NEON ALGORITHM THEORETICAL BASIS DOCUMENT (ATBD): TIS SOIL WATER CONTENT AND WATER SALINITY

PREPARED BY	ORGANIZATION	DATE
Edward Ayres	FIU	09/15/2016
Josh Roberti	FIU	09/15/2016

APPROVALS	ORGANIZATION	APPROVAL DATE
Kate Thibault	SCI	04/20/2022

RELEASED BY	ORGANIZATION	RELEASE DATE
Tanisha Waters	CM	04/20/2022

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Change Record

REVISION	DATE	ECO #	DESCRIPTION OF CHANGE
A	10/28/2016	ECO-04217	Initial release
B	11/15/2017	ECO-05214	Added soil water content measurement precision
C	01/24/2018	ECO-05386	Added Valid calibration, Science review, and Signal Despiking and Time Series Analysis flag to table of QA/QC flags associated with this data product.
D	04/20/2022	ECO-06809	• Update to reflect change in terminology from relocatable to gradient sites • Added NEON to document title

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1 DESCRIPTION

Contained in this document are details concerning soil water content and salinity 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 water content and water salinity will be ascertained by deploying sensors across a range of depths in the TIS soil plots at each NEON terrestrial site.

1.1 Purpose

This document details the algorithms used for creating NEON Level 1 data products for soil water content and water salinity from Level 0 data, and ancillary data as defined in this document (such as calibration data) obtained via instrumental measurements made by the soil water content and water salinity 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 water content and water salinity is described in this document. The soil water content and water salinity sensor employed is the Sentek TriSCAN. 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.011081	ATBD QA/QC Plausibility Tests
AD[06]	NEON.DOC.000783	ATBD De-spiking and Time Series Analyses
AD[07]	NEON.DOC.000746	Calibration Fixture and Sensor Uncertainty Analysis (CVAL)
AD[08]	NEON.DOC.000785	TIS Level 1 Data Products Uncertainty Budget Estimation Plan
AD[09]	NEON.DOC.000927	NEON Calibration and Sensor Uncertainty Values [1]
AD[10]	NEON.DOC.001113	Quality Flags and Quality Metrics for TIS Data Products
AD[11]	NEON.DOC.000746	Evaluating Uncertainty (CVAL)
AD[12]	NEON.DOC.001084	Soil Moisture Profile Normalization Fixture L1W300
AD[13]	NEON.DOC.000785	TIS Level 1 Data Products Uncertainty Budget Estimation Plan
AD[14]	NEON.DOC.000927	NEON Calibration and Sensor Uncertainty Values (CVAL)
AD[15]	NEON.DOC.001571	NEON Algorithm Theoretical Basis Document – Soil Temperature
AD[16]	TBD	Soil Moisture Sensor Calibration Procedure
AD[17]	NEON.DOC.000613	C^3 Soil Water Content Profile
AD[18]	NEON.DOC.003146	Soil Sensor Depth Selection
AD[19]		NEON Data Publication Workbook for TIS Soil Water Content and Water Salinity

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

2.2 Reference Documents

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

2.3 Acronyms

Acronym	Explanation
AIS	Aquatic Instrument System
ATBD	Algorithm Theoretical Basis Document
CI	NEON Cyberinfrastructure
CVAL	NEON Calibration, Validation, and Audit Laboratory
DAS	Data Acquisition System
DP	Data Product

FDAS	Field Data Acquisition System
GRAPE	Grouped Remote Analog Peripheral Equipment
Hz	Hertz
L0	Level 0
L1	Level 1
PRT	Platinum resistance thermometer
QA/QC	Quality assurance and quality control

2.4 Variable Nomenclature

The symbols used to display the various inputs in the ATBD, e.g., calibration coefficients and uncertainty estimates, were chosen so that the equations can be easily interpreted by the reader. However, the symbols provided will not always reflect NEON's internal notation, which is relevant for CI's use, and/or the notation that is used to present variables on NEON's data portal. Therefore a lookup table is provided in order to distinguish what symbols specific variables can be tied to in the following document.

Prior to July 2016, the CVAL xml files for the soil water content sensors were sometimes missing calibration coefficients CVALA1, CVALA2, and CVALA3, while the uncertainty coefficients (U_CVALA1 and U_CVALA3) were set to 0 as the true values were unknown at that time. In these cases, CVALA1, CVALA2, and CVALA3 shall be set to the manufacturer default values (Sentek 2011), and the uncertainty coefficients shall be set to the values shown in the table below, which assume that the sensor was using the default manufacturer calibration coefficients. This will allow the algorithms in this document to process data from sensors that were deployed with older xml files.

