ALGORITHM THEORETICAL BASIS DOCUMENT (ATBD):

SOIL CO_2 CONCENTRATION
(REDACTED)

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Change Record

REVISION	DATE	ECO #	DESCRIPTION OF CHANGE
A	06/22/2017	ECO-04911	Initial release
B	09/27/2017	ECO-05054	Clarifying approach to determine the final quality flag (finalQF)

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LIST OF TABLES AND FIGURES

1 DESCRIPTION

Contained in this document are details concerning temperature measurements made at all NEON sites. Specifically, the processes necessary to convert "raw" sensor measurements into meaningful scientific units and their associated uncertainties are described. Soil CO_2 concentration profiles will be ascertained by installing sensors at various depths below the soil surface in each of the 5 TIS soil plots at NEON core and relocatable terrestrial sites.

1.1 Purpose

This document details the algorithms used for creating NEON Level 1 data products for soil CO_2 concentration from Level 0 data, and ancillary data as defined in this document (such as calibration data) obtained via instrumental measurements made by the soil CO_2 concentration sensor. It includes a detailed discussion of measurement theory and implementation, appropriate theoretical background, data product provenance, quality assurance and control methods used, approximations and/or assumptions made, and a detailed exposition of uncertainty resulting in a cumulative reported uncertainty for this product.

1.2 Scope

The theoretical background and entire algorithmic process used to derive Level 1 data from Level 0 data for soil CO_2 concentration is described in this document. The soil CO_2 concentration sensor employed is the Vaisala GMP343 diffusion model 0-20,000 ppm CO_2 concentration range. This document does not provide computational implementation details, except for cases where these stem directly from algorithmic choices explained here.

2 RELATED DOCUMENTS, ACRONYMS AND VARIABLE NOMENCLATURE

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.002652	NEON Level 1, Level 2 and Level 3 Data Products Catalog
AD[04]	NEON.DOC.005005	NEON Level 0 Data Products Catalog
AD[05]	NEON.DOC.000782	ATBD QA/QC Data Consistency
AD[06]	NEON.DOC.011081	ATBD QA/QC Plausibility Tests
AD[07]	NEON.DOC.000783	ATBD De-spiking and Time Series Analyses
AD[08]	NEON.DOC.000746	Calibration Fixture and Sensor Uncertainty Analysis (CVAL)
AD[09]	NEON.DOC.000785	TIS Level 1 Data Products Uncertainty Budget Estimation Plan
AD[10]	NEON.DOC.000927	NEON Calibration and Sensor Uncertainty Values[1]
AD[11]	NEON.DOC.001113	Quality Flags and Quality Metrics for TIS Data Products
AD[12]	NEON.DOC.003146	Soil sensor depth selection
AD[13]	NEON.DOC.000653 Pressure	NEON Algorithm Theoretical Basis Document – Barometric

[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
N/A	Not Applicable
CO2	Carbon dioxide

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**
A_{T1}	CVALA2	Manufacturer specified sensor-specific temperature compensation value recorded by CVAL and sent to CI data store
B_{T1}	CVALB2	Manufacturer specified sensor-specific temperature compensation value recorded by CVAL and sent to CI data store
C_{T1}	CVALC2	Manufacturer specified sensor-specific temperature compensation value recorded by CVAL and sent to CI data store
A_{T2}	CVALA3	Manufacturer specified sensor-specific temperature compensation value recorded by CVAL and sent to CI data store
B_{T2}	CVALB3	Manufacturer specified sensor-specific temperature compensation value recorded by CVAL and sent to CI data store
C_{T2}	CVALC3	Manufacturer specified sensor-specific temperature compensation value recorded by CVAL and sent to CI data store
A_{T3}	CVALA4	Manufacturer specified sensor-specific temperature compensation value recorded by CVAL and sent to CI data store
B_{T3}	CVALB4	Manufacturer specified sensor-specific temperature compensation value recorded by CVAL and sent to CI data store
C_{T3}	CVALC4	Manufacturer specified sensor-specific temperature compensation value recorded by CVAL and sent to CI data store
L_0	CVALL0	Calibration coefficient (ppm) from CVAL via calibration XML file for <1000 ppm range
L_1	CVALL1	Calibration coefficient (unitless) from CVAL via calibration XML file for <1000 ppm range

