ex}	$u_{A_{ex}}$	$u_{A_{ex}}$	Equation 24	Equation 23
A_{em}	$u_{A_{em}}$	$u_{A_{em}}$	Equation 26	Equation 25
l	$u_{A1,l_{fDOM}}$	$u_{A1,l_{fDOM}}$	Equation 28	Equation 27
ρ	$u_{A1,\rho_{fDOM}}$	$u_{A1,\rho_{fDOM}}$	Equation 22	Equation 21

Table 7: Uncertainty budget for temperature only corrected individual measurements of fDOM. Shaded rows denate the order of uncertainty propagation (from lightest to darkest).

Source of Measurement Uncertainty	**Measurement Uncertainty Component** $u(x_i)$	**Measurement Uncertainty Value**	$\frac{\partial f}{\partial x_i}$	$u_{x_i}(Y) \equiv \lvert\frac{\partial f}{\partial x_i}\rvert u(x_i)$
fDOM	$u_{A1,fDOM}$	$u_{A1,fDOM}$	Equation 40	Equation 39
temperature	$u_{A1,temp}$	$u_{A1,temp}$	Equation 42	Equation 41
ρ	$u_{A1,\rho_{fDOM}}$	$u_{A1,\rho_{fDOM}}$	Equation 44	Equation 43

Table 8: Uncertainty budget for absorbance only corrected individual measurements of fDOM. Shaded rows denate the order of uncertainty propagation (from lightest to darkest).

Source of Measurement Uncertainty	**Measurement Uncertainty Component** $u(x_i)$	**Measurement Uncertainty Value**	$\frac{\partial f}{\partial x_i}$	$u_{x_i}(Y) \equiv \lvert\frac{\partial f}{\partial x_i}\rvert u(x_i)$
fDOM	$u_{A1,fDOM}$	$u_{A1,fDOM}$	Equation 31	Equation 30
A_{ex}	$u_{A_{ex}}$	$u_{A_{ex}}$	Equation 33	Equation 32
A_{em}	$u_{A_{em}}$	$u_{A_{em}}$	Equation 35	Equation 34
l	$u_{A1,l_{fDOM}}$	$u_{A1,l_{fDOM}}$	Equation 37	Equation 36

Table 9: Uncertainty budget for un-corrected individual measurements of fDOM. Shaded rows denate the order of uncertainty propagation (from lightest to darkest).

Source of Measurement Uncertainty	**Measurement Uncertainty Component $u(x_i)$**	**Measurement Uncertainty Value**	$\frac{\partial f}{\partial x_i}$	$u_{x_i}(Y) \equiv \lvert\frac{\partial f}{\partial x_i}\rvert u(x_i)$
fDOM	$u_{A1,fDOM}$	$u_{A1,fDOM}$	1	Equation 46

QA/QC tests may be expanded to include consistency analyses among similar measurement streams.

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