Symbol	**Internal Notation**	**Description**
C_1	CVALA1	Soil water content calibration coefficient A from the CVAL water content xml file. If not present in CVAL xml set it to 0.1957 (Sentek 2011).
C_2	CVALA2	Soil water content calibration coefficient B from the CVAL water content xml file. If not present in CVAL xml set it to 0.404 (Sentek 2011).
C_3	CVALA3	Soil water content calibration coefficient C from the CVAL water content xml file. If not present in CVAL xml set it to 0.02852 (Sentek 2011).
u_{A1}	U_CVALA1	Combined uncertainty soil moisture from the CVAL water content xml file. If U_CVALA1 = 0 in CVAL xml set it to 0.1068177.
u_{A3}	U_CVALA3	Combined uncertainty (truth and trueness *only*) soil moisture from the CVAL water content xml file. If U_CVALA3 = 0 in CVAL xml set it to 0.1067726.

3 DATA PRODUCT DESCRIPTION

3.1 Variables Reported

The soil water content and water salinity-related L1 DPs provided by the algorithms documented in this ATBD are displayed in the accompanying file AD[19]. Note that soil water content is sometimes referred to as moisture, while salinity is sometimes referred to as ion content.

3.2 Input Dependencies

Table 1 details the DPs used to produce soil water content and salinity-related L1 DPs in this ATBD. Note that depending on soil depth at the site, the number of sensors in the depth profile may be less than the number shown in **Table 1**.

Table 1. List of DPs used to produce Soil Water Content and Water Salinity-related L1 DPs via this ATBD.

Description	Sample Frequency	Units	Data Product Number
Volumetric soil water content (θ) from shallowest depth	0.1 Hz	%	NEON.DOM.SITE.DP0.00094.001.02081.HOR.501.000
Soil volumetric water ion content (S) from shallowest depth	0.1 Hz	Unitless	NEON.DOM.SITE.DP0.00094.001.02082.HOR.501.000
Volumetric soil water content (θ) from 2nd shallowest depth	0.1 Hz	%	NEON.DOM.SITE.DP0.00094.001.02083.HOR.501.000
Soil volumetric water ion content (S) from 2nd shallowest depth	0.1 Hz	Unitless	NEON.DOM.SITE.DP0.00094.001.02084.HOR.501.000
Volumetric soil water content (θ) from 3rd shallowest depth	0.1 Hz	%	NEON.DOM.SITE.DP0.00094.001.02085.HOR.501.000
Soil volumetric water ion content (S) from 3rd shallowest depth	0.1 Hz	Unitless	NEON.DOM.SITE.DP0.00094.001.02086.HOR.501.000
Volumetric soil water content (θ) from 4th shallowest depth	0.1 Hz	%	NEON.DOM.SITE.DP0.00094.001.02087.HOR.501.000
Soil volumetric water ion content (S) from 4th shallowest depth	0.1 Hz	Unitless	NEON.DOM.SITE.DP0.00094.001.02088.HOR.501.000
Volumetric soil water content (θ) from 5th shallowest depth	0.1 Hz	%	NEON.DOM.SITE.DP0.00094.001.02089.HOR.501.000
Soil volumetric water ion content (S) from 5th shallowest depth	0.1 Hz	Unitless	NEON.DOM.SITE.DP0.00094.001.02090.HOR.501.000
Volumetric soil water content (θ) from 6th shallowest depth	0.1 Hz	%	NEON.DOM.SITE.DP0.00094.001.02091.HOR.501.000
Soil volumetric water ion content (S) from 6th shallowest depth	0.1 Hz	Unitless	NEON.DOM.SITE.DP0.00094.001.02092.HOR.501.000

Description	Sample Frequency	Units	Data Product Number
Volumetric soil water content (θ) from 7th shallowest depth	0.1 Hz	%	NEON.DOM.SITE.DP0.00094.001.02093.HOR.501.000
Soil volumetric water ion content (S) from 7th shallowest depth	0.1 Hz	Unitless	NEON.DOM.SITE.DP0.00094.001.02094.HOR.501.000
Volumetric soil water content (θ) from 8th shallowest depth	0.1 Hz	%	NEON.DOM.SITE.DP0.00094.001.02095.HOR.501.000
Soil volumetric water ion content (S) from 8th shallowest depth	0.1 Hz	Unitless	NEON.DOM.SITE.DP0.00094.001.02096.HOR.501.000
Soil temperature	1-min	°C	NEON.DOM.SITE.DP1.00041.001.00933.HOR.VER.001
Soil temperature expanded uncertainty	1-min	°C	NEON.DOM.SITE.DP1.00041.001.00938.HOR.VER.001
Soil temperature final quality flag	1-min	Unitless	NEON.DOM.SITE.DP1.00041.001.00314.HOR.VER.001

The level 0 data products shall be converted to their corresponding Level 1 Data Products as shown in **Table 2**.

Table 2. Corresponding Level 0 and Level 1 soil water content and water salinity data products.