Symbol	Internal Notation	Description
L_2	CVALL2	Calibration coefficient (ppm^{-1}) from CVAL via calibration XML file for <1000 ppm range
M_0	CVALM0	Calibration coefficient (ppm) from CVAL via calibration XML file for ≥1000 and <5000 ppm range
M_1	CVALM1	Calibration coefficient (unitless) from CVAL via calibration XML file for ≥1000 and <5000 ppm range
M_2	CVALM2	Calibration coefficient (ppm^{-1}) from CVAL via calibration XML file for ≥1000 and <5000 ppm range
H_0	CVALH0	Calibration coefficient (ppm) from CVAL via calibration XML file for ≥5000 ppm range
H_1	CVALH1	Calibration coefficient (unitless) from CVAL via calibration XML file for ≥5000 ppm range
H_2	CVALH2	Calibration coefficient (ppm^{-1}) from CVAL via calibration XML file for ≥5000 ppm range
t	t_degreesC	Temperature test threshold from the soil CO2 ATBD-specific threshold file in the CI data store
RH	RH	Soil air relative humidity value from the soil CO2 ATBD-specific threshold file in the CI data store
G	O2Conc	Soil air oxygen concentration value from the soil CO2 ATBD-specific threshold file in the CI data store
u_{A1}	U_CVALA1	Combined, relative uncertainty of sensor (%)
u_{A3}	U_CVALA3	Combined, relative uncertainty (truth and trueness only) of sensor (%)
u_{R1}	U_CVALR1	Combined, relative uncertainty of Field DAS resistance readings (%)
u_{R3}	U_CVALR3	Combined, relative uncertainty (truth and trueness only) of Field DAS resistance readings (%)
${V_{eff}}_{A1}$	U_CVALD1	Effective degrees of freedom relating to U_CVALA1 (unitless)
${V_{eff}}_{A3}$	U_CVALD3	Effective degrees of freedom relating to U_CVALA3 (unitless)
${V_{eff}}_{R1}$	U_CVALF1	Effective degrees of freedom relating to U_CVALR1 (unitless)
${V_{eff}}_{R3}$	U_CVALF3	Effective degrees of freedom relating to U_CVALR3 (unitless)

3 DATA PRODUCT DESCRIPTION

4 DATA PRODUCT DESCRIPTION

4.1 Variables Reported

The soil CO_2 concentration related L1 DPs provided by the algorithms documented in this ATBD are displayed in the accompanying file NEON.DOC.003916.txt.

4.2 Input Dependencies

Table 4-1 details the soil CO_2 concentration-related L0 DPs used to produce L1 soil CO_2 concentration DPs in this ATBD. Since the soil CO_2 concentration data product relies on the barometric pressure ATBD (AD[13]), the inputs that are required to calculate barometric pressure are also needed in this ATBD but these are not listed in Table 4-1 to avoid duplication.

Table 4-1: List of soil CO_2 concentration-related L0 DPs that are transformed into L1 soil CO_2 concentration DPs in this ATBD.

Description	Sample Frequency	Units	Data Product Number
Raw CO_2 sensor measurement (c_{raw})	0.1 Hz	µmol mol^{-1}	NEON.DOM.SITE.DP0.00095.REV.01729.HOR.501.001
Soil CO_2 sensor headspace temperature (T)	0.1 Hz	°C	NEON.DOM.SITE.DP0.00095.REV.01730.HOR.501.001
Soil CO_2 sensor error status (QF_E)	0.1 Hz	N/A	NEON.DOM.SITE.DP0.00095.REV.01731.HOR.501.001
Raw CO_2 sensor measurement (c_{raw})	0.1 Hz	µmol mol^{-1}	NEON.DOM.SITE.DP0.00095.REV.01729.HOR.502.001
Soil CO_2 sensor headspace temperature (T)	0.1 Hz	°C	NEON.DOM.SITE.DP0.00095.REV.01730.HOR.502.001
Soil CO_2 sensor error status (QF_E)	0.1 Hz	N/A	NEON.DOM.SITE.DP0.00095.REV.01731.HOR.502.001
Raw CO_2 sensor measurement (c_{raw})	0.1 Hz	µmol mol^{-1}	NEON.DOM.SITE.DP0.00095.REV.01729.HOR.503.001

Description	Sample Frequency	Units	Data Product Number
Soil CO_2 sensor headspace temperature (T_{CO2})	0.1 Hz	°C	NEON.DOM.SITE.DP0.00095.REV. 01730.HOR.503.001
Soil CO_2 sensor error status (QF_E)	0.1 Hz	N/A	NEON.DOM.SITE.DP0.00095.REV. 01731.HOR.503.001
Level 1 1-minute mean soil temperature profile (T_{Soil})	1-min	°C	NEON.DOM.SITE.DP1.00041. REV.00933.HOR.VER.001
Level 1 1-minute soil temperature final quality flag (QF_T)	1-min	NA	NEON.DOM.SITE.DP1.00041.REV.00314. HOR.VER.001
One-minute mean station pressure	NA	kPa	NEON.DOM.SITE.DP1.00004.REV.00451. HOR.VER.001
One-minute station pressure final quality flag	NA	binary	NEON.DOM.SITE.DP1.00004.REV.00490. HOR.VER.001
One-minute station pressure expanded uncertainty	NA	kPa	NEON.DOM.SITE.DP1.00004.REV.00456. HOR.VER.001
One-minute mean temperature (soil plot HMP155)	NA	◦C	NEON.DOM.SITE.DP1.00098.REV.00693. HOR.000.001
One-minute temperature final quality flag (soil plot HMP155)	NA	binary	NEON.DOM.SITE.DP1.00098.REV.00732. HOR.000.001
One-minute temperature expanded uncertainty (soil plot HMP155)	NA	◦C	NEON.DOM.SITE.DP1.00098.REV.00698. HOR.000.001
One-minute mean temperature (tower HMP155)	NA	◦C	NEON.DOM.SITE.DP1.00098.REV.00693. 000.VER.001
One-minute temperature final quality flag (tower HMP155)	NA	binary	NEON.DOM.SITE.DP1.00098.REV.00732. 000.VER.001
One-minute temperature expanded uncertainty (tower HMP155)	NA	◦C	NEON.DOM.SITE.DP1.00098.REV.00698. 000.VER.001