Level 0 Data Product	Level 1 Data Product
NEON.DOM.SITE.DP0.00094.001.02081.HOR.501.000	NEON.DOM.SITE.DP1.00094.001.01005.HOR.501.TMI
NEON.DOM.SITE.DP0.00094.001.02082.HOR.501.000	NEON.DOM.SITE.DP1.00094.001.01045.HOR.501.TMI
NEON.DOM.SITE.DP0.00094.001.02083.HOR.501.000	NEON.DOM.SITE.DP1.00094.001.01005.HOR.502.TMI
NEON.DOM.SITE.DP0.00094.001.02084.HOR.501.000	NEON.DOM.SITE.DP1.00094.001.01045.HOR.502.TMI
NEON.DOM.SITE.DP0.00094.001.02085.HOR.501.000	NEON.DOM.SITE.DP1.00094.001.01005.HOR.503.TMI
NEON.DOM.SITE.DP0.00094.001.02086.HOR.501.000	NEON.DOM.SITE.DP1.00094.001.01045.HOR.503.TMI
NEON.DOM.SITE.DP0.00094.001.02087.HOR.501.000	NEON.DOM.SITE.DP1.00094.001.01005.HOR.504.TMI
NEON.DOM.SITE.DP0.00094.001.02088.HOR.501.000	NEON.DOM.SITE.DP1.00094.001.01045.HOR.504.TMI
NEON.DOM.SITE.DP0.00094.001.02089.HOR.501.000	NEON.DOM.SITE.DP1.00094.001.01005.HOR.505.TMI
NEON.DOM.SITE.DP0.00094.001.02090.HOR.501.000	NEON.DOM.SITE.DP1.00094.001.01045.HOR.505.TMI
NEON.DOM.SITE.DP0.00094.001.02091.HOR.501.000	NEON.DOM.SITE.DP1.00094.001.01005.HOR.506.TMI
NEON.DOM.SITE.DP0.00094.001.02092.HOR.501.000	NEON.DOM.SITE.DP1.00094.001.01045.HOR.506.TMI
NEON.DOM.SITE.DP0.00094.001.02093.HOR.501.000	NEON.DOM.SITE.DP1.00094.001.01005.HOR.507.TMI
NEON.DOM.SITE.DP0.00094.001.02094.HOR.501.000	NEON.DOM.SITE.DP1.00094.001.01045.HOR.507.TMI
NEON.DOM.SITE.DP0.00094.001.02095.HOR.501.000	NEON.DOM.SITE.DP1.00094.001.01005.HOR.508.TMI
NEON.DOM.SITE.DP0.00094.001.02096.HOR.501.000	NEON.DOM.SITE.DP1.00094.001.01045.HOR.508.TMI

3.3 Product Instances

Soil water content and water salinity sensors will be deployed at multiple depths in each of the 5 soil plots at every NEON core and gradient sites. The number of sensors deployed at a site may vary depending on site-specific soil properties.

3.4 Temporal Resolution and Extent

One- and thirty-minute averages of soil water content and water salinity will be calculated to form L1 DPs.

3.5 Spatial Resolution and Extent

According to the manufacturer specifications the soil water content and water salinity sensor integrates over 10 cm vertically (i.e., 5 cm above and below the mid-point of the sensor) and 14 cm horizontally from the outer edge of the sensor tube, but is more sensitive to the soil immediately surrounding the sensor location (Sentek 2011).

4 SCIENTIFIC CONTEXT - SOIL WATER CONTENT

Soil water content is a key meteorological and ecological variable and is the primary determinant of water availability to plants and soil organisms. Prolonged very low soil water contents typically reduce primary production and biological activity in the soil due to water stress, while very high soil water contents reduce biological activity in the soil due to a reduction in oxygen supply. Soil water content also influences the severity of heat waves due to the water's high latent heat of vaporization. As a result, NEON's soil water content measurements will be useful when interpreting changes in other environmental measurements.

4.1 Theory of Measurement

The Sentek TriSCAN is a capacitance-type sensor (also known as a frequency domain reflectometry sensor, FDR). According to Evett and Cepuder (2008), "The common characteristics of this type of sensor include the use of a capacitor consisting of two hollow cylindrical metal electrodes arranged coaxially but separated by several millimeters with an insulating plastic, and the use of an electronic oscillator that produces a sinusoidal waveform. The capacitor forms part of the oscillating circuit, and the electrodes are arranged so as to be very close to the inside of the access tube, the idea being that the fringing field of the capacitor will interact with the soil outside of the tube such that the capacitance is influenced by the soil bulk electrical permittivity and thus by soil water content. In any of these systems, the frequency of oscillation decreases as soil water content increases."

The electronic oscillator in the Sentek TriSCAN produces waveforms at two different frequencies. Measurements at one frequency result in a raw count, which is internally normalized by the sensor against measurements made when the sensor was surrounded by air and water (AD[12]) and then converted to volumetric water content using the user-defined calibration equation (Sentek 2003). Note that a study of Sentek EnviroSCAN sensors, which use similar technology to the TriSCAN sensors, found that the normalization values have a small temperature dependency that resulted in a volumetric water content error of approximately 0.005 cm^3 cm^{-3} for every 10 °C difference in the temperature in the field versus the temperature at which the sensor was normalized (Paltineanu and Starr 1997).

The Senteks used throughout the NEON Observatory undergo site- and depth-specific calibrations. Resulting, soil-specific calibration coefficients are programmed into the Sentek sensors prior to field deployment, and because of this, individual moisture and salinity measurements output by the sensor are considered calibrated. When the site- and depth-specific calibration coefficients are not available prior to deployment of a sensor, the manufacturer default calibration coefficients are loaded into the sensor, which results in greater measurement uncertainty.

The TriSCAN sensor uses an internal proprietary algorithm to convert the data generated from both measurement frequencies to the volumetric ion content measurement, which is an index of soil salinity (Sentek 2003). The TriSCAN volumetric ion content measurements are only supported by the manufacturer for soil with a salinity of 0-17 dSm^{-1} (deci Siemens per meter) and a texture class of sand, loamy sand, and sandy loam as defined in the Australian Soil and Land Survey Field Handbook (Sentek 2003). Note that the manufacturer states that "there is minor positive relationship between [volumetric ion content] and soil temperature", which is not currently accounted for by the sensor (Sentek 2003).

The Sentek TriSCAN sensor, like most soil water content sensors, is unable to measure water content when the water is frozen. Since the water content measurement is needed to calculate the volumetric ion content, neither data products will be produced when soil water is likely to be frozen.

Additional information about the sensor can be found in Buss et al. (2004).

4.2 Theory of Algorithm

The sensor reports volumetric soil water content in percent units ($\theta_{\%}$). These values are derived internally by the sensor but do not account for the effect of temperature on the normalization values (Paltineanu and Starr 1997).

To convert volumetric water content in percent units ($\theta_{\%}$) to volumetric water content in cm^3 cm^{-3} units ($\theta_{\mathrm{cm3\ cm-3}}$) the following equation is used:

$$\theta_{\mathrm{cm3\ cm-3}\,i} = \frac{\theta_{\%\,i}}{100} \tag{1}$$

One-minute ($\bar{\theta}_1$) and thirty-minute ($\bar{\theta}_{30}$) averages of volumetric soil water content will be determined as follows to create the L1 DPs listed in AD[19].

$$\bar{\theta}_1 = \frac{1}{n}\sum_{i=1}^{n} \theta_{\mathrm{cm3\ cm-3}\,i} \tag{2}$$

where, for each 1-minute average, n is the number of measurements during the averaging period and $\theta_{\mathrm{cm3\ cm-3}\,i}$ is a 0.1 Hz volumetric water content during the 60-second averaging period (0, 60).

And

$$\bar{\theta}_{30} = \frac{1}{n}\sum_{i=1}^{n} \theta_{\mathrm{cm3\ cm-3}\,i} \tag{3}$$

where, for each 30-minute average, n is the number of measurements during the averaging period and $\theta_{\mathrm{cm3\ cm-3}\,i}$ is a 0.1 Hz volumetric water content during the 1800-second averaging period (0, 1800).

5 ALGORITHM IMPLEMENTATION – SOIL WATER CONTENT

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

1. The temperature from the soil temperature sensor that is closest to the depth of the soil water content and water salinity sensor and in the same soil plot will be used to determine if the soil water content data product needs to be calculated.
2. QA/QC Plausibility tests will be applied to the data stream in accordance with AD[05]. The details are provided below.
3. Signal de-spiking and time series analysis will be applied to the data stream in accordance with AD[06].
4. The calibration coefficients used by the sensor to calculate the volumetric soil water content will be checked to determine whether the manufacturer default or the site- and depth-specific calibration coefficients were used. This information will be used to determine the default calibration flag setting.
5. One- and thirty-minute averages will be calculated using Eq. (2) and (3).
6. Descriptive statistics, i.e. minimum, maximum, and variance, will be determined for both one- and thirty-minute averages.
7. Quality metrics, quality flags, and the final quality flag will be produced for one- and thirty-minute averages according to AD[10].

<u>**QA/QC Procedure**</u>:

1. **Temperature test** – If the 1-minute averaged soil temperature (T, NEON.DOM.SITE.DP1.00041.001.00933.HOR.VER.001) from the sensor closest to the depth of and in the same soil plot as the soil moisture and salinity sensor is $\leq U_{95}(T)$ °C for any soil water content measurement within the averaging period, the Level 1 soil water content data product shall not be calculated. $U_{95}(T)$ is defined as the Level 1 1-minute soil temperature expanded uncertainty (NEON.DOM.SITE.DP1.00041.001.00938.HOR.VER.001) from the same soil temperature sensor at the corresponding time. If the temperature is $> U_{95}(T)$ °C or the temperature data are not available, the L1 soil water content data product shall be calculated. This test will be applied to every L0 datum and an associated flag of:
   - 0 will be generated when the soil temperature is $> U_{95}(T)$ °C,
   - 1 will be generated when the soil temperature is $\leq U_{95}(T)$ °C, and
   - -1 will be generated when the soil temperature is not available and/or the soil temperature final quality flag (QF_T, NEON.DOM.SITE.DP1.00041.001.00314.HOR.VER.001) equals 1.