Description	Sample Frequency	Units	Data Product Number
One-minute mean dewpoint temperature (soil plot HMP155)	NA	◦C	NEON.DOM.SITE.DP1.00098.REV.00733.HOR.000.001
One-minute dewpoint temperature final quality flag (soil plot HMP155)	NA	binary	NEON.DOM.SITE.DP1.00098.REV.00772.HOR.000.001
One-minute dewpoint temperature expanded uncertainty (soil plot HMP155)	NA	◦C	NEON.DOM.SITE.DP1.00098.REV.00738.HOR.000.001
One-minute mean dewpoint temperature (tower HMP155)	NA	◦C	NEON.DOM.SITE.DP1.00098.REV.00733.000.VER.001
One-minute dewpoint temperature final quality flag (tower HMP155)	NA	binary	NEON.DOM.SITE.DP1.00098.REV.00772.000.VER.001
One-minute dewpoint temperature expanded uncertainty (tower HMP155)	NA	◦C	NEON.DOM.SITE.DP1.00098.REV.00738.000.VER.001

4.3 Product Instances

Three soil CO_2 concentration sensors will be deployed in each of the five TIS soil plots at NEON core and relocatable terrestrial sites.

4.4 Temporal Resolution and Extent

The soil CO_2 concentration sensor will make CO_2 concentration measurements at 10 second intervals and one- and thirty-minute averages of soil CO_2 will be calculated to form L1 DPs.

4.5 Spatial Resolution and Extent

The soil CO_2 concentration measurements represent the CO_2 concentration of the air that has diffused to the sensor headspace via holes drilled around a ~11 cm diameter access tube. Each TIS soil plot will contain a profile of soil CO_2 sensors ranging in depth from approximately 2 cm below the soil surface to approximately 6-30 cm deep. Sensor installation depths will vary among sites based on soil horizon thicknesses, expected soil CO_2 concentration, and other site-specific variables (AD[12]). The different installation depths of soil CO_2 concentration sensors within an individual soil plot provide vertical spatial information. The CO_2 sensors installed across the five TIS soil plots at each NEON core and relocatable site provides horizontal spatial information. Horizontal spatial variability among the soil CO_2 sensors within a soil plot is assumed to be negligible as the sensors are typically ~1 m apart.

Each soil CO_2 concentration sensor location will represent the point at which it is placed in the soil. Ultimately, a CO_2 concentration profile will be developed for each soil plot from the soil CO_2 concentration sensors installed at different depths. The CO_2 concentration profile will be used to determine soil CO_2 efflux rates.

5 SCIENTIFIC CONTEXT

Measuring soil CO_2 efflux rates is an important component of NEON's terrestrial carbon cycling measurements because it represents one of the largest fluxes of carbon from ecosystems to the atmosphere. The vast majority of CO_2 leaving the soil and entering the atmosphere is produced via respiration by organisms living in the soil, including plant roots, microorganisms, and soil animals. As a result, soil CO_2 efflux is an indicator of total belowground biological activity. In addition, since soils store large amounts of carbon and soil respiration is the primary pathway for this carbon to enter the atmosphere, long-term changes in soil CO_2 efflux rates over large areas could influence CO_2 concentrations in the atmosphere.

5.1 Theory of Measurement

The Vaisala GMP343 is a nondispersive infrared sensor (Vaisala 2013). The sensor consists of a miniature filament lamp that shines into the sensor headspace (which is open to the surrounding air), with a mirror and an infrared detector positioned behind a Fabry-Perot Interferometer. The Fabry-Perot Interferometer changes its measurement wavelength between the absorption band of CO_2 and a reference band. When the Fabry-Perot Interferometer is set to the CO_2 absorption band the detector receives less light than when it is set to the reference band, and the reduction in light transmission is proportional to the abundance of CO_2 molecules in the sensor headspace.

In addition, the sensor has a temperature probe located in the sensor headspace that is used to compensate for temperature changes on the CO_2 measurements. Compensations for air pressure, relative humidity, and oxygen concentration are also applied as specified below.

5.2 Theory of Algorithm

Note that some of the information in this section is redacted in the public version because the manufacturer did not want the proprietary equations made public. NEON used the equations provided by the manufacturer to apply the compensations for temperature, pressure, relative humidity, and oxygen concentration.

The compensations necessary to convert the sensor readings to CO_2 concentration (ppm) depends on environmental parameters (temperature, pressure, relative humidity and oxygen concentration), as well as the CO_2 concentration. As a result, the compensation factors must be calculated via the following equations [[redacted] and [redacted]] until *i*=10 (Vaisala pre 2014).

[redacted]

Do not calculate the soil CO_2 concentration data product if 1) 1-minute pressure corrected to the ground surface (*p*) is missing or has a final quality flag of 1; or 2) if the temperature reported by the sensor (T_{CO2}) is unavailable.

After completing [redacted], the equation is modified to [redacted] and repeated iteratively until *i*=10.

[redacted]

[redacted]

The equation above, as well as subsequent equations, assume that barometric pressure adjusted to the elevation of the soil plot surface where the CO_2 concentration sensor is installed, is representative of pressure in the sensor's headspace. This assumption is reasonable since the TIS soil plots are located within a few hundred meters horizontally and <100 m vertically of the barometric pressure sensor, and the soil CO_2 concentration sensors are installed ≤0.5 m below the soil surface. Moreover, soil air pressure is often in equilibrium with atmospheric pressure. For example, over ~120 days soil air pressure at 0.1, 0.3, 0.4 and 0.75 m was usually in equilibrium with atmospheric pressure and when it was not in equilibrium it differed by less than 2.5 kPa (Renault et al. 1998).

Pressure at the soil plot surface will be calculated following AD[13]. Elevation above sea level (m) of each soil plot, which is used in the pressure calculation (AD[13]), shall be calculated as the average elevation of the four corners of that plot:

$$h_{soil,i} = \frac{h_{soil_{c1},i} + h_{soil_{c2},i} + h_{soil_{c3},i} + h_{soil_{c4},i}}{4}$$ **Equation 3**

Where:

$h_{soil,i}$	elevation of soil plot *i* (m ASL)
$h_{soil_{c1},i}$	elevation of corner 1 of soil plot *i* (m ASL), stored in the CI data store
$h_{soil_{c2},i}$	elevation of corner 2 of soil plot *i* (m ASL), stored in the CI data store
$h_{soil_{c3},i}$	elevation of corner 3 of soil plot *i* (m ASL), stored in the CI data store
$h_{soil_{c4},i}$	elevation of corner 4 of soil plot *i* (m ASL), stored in the CI data store

According to the manufacturer [redacted] and [redacted] apply to pressure ranges of 700 to 1300 hPa, temperature ranges of -40 to +60 °C, relative humidity ranges of 0 to 100%, and oxygen concentrations of 0 to 100%. Note that a data quality flag will be applied to the data product indicating instances when pressure is outside this range, which will likely occur frequently or occasionally at a few high elevation sites.

[redacted] [redacted]

[redacted]

[redacted]

[redacted]

[redacted]	[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]	[redacted]

[redacted] [redacted]

[redacted]

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[redacted] [redacted]

[redacted]

[redacted]

[redacted] [redacted]

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[redacted]

[redacted] [redacted]

[redacted]

[redacted]

[redacted] [redacted]

[redacted]

[redacted]

The present NEON design does not include measurements of relative humidity in soil air. Fortunately, according to the manufacturer, the compensation for relative humidity is much less important than the compensation for temperature and pressure (Vaisala 2013). For example, an extreme change in relative humidity from 0 to 100 % changes the compensated CO_2 concentration from 10,193 to 9,913 ppm, respectively, with a raw CO_2 measurement of 10,000 ppm at 25 °C, 101.3 kPa, and 21 % oxygen concentration. In a closed system under constant pressure and temperature, soil air relative humidity would equilibrate at 100% since there is usually some liquid water present in the soil. Of course soil air is not a closed system, however, several attributes of soil allow for relatively long amounts of time for equilibration to occur, including the high tortuosity of soil pores that reduces mixing of soil air with the atmosphere, and the relatively high thermal capacity of soil, which buffers soils against rapid temperature changes. A value of 75% relative humidity was chosen for all sensors initially but may be updated in the future if soil relative humidity data become available.

[redacted] [redacted]

[redacted]

[redacted]

[redacted] [redacted]

[redacted]

[redacted]

[redacted] [redacted]

[redacted]

[redacted]

[redacted] [redacted]

[redacted]

[redacted]

The present NEON design does not include measurements of oxygen concentration in soil air. Fortunately, according to the manufacturer, the compensation for oxygen concentration is much less important than the compensation for temperature and pressure (Vaisala 2013). For example, an extreme change in oxygen concentration from 0 to 21 % changes the compensated CO_2 concentration from 9790 to 9976 ppm, respectively, with a raw CO_2 measurement of 10,000 ppm at 25 °C, 101.3 kPa, and 75 % relative humidity. Since photosynthesis cannot occur in the soil due to light limitation no oxygen is produced in the soil. However, soil organisms use oxygen during respiration which depletes the oxygen concentration and creates an oxygen diffusion gradient with the atmosphere. The high tortuosity of pores in the soil reduces mixing of soil air with the atmosphere and results in a decrease in oxygen concentration with depth relative to the concentration in the atmosphere. Since soil air oxygen concentration is unknown at most NEON sites we will initially use the atmospheric oxygen concentration, 20.95 %, but may update this value in the future if soil oxygen data become available. This value may overestimate the oxygen concentration at some sites, particularly deeper in the soil profile and when soil moisture is high (i.e., diffusion of atmospheric air into the soil is slow).