The logic for the temperature test is summarized in **Table 3**.

Table 3. Summary of temperature test logic.

Soil Temperature parameters	Level 1 soil water content & water salinity data product	Soil water content & water salinity temperature flag setting	Soil water content & water salinity final quality flag setting
n = 1 (i.e., data present) $T > U_{95}(T)$ QF_T = 0	Calculate	0	0
n = 1 (i.e., data present) $T \leq U_{95}(T)$ QF_T = 0	Don't calculate	1	0
n = 0 (i.e., missing data)	Calculate	-1	1
QF_T = 1	Calculate	-1	1

At most NEON sites and soil plots there will be a soil temperature sensor installed at the same depth as each soil water content and salinity sensor (AD[18]). However, the installation depths of soil temperature and soil water content and salinity sensors may differ if an obstacle (e.g., boulder) was encountered during the installation of one or both profiles. Since the installation depths for the temperature and water content sensors were not known for all soil plots at the time of writing, the data products that will be used for the temperature QA/QC test were specified based on the vertical index (**Table 4**). In most cases this will result in soil temperature measurements from the same depth as the soil water content and salinity sensor being used for the temperature test, however, there are likely to be a few exceptions where the temperature sensor will be at a different depth.

Table 4. Soil temperature data products that will be used for the temperature QA/QC test. Assumes "DOM", "SITE", and "HOR" are identical within each row.

Soil water content data product	Soil salinity data product	1-minute averaged soil temperature data product	1-minute soil temperature expanded uncertainty	1-minute soil temperature final quality flag
NEON.DOM.SITE.DP0.00094.001.02081.HOR.VER.000	NEON.DOM.SITE.DP0.00094.001.02082.HOR.VER.000	NEON.DOM.SITE.DP1.00041.001.00933.HOR.502.001	NEON.DOM.SITE.DP1.00041.001.00938.HOR.502.001	NEON.DOM.SITE.DP1.00041.001.00314.HOR.502.001
NEON.DOM.SITE.DP0.00094.001.02083.HOR.VER.000	NEON.DOM.SITE.DP0.00094.001.02084.HOR.VER.000	NEON.DOM.SITE.DP1.00041.001.00933.HOR.503.001	NEON.DOM.SITE.DP1.00041.001.00938.HOR.503.001	NEON.DOM.SITE.DP1.00041.001.00314.HOR.503.001
NEON.DOM.SITE.DP0.00094.001.02085.HOR.VER.000	NEON.DOM.SITE.DP0.00094.001.02086.HOR.VER.000	NEON.DOM.SITE.DP1.00041.001.00933.HOR.504.001	NEON.DOM.SITE.DP1.00041.001.00938.HOR.504.001	NEON.DOM.SITE.DP1.00041.001.00314.HOR.504.001

NEON.DOM.SITE.DP0.00094.001.02087.HOR.VER.000	NEON.DOM.SITE.DP0.00094.001.02088.HOR.VER.000	NEON.DOM.SITE.DP1.00041.001.00933.HOR.505.001	NEON.DOM.SITE.DP1.00041.001.00938.HOR.505.001	NEON.DOM.SITE.DP1.00041.001.00314.HOR.505.001
NEON.DOM.SITE.DP0.00094.001.02089.HOR.VER.000	NEON.DOM.SITE.DP0.00094.001.02090.HOR.VER.000	NEON.DOM.SITE.DP1.00041.001.00933.HOR.506.001	NEON.DOM.SITE.DP1.00041.001.00938.HOR.506.001	NEON.DOM.SITE.DP1.00041.001.00314.HOR.506.001
NEON.DOM.SITE.DP0.00094.001.02091.HOR.VER.000	NEON.DOM.SITE.DP0.00094.001.02092.HOR.VER.000	NEON.DOM.SITE.DP1.00041.001.00933.HOR.507.001	NEON.DOM.SITE.DP1.00041.001.00938.HOR.507.001	NEON.DOM.SITE.DP1.00041.001.00314.HOR.507.001
NEON.DOM.SITE.DP0.00094.001.02093.HOR.VER.000	NEON.DOM.SITE.DP0.00094.001.02094.HOR.VER.000	NEON.DOM.SITE.DP1.00041.001.00933.HOR.508.001	NEON.DOM.SITE.DP1.00041.001.00938.HOR.508.001	NEON.DOM.SITE.DP1.00041.001.00314.HOR.508.001
NEON.DOM.SITE.DP0.00094.001.02095.HOR.VER.000	NEON.DOM.SITE.DP0.00094.001.02096.HOR.VER.000	NEON.DOM.SITE.DP1.00041.001.00933.HOR.509.001	NEON.DOM.SITE.DP1.00041.001.00938.HOR.509.001	NEON.DOM.SITE.DP1.00041.001.00314.HOR.509.001

2. **Plausibility Tests** AD[11] – All plausibility tests will be determined for soil water content. Test parameters will be provided by FIU and maintained in the CI data store. All plausibility tests will be applied to the sensor's converted L0 DP and an associated pass/fail flag will be generated for each test.