Once the compensations for temperature, pressure, oxygen concentration, and relative humidity have been applied using the algorithms above, one of the following calibration equations shall be applied to each datum depending on its value:

If c_{10} < 1000 ppm: $$C_j = L_2 {c_{10}}^2 + L_1 c_{10} + L_0$$ **Equation 14**

If 1000 ≤ c_{10} < 5000 ppm: $$C_j = M_2 {c_{10}}^2 + M_1 c_{10} + M_0$$ **Equation 15**

If c_{10} ≥ 5000 ppm: $$C_j = H_2 {c_{10}}^2 + H_1 c_{10} + H_0$$ **Equation 16**

Where:

c_{10} output of [redacted] after 10 iterations. This represents the sensor's CO_2 reading after compensation for temperature, pressure, oxygen concentration, and relative humidity;
L_0 calibration coefficient provided by CVAL and stored in the CI data store;
L_1 calibration coefficient provided by CVAL and stored in the CI data store;
L_2 calibration coefficient provided by CVAL and stored in the CI data store;
M_0 calibration coefficient provided by CVAL and stored in the CI data store;
M_1 calibration coefficient provided by CVAL and stored in the CI data store;
M_2 calibration coefficient provided by CVAL and stored in the CI data store;
H_0 calibration coefficient provided by CVAL and stored in the CI data store;
H_1 calibration coefficient provided by CVAL and stored in the CI data store;
H_2 calibration coefficient provided by CVAL and stored in the CI data store;
C_j CO_2 concentration (ppm, wet mole fraction) in the sensor headspace.

Once the compensated and calibrated soil CO_2 concentrations have been calculated using the above equations, one-minute ($\bar{C}_1$) and thirty-minute ($\bar{C}_{30}$) averages of CO_2 concentration will be determined accordingly to create L1 soil temperature DPs:

$$\bar{C}_1 = \frac{1}{n}\sum_{j=x}^{n} C_j$$ **Equation 17**

where:

C_j is the compensated and calibrated soil CO_2 concentration;
$\bar{C}_1$ is the one-minute average of C_j;
T is defined as $0 \leq T < 60$ seconds;
n is the number of measurements in the averaging period T;

and

$$\bar{C}_{30} = \frac{1}{n}\sum_{j=x}^{n} C_j$$ **Equation 18**

where:

C_j is the compensated and calibrated soil CO2 concentration;
$\bar{C}_{30}$ is the one-minute average of C_j;
T is defined as $0 \leq T < 1800$ seconds;
n is the number of measurements in the averaging period T;

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.

6 ALGORITHM IMPLEMENTATION

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

1. 0.1 Hz data will be converted to compensated and calibrated soil CO_2 concentration, c_j, according to the equations above.
2. The warm-up/installation, sensor error status, temperature, and pressure range tests will be applied to the data stream as described below.
3. QA/QC Plausibility tests will be applied to the data stream in accordance with AD[06], details are provided below.
4. Signal de-spiking and time series analysis will be applied to the data stream in accordance with AD[07].

5. One- and thirty-minute temperature averages will be calculated using Equation 17 and Equation 18.
6. Descriptive statistics, i.e. minimum, maximum, and variance, will be determined for both one- and thirty-minute averages.
7. QA/QC Summary (Qsum) will be produced for one- and thirty-minute averages according to AD[11].

QA/QC Procedure:

1. **Warm-up/installation Test** – Since the manufacturer specifies that the GMP343 sensor requires a warm-up time of 30 minutes to achieve full accuracy (Vaisala 2013) and the 90% response time of the sensor in the NEON assembly is expected to be approximately 90 minutes at the time of writing, a flag will be applied based on time since last L0 measurement. This is because a long gap since the last measurement may indicate that the sensor was shut down and/or removed from the assembly. If there was a continuous gap (or gaps) of >5 minutes in both the L0 CO_2 (c_{raw}) and temperature (T_{CO2}) measurements within the 90 minutes preceding the measurement, set the warm-up/installation flag to "1"; whereas if there was not a gap of >5 minutes in the L0 CO_2 (c_{raw}) or temperature (T_{CO2}) measurements, set the warm-up/installation flag to 0.

2. **Sensor Error Status Test** – The sensor error status shall be used to assign a flag to the soil CO_2 concentration data product. If the sensor error status does not indicate an error (i.e., "0") the data passes the test and is set to "0". Whereas, if the sensor error status indicates an error (i.e., "1") the data fails the test and shall be set to "1". If the sensor error status test cannot be run (e.g., because sensor error status is unavailable), the flag shall be set to "-1".

3. **Temperature Test** – The headspace temperature reported by the soil CO_2 concentration sensor (T_{CO2}) shall be compared to temperature measured from the soil temperature profile sensors (T_{Soil}) in the same soil plot and at the nearest depth to the soil CO_2 concentration sensor as specified in Table 6-1. If the temperature reported by the CO_2 sensor is within $\pm t$ °C of the temperature reported by the soil temperature profile the datum passes the test and the flag = 0 (Table 6-2). If it is outside of this range the datum fails the test and the flag = 1. While if the test cannot be performed (e.g., soil temperature data is not available for the corresponding time) or the final quality flag of the soil temperature measurement (QF_T) is "1" the temperature test flag = -1 (Table 6-2). Due to expected spatial variability, both horizontal and vertical, in soil temperature between the temperature and CO_2 sensor locations, a relatively large tolerance is needed for this test to avoid erroneously flagging "good" soil CO_2 data. As a result this test threshold is sufficient to identify major discrepancies in temperature measurements, which may indicate a malfunctioning soil CO_2 sensor, however, it is likely insufficient to identify smaller biases in the soil CO_2 sensor's temperature measurement.

Table 6-1. Corresponding soil temperature data product for the Temperature Test.

Soil CO_2 sensor temperature DP number	Soil temperature DP number	Sites
NEON.DOM.SITE.DP0.00095.001.01730.HOR.501.000	NEON.DOM.SITE.DP1.00041.001.00933.HOR.501.001	ABBY, BARR, BART, BLAN, BONA, CLBJ, CPER, DCFS, DEJU, DELA, DSNY, GRSM, GUAN, HARV, HEAL, JERC, JORN, KONA, KONZ, LAJA, LENO, MLBS, MOAB, NIWO, NOGP, OAES, OLAA, ONAQ, ORNL, OSBS, RMNP, SCBI, SERC, SJER, SOAP, SRER, STEI, STER, TALL, TEAK, TOOL, TREE, UKFS, UNDE, WOOD, WREF, YELL
NEON.DOM.SITE.DP0.00095.001.01730.HOR.502.000	NEON.DOM.SITE.DP1.00041.001.00933.HOR.502.001	ABBY, BARR, BART, BLAN, CPER, DCFS, DEJU, DELA, DSNY, GRSM, GUAN, HARV, HEAL, JERC, JORN, KONA, KONZ, LENO, MLBS, MOAB, NIWO, NOGP, OAES, ONAQ, ORNL, OSBS, RMNP, SCBI, SERC, SRER, STEI, STER, TALL, TOOL, TREE, UKFS, UNDE, WOOD
NEON.DOM.SITE.DP0.00095.001.01730.HOR.502.000	NEON.DOM.SITE.DP1.00041.001.00933.HOR.503.001	LAJA
NEON.DOM.SITE.DP0.00095.001.01730.HOR.502.000	TBD	BONA, CLBJ, OLAA, SJER, SOAP, TEAK, WREF, YELL
NEON.DOM.SITE.DP0.00095.001.01730.HOR.503.000	NEON.DOM.SITE.DP1.00041.001.00933.HOR.502.001	BART, CPER, DCFS, DSNY, HARV, KONA, KONZ, LENO, MLBS, NOGP, OAES, TALL, UKFS, WOOD
NEON.DOM.SITE.DP0.00095.001.01730.HOR.503.000	NEON.DOM.SITE.DP1.00041.001.00933.HOR.503.001	ABBY, BARR, BLAN, DEJU, DELA, GUAN, HEAL, JORN, MOAB, NIWO, ONAQ, ORNL, SCBI, SERC, SRER, STEI, STER, TOOL, TREE, UNDE
NEON.DOM.SITE.DP0.00095.001.01730.HOR.503.000	NEON.DOM.SITE.DP1.00041.001.00933.HOR.504.001	GRSM, JERC, LAJA, OSBS, RMNP
NEON.DOM.SITE.DP0.00095.001.01730.HOR.503.000	TBD	BONA, CLBJ, OLAA, SJER, SOAP, TEAK, WREF, YELL

Table 6-2. Summary of temperature test logic.

Soil Temperature parameters	Level 1 soil CO_2 data product	Soil CO_2 temperature flag setting
n = 1 (i.e., data present) $-t < (T_{CO2} - T_{Soil}) < t$ QF_T = 0	Calculate	0
n = 1 (i.e., data present) $-t > (T_{CO2} - T_{Soil})$ OR $t < (T_{CO2} - T_{Soil})$ QF_T = 0	Calculate	1
n = 0 (i.e., missing data)	Calculate	-1
QF_T = 1	Calculate	-1

4. **Pressure Range Test** – Apply a flag to identify when the barometric pressure value used in the compensation fall outside of 70.0-130.0 kPa, which is the pressure range certified by the manufacturer. Flag = 0 if soil plot pressure is ≥70.0 kPa and ≤130.0 kPa; Flag = 1 if soil plot pressure is <70.0 kPa or >130.0 kPa; and Flag = -1 if barometric pressure data is not available or has a final quality flag of 1.