3. **Signal De-spiking** – The de-spiking QA/QC routine will be run on defined time segments of data, as specified by FIU and maintained in the CI data store. Utilizing the median absolute deviation for a segment of data, the routine will identify and disregard large spikes from the timeseries. For data values that are "de-spiked" a de-spiking flag will be applied according to AD[06].

4. **Default calibration test** – If C_1, C_2, and C_3 are 0.1957, 0.404, and 0.02852, respectively, for any datum in an averaging period, the default calibration flag for that averaging period shall be set to "1". If one or more of C_1, C_2, and C_3 are numbers that are not 0.1957, 0.404, and 0.02852, respectively, for any datum in an averaging period, the default calibration flag for that averaging period shall be set to "0". Values for C_1, C_2, and C_3 are found in the CVAL soil water content xml file, not in the soil water salinity xml file. Values for C_1, C_2, and C_3 for each soil water content data product are found in the CVAL soil water content xml file that corresponds to the same named location and the Stream ID shown in **Table 5**.

Table 5. Stream ID in the xml file used for the soil water salinity default calibration test.

Stream ID in CVAL xml file	Soil water content data product
0	NEON.DOM.SITE.DP0.00094.001.02081.HOR.VER.000
2	NEON.DOM.SITE.DP0.00094.001.02083.HOR.VER.000
4	NEON.DOM.SITE.DP0.00094.001.02085.HOR.VER.000

6	NEON.DOM.SITE.DP0.00094.001.02087.HOR.VER.000
8	NEON.DOM.SITE.DP0.00094.001.02089.HOR.VER.000
10	NEON.DOM.SITE.DP0.00094.001.02091.HOR.VER.000
12	NEON.DOM.SITE.DP0.00094.001.02093.HOR.VER.000
14	NEON.DOM.SITE.DP0.00094.001.02095.HOR.VER.000

4. **Quality Flags (QFs) and Quality Metrics (QMs)** AD[15] – If a datum has failed one of the following tests it will not be used to create a L1 DP, ***range, de-spiking, persistence***, or ***step*** or has a ***temperature*** flag set to "1". α and β QFs and QMs will be determined for all of the external flags, **Table 6**. In addition, L1 DPs will have a QA/QC report and quality metrics associated with each flag listed in **Table 6** as well as a final quality flag, as detailed in AD[10]. Ancillary information needed for the algorithm and other information maintained in the CI data store is shown in **Table 7**.
    1. **Final Quality: Soil water content** - The final quality flag for soil water content (i.e., VSWCFinalQF; NEON.DOM.SITE.DP1.00094.001.01044.HOR.VER.001 and NEON.DOM.SITE.DP1.00094.001.01044.HOR.VER.030) shall be set to 1 if any datum within the averaging period had a temperature test flag of -1 and/or a default calibration flag of 1, otherwise the final quality flag will be set according to the procedure defined in AD[10].

Table 6. Flags associated with soil water content measurements.

Tests
Temperature
Default calibration
Range
Persistence
Step
Null
Gap
Signal Despiking and Time Series Analysis
Valid calibration
Science review
Final quality flag

Table 7. Information maintained in the CI data store for the soil water content.

Tests/Values	**CI Data Store Contents**
Temperature	Temperature threshold
Range	Minimum and maximum values
Persistence	Window size, threshold values and maximum time length
Step	Threshold values
Null	Test limit
Gap	Test limit
Signal Despiking	Time segments and threshold values
Default calibration	CVAL and FIU sensor specific calibration coefficients
Uncertainty	AD[14]
Final Quality Flag	AD[10]

6 SCIENTIFIC CONTEXT - SOIL WATER SALINITY

Soil water salinity (i.e., ion content) can directly impact primary production and the activity of soil organisms. High soil water salinity can inhibit plant growth and the activity of soil organisms. In addition, soil water salinity can be indicative of soil nutrient availability (e.g., soil water ion content typically increases following the addition of inorganic fertilizers).

6.1 Theory of Measurement

See Theory of Measurement for soil water content measurements above.

6.2 Theory of Algorithm

The sensor reports a unitless volumetric ion content value (S_i). This value is calculated internally by the sensor, in part based on the sensor's soil water content measurement, using a proprietary algorithm that is not available to NEON. As a result, there is little additional processing that NEON can do. However, the measure provides a qualitative assessment of ion content (salinity) that can be tracked over time to observe changes at a particular location. Since the soil water salinity values cannot be converted to standard units, the data cannot easily be compared among sites.

One-minute ($\bar{S}_1$) and thirty-minute ($\bar{S}_{30}$) averages of soil water salinity will be determined as follows to create the L1 DPs listed in AD[19].

$$\bar{S}_1 = \frac{1}{n}\sum_{i=1}^{n} S_i \tag{4}$$

where, for each 1-minute average, n is the number of measurements during the averaging period and S_i is a 0.1-Hz temperature measurement taken during the 60-second averaging period [0, 60). For a 1-minute average, n = 6 if all data points are included.

and

$$\bar{S}_{30} = \frac{1}{n}\sum_{i=1}^{n} S_i \tag{5}$$

where, for each 30-minute average, n is the number of measurements during the averaging period and S_i is a 0.1-Hz measurement taken during the 1800-second averaging period [0, 1800).

7 ALGORITHM IMPLEMENTATION – SOIL WATER SALINITY

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

1. The temperature from the soil temperature sensor that is closest to the depth of the soil water content and soil water salinity sensor and in the same soil plot will be used to determine if the soil water content and water salinity data product needs to be calculated.
2. QA/QC Plausibility tests will be applied to the data stream in accordance with AD[05]. The details are provided below.
3. Signal de-spiking and time series analysis will be applied to the data stream in accordance with AD[06].
4. The calibration coefficients used by the sensor to calculate the volumetric soil water content will be checked to determine whether the manufacturer default or the site- and depth-specific calibration coefficients were used. This information will be used to determine the default calibration flag setting.
5. One- and thirty-minute soil water salinity averages will be calculated using Eq. (4) and (5).
6. Descriptive statistics, i.e. minimum, maximum, and variance, will be determined for both one- and thirty-minute averages.
7. Quality metrics, quality flags, and the final quality flag will be produced for one- and thirty-minute averages according to AD[10].

QA/QC Procedure:

1. **Temperature test** – If the 1-minute averaged, soil temperature (T, NEON.DOM.SITE.DP1.00041.001.00933.HOR.VER.001) from the sensor closest to the depth of and in the same soil plot as the soil moisture and salinity sensor is $\leq U_{95}(T)$ °C for any soil water content measurement within the averaging period, the Level 1 soil water salinity data product shall not be calculated. $U_{95}(T)$ is defined as the Level 1 1-minute soil temperature expanded uncertainty (NEON.DOM.SITE.DP1.00041.001.00938.HOR.VER.001) from the same soil temperature sensor at the corresponding time. If the temperature is $> U_{95}(T)$ °C or the temperature data are not available, the L1 soil water content and water salinity data product shall be calculated. This test will be applied to every L0 datum and an associated flag will be generated where 0 = the soil temperature is $> U_{95}(T)$ °C, 1 = the soil temperature is $\leq U_{95}(T)$ °C, and -1 = the soil temperature is not available and/or the soil temperature final quality flag (QF_T, NEON.DOM.SITE.DP1.00041.001.00314.HOR.VER.001) equaled 1. The logic for the temperature test is summarized in **Table 3**. The temperature data products to be used for this test are shown in **Table 4**.

2. **Plausibility Tests** AD[05] – All plausibility tests will be determined for soil water salinity. Test parameters will be provided by FIU and maintained in the CI data store. All plausibility tests will

be applied to the sensor's converted L0 DP and an associated pass/fail flag will be generated for each test.

3. **Signal De-spiking** – The de-spiking QA/QC routine will be run on defined time segments of data, as specified by FIU and maintained in the CI data store. Utilizing the median absolute deviation for a segment of data, the routine will identify and disregard large spikes from the timeseries. For data values that are "de-spiked" a de-spiking flag will be applied according to AD[06].

5. **Default calibration test** – If C_1, C_2, and C_3 are 0.1957, 0.404, and 0.02852, respectively, for any datum in an averaging period, the default calibration flag for that averaging period shall be set to "1". If one or more of C_1, C_2, and C_3 are numbers that are not 0.1957, 0.404, and 0.02852, respectively, for any datum in an averaging period, the default calibration flag for that averaging period shall be set to "0". Values for C_1, C_2, and C_3 for each soil water salinity data product are found in the CVAL soil water content xml file that corresponds to the same named location and the StreamID shown in **Table 8**.

Table 8. Stream ID in the xml file used for the soil water salinity default calibration test.

Stream ID in CVAL xml file	Soil water salinity data product
0	NEON.DOM.SITE.DP0.00094.001.02082.HOR.VER.000
2	NEON.DOM.SITE.DP0.00094.001.02084.HOR.VER.000
4	NEON.DOM.SITE.DP0.00094.001.02086.HOR.VER.000
6	NEON.DOM.SITE.DP0.00094.001.02088.HOR.VER.000
8	NEON.DOM.SITE.DP0.00094.001.02090.HOR.VER.000
10	NEON.DOM.SITE.DP0.00094.001.02092.HOR.VER.000
12	NEON.DOM.SITE.DP0.00094.001.02094.HOR.VER.000
14	NEON.DOM.SITE.DP0.00094.001.02096.HOR.VER.000