5. **Plausibility Tests** AD[06] – All plausibility tests will be determined for the soil CO_2 concentration data. 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.

6. **Signal Despiking and Time Series Analysis** – Time segments and threshold values for the automated despiking QA/QC routine will be specified by FIU and maintained in the CI data store. QFs from the despiking analysis will be applied according to AD[07].

7. **Quality Flags (QFs) and Quality Metrics (QMs)** AD[11] – If a datum has failed one of the following tests it will not be used to create a L1 DP, ***range, de-spiking, persistence, step, sensor error status***. Flags associated with the soil CO_2 concentration L1 data product are listed in Table 6-3. Ancillary information needed for the algorithm and other information maintained in the CI data store is shown in Table 6-4.

    a. **Setting the Final Quality Flag**– If <50% of data in the averaging period fail the warm-up/installation test flag, temperature test flag, and the pressure range test (i.e., warmUpInstallationFailQM, temperatureSCO2FailQM, and pressureRangeFailQM <50), the soil CO_2 concentration final quality flag (finalQF) shall be determined using α and β according to AD[11]. If ≥50% of data in the averaging period fail the warm-up/installation test flag, temperature test flag, or the pressure range test (i.e., warmUpInstallationFailQM, temperatureSCO2FailQM, or pressureRangeFailQM ≥50), the soil CO_2 concentration final quality flag (finalQF) shall be set to "1".

Table 6-3. Flags associated with soil CO_2 concentration measurements.

Tests
Warm-up/installation
Sensor error status
Temperature
Pressure range
Range
Persistence
Step
Null
Gap
Signal Despiking and Time Series Analysis
Final quality flag

Table 6-4. Information maintained in the CI data store for soil CO_2 concentration.

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
Gap	Test limit
Signal Despiking and Time Series Analysis	Time segments and threshold values
Temperature	Temperature test threshold values
Calibration	CVAL sensor specific calibration coefficients
Uncertainty	AD[10]
Final Quality Flag	AD[11]

7 UNCERTAINTY

Uncertainty of measurement is inevitable; therefore, measurements should be accompanied by a statement of their uncertainty for completeness (JCGM 2008; Taylor 1997). To do so, it is imperative to identify all sources of measurement uncertainty related to the quantity being measured. Quantifying the uncertainty of TIS measurements will provide a measure of the reliability and applicability of individual measurements and TIS data products. This portion of the document serves to identify, evaluate, and quantify sources of uncertainty relating to individual, calibrated soil CO_2 concentration measurements as well as L1 mean data products. It is a reflection of the information described in AD[13], and is explicitly described for the soil CO_2 assembly in the following sections.

7.1.1 Measurement Uncertainty

The following subsections present the uncertainties associated with *individual 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[13] 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

$x_i \ (i = 1, \dots, n),\ i.e., y = f(x_1, x_2, \dots, x_n)$, the combined measurement uncertainty of *y*, assuming the inputs are independent, can be calculated as follows:

$$u_c(y) = \left(\sum_{i=1}^{N} \left(\frac{\partial f}{\partial x_i} \right)^2 u^2(x_i) \right)^{\frac{1}{2}} \quad (19)$$

where

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

$u(x_i)$ = combined standard uncertainty of x_i.

Thus, the uncertainty of the measurand can be found be summing the input uncertainties in quadrature. The calculation of these input uncertainties is discussed below.

7.1.1.1 Combined Measurement Uncertainty

Until further notice, an average, relative, uncertainty estimate will be used for all calibrated, soil CO_2 measurements. This uncertainty comprises the uncertainties of all the input variables: raw CO_2, soil temperature, pressure at soil surface, oxygen content, relative humidity, and calibration uncertainty, and is a result of a sensitivity analysis of over 38,000 scenarios where the input variables were altered on each scenario run. This uncertainty is 0.007 (unitless).

The combined, standard, measurement uncertainty resulting from the aforementioned uncertainties above is calculated as follows:

$$u_C(C_i) = 0.007 * C_i \tag{20}$$

7.1.1.2 Expanded Measurement Uncertainty

The expanded measurement uncertainty is calculated as:

$$U_{95}(C_i) = k_{95} * u_c(C_i) \tag{21}$$

Where:

$U_{95}(C_i)$ = expanded measurement uncertainty at 95% confidence (ppm)

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

7.1.2 Uncertainty of L1 Mean Data Product

The following subsections discuss uncertainties associated with temporally averaged, i.e., L1 mean, data products. As stated previously, it is important to note the differences between the *measurement uncertainties* presented in Section 6.1.1 and the uncertainties presented in the following subsections. The uncertainties presented in the following subsections reflect the uncertainty of a time-averaged mean value; that is, they reflect the uncertainty of a distribution of measurements collected under non-controlled conditions (i.e., those found in the field), as well as any uncertainties, in the form of *Truth* and *Trueness*, related to the accuracy of the field assembly.

7.1.2.1 Repeatability (natural variation)

To determine the validity of the L1 mean soil CO_2 DP, its uncertainty must be calculated. The distribution of the individual measurements is used as metric to quantify this uncertainty. Specifically, the *estimated standard error of the mean (natural variation)* is computed. This value reflects the repeatability of insolation measurements for a specified time period:

$$u_{NAT}(\bar{C}) = \frac{s(C_i)}{\sqrt{n}} \tag{22}$$

Where,

$u_{NAT}(\bar{C})$ = standard error of the mean (natural variation) (ppm)

$s(C_i)$ = experimental standard deviation of individual observations for the defined time period (ppm)

n = number of observations made during the defined time period. (unitless)

7.1.2.2 Combined Uncertainty

The combined uncertainty for our L1 mean soil CO_2 data product, $u_c(\bar{C})$, given in units of ppm, is computed by summing the uncertainties from Sections 6.1.2.1 through 6.1.2.3 in quadrature:

$$u_c(\bar{C}) = \left(u_{NAT}^2(\bar{C}) + u_C^2(C_i)\right)^{\frac{1}{2}} \tag{23}$$

7.1.2.3 Expanded Uncertainty

The expanded uncertainty is calculated as:

$$U_{95}(\bar{C}) = k_{95} * u_c(\bar{C}) \tag{24}$$

Where:

$U_{95}(\bar{C})$ = expanded L1 mean data product uncertainty at 95% confidence (ppm)

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

7.1.2.4 Communicated Precision

In-house calibrations completed by NEON's CVAL revealed that the repeatability of soil CO_2 concentration measurements is significant to 0.845% of the measurement. As such, the communicated precision of L1, mean, CO_2 concentration data will be 0.845% of the measurement.

7.1.3 Uncertainty Budget

The uncertainty budget is a visual aid detailing i) quantifiable sources of uncertainty, ii) means by which they are derived, and iii) the order of their propagation. Uncertainty values denoted in this budget are either derived within this document or are provided by other NEON teams (e.g., CVAL), and stored in the CI data store.

Table 6-1: Uncertainty budget for an individual soil CO_2 measurement. Shaded rows denote the order of uncertainty propagation (from lightest to darkest).

Source of measurement uncertainty	**Measurement uncertainty component $u(x_i)$**	**Measurement uncertainty value**	$\frac{\partial f}{\partial x_i}$	$u_{x_i}(Y) \equiv \left\lvert\frac{\partial f}{\partial x_i}\right\rvert u(x_i)$ $[\mu mol\ m^{-2}\ s^{-1}]$
0.11 Hz soil CO_2	$u_c(C_i)$	Eq. (20) $[ppm]$	n/a	n/a

Table 6-2: Uncertainty budget for L1 mean soil CO_2 measurements. Shaded rows denote the order of uncertainty propagation (from lightest to darkest).

Source of uncertainty	**Uncertainty component $u(x_i)$**	**Uncertainty value**	$\frac{\partial f}{\partial x_i}$	$u_{x_i}(Y) \equiv \left\lvert\frac{\partial f}{\partial x_i}\right\rvert u(x_i)$ $[\mu mol\ m^{-2}\ s^{-1}]$
L1 mean soil CO_2	$u_c(\bar{C})$	Eq. (23) $[ppm]$	n/a	n/a
Natural variation	$u_{NAT}(\bar{C})$	Eq. (22) $[ppm]$	1	Eq. (22)
0.1 Hz soil CO_2	$u_c(C_i)$	Eq. (20) $[ppm]$	1	Eq. (20)

8 FUTURE PLANS AND MODIFICATIONS

The value of the relative humidity and oxygen parameter may be changed to a site- and/or depth-specific value, or even a dynamic value, if additional information on these soil air parameters becomes available in the future.

The threshold for the soil temperature QA/QC test may be updated to a site- and/or depth-specific value. In addition, the temperature test may be updated to use data from the soil temperature sensor that has the closest depth to soil CO_2 sensor, or even interpolated soil temperature at the same depth as the CO_2 sensor if that becomes available.

When atmospheric pressure with a final quality flag of 0 is unavailable, a time threshold may be added specify whether the most recent pressure reading with a final quality flag of 0 should be used. For example, use the most recent pressure reading with a final quality flag of 0 if this is less than 24 hours old; otherwise use X (where X is average site-specific pressure).

A correction for the response time for the sensor assembly may be added to account for the lag time needed for CO_2 in soil air to diffuse into the sensor assembly.

Future system flags may be incorporated into the data stream and included in the QA/QC summary. For example, a consistency test may be added to compare CO_2 concentrations at different depths within a soil plot and at the same depth among plots within each site.

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

Dynamic uncertainty estimates will be generated once autocorrelation and Monte Carlo frameworks are set up in the Docker environment.

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