5. **Quality Flags (QFs) and Quality Metrics (QMs)** AD[10] – If a datum has failed one of the following tests it will not be used to create a L1 DP, ***range, de-spiking, persistence,*** or ***step*** or has a ***temperature*** flag set to "1". α and β QFs and QMs will be determined for all of the external flags, **Table 9**. In addition, L1 DPs will have a QA/QC report and quality metrics associated with each flag listed in **Table 9** as well as a final quality flag, as detailed in AD[10]. Ancillary information needed for the algorithm and other information maintained in the CI data store is shown in **Table 10**.
    a. **Final Quality: Soil water salinty** - The final quality flag for soil water salinity (i.e., VSICFinalQF; NEON.DOM.SITE.DP1.00094.001.01084.HOR.VER.001 and NEON.DOM.SITE.DP1.00094.001.01084.HOR.VER.030) shall be set to 1 if any datum within the averaging period had a temperature test flag of -1 and/or a default calibration flag of 1, otherwise the final quality flag will be set according to the procedure defined in AD[10].

Table 9. Flags associated with soil water salinity measurements.

Tests
Temperature
Default calibration
Range
Persistence
Step
Null
Gap
Signal Despiking and Time Series Analysis
Valid calibration
Science review
Final quality flag

Table 10. Information maintained in the CI data store for the soil water salinity.

Tests/Values	CI Data Store Contents
Temperature	Temperature threshold
Range	Minimum and maximum values
Persistence	Window size, threshold values and maximum time length
Step	Threshold values
Null	Test limit
Gap	Test limit
Signal Despiking	Time segments and threshold values
Default calibration	CVAL and FIU sensor specific calibration coefficients
Uncertainty	AD[14]
Final Quality Flag	AD[10]

8 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 water and salinity 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 water and salinity assembly in the following sections.

8.1 Uncertainty of Soil Water and Salinity Measurements

Uncertainty of the soil water and salinity assembly is broken down into two sections. The first details the sources of *measurement* uncertainty, i.e., those associated with *individual measurements*. The second discusses uncertainties associated with temporally averaged data products.

Regarding the salinity of soil, the internal algorithms of the Sentek TriSCAN are proprietary. Thus, we must assume that the manufacturer's specifications are an accurate and reliable source by which uncertainty of soil salinity is represented.

8.1.1 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 8.2. We urge the reader to refer to AD[10] 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

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

$$u_c(y) = \left(\sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i)\right)^{\frac{1}{2}} \quad (6)$$

where

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

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

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

8.1.2 Calibration

An outside laboratory will be calibrating volumetric soil water content measurements of the sensors to those derived from gravimetric soil water measurements. This calibration will result in the derivation of site-and depth-specific coefficients that will be programmed into each Sentek TriSCAN prior to field deployment. Identification and quantification of the uncertainties associated with these calibrations processes are detailed in AD[16].

Initially, many of the sensors will quantify volumetric water content using the manufacturer provided calibration coefficients. Because the manufacturer coefficients were derived using only three soil types (see Sentek (2011)), it is expected that the resulting volumetric water contents for many of the sites and depths will carry a great deal of uncertainty. To quantify these uncertainties, volumetric water content measurements derived from water weight and volumetric measurements of individual soil blocks collected throughout the Observatory (considered "truth") were compared to those derived by the Sentek calibration coefficients using the observed scaled moisture frequency. This was completed for 33 soil blocks comprising various soil horizons from many sites. The average of these calibration uncertainties was computed and applied to all soil moisture measurements that were computed using the manufacturer's coefficients.

Uncertainties associated with the calibration process propagate into a standard, combined measurement uncertainty. This combined uncertainty, u_{A1}, represents

i) the repeatability and reproducibility of the sensor and the lab DAS and
ii) uncertainty of the calibration procedures and coefficients. It is a constant value that will be applied to individual measurements soil water content measurements (that is, it does not vary with any specific sensor, DAS component, location, etc.).

A detailed summary of the calibration procedures and corresponding uncertainty estimates can be found in AD[16].

8.1.3 Field DAS

Sentek TriSCAN soil sensors have an internal Analog to Digital (A/D) converter and output data in digital form. Therefore, measurement noise introduced by the field DAS can be considered negligible (please refer to AD[13] for further explanation).

8.1.4 Combined Measurement Uncertainty

Soil Water Content:

The combined measurement uncertainty for the calibrated, volumetric soil water content is simply:

$$u_c(G_i) = u_{A1} \tag{7}$$

Soil Salinity:
The Sentek sensor uses proprietary algorithms to quantify soil salinity and the manufacturer does not provide a measurement uncertainty for salinity measurements. As such, the end-user should exercise caution when working with these data.

8.1.5 Expanded Measurement Uncertainty

The expanded measurement uncertainties are calculated as:

$$U_{95}(Y_i) = k_{95} \; * u_c(Y_i) \tag{8}$$

Where:

$U_{95}(Y_i)$ = expanded measurement uncertainty at 95% confidence
k_{95} = 2; coverage factor for 95% confidence (unitless)

8.2 Uncertainty of L1 Mean Data Product

The following subsections discuss uncertainties associated with L1 mean temperature data products. As stated previously, it is important to note the differences between the *measurement uncertainties* presented in Section 8.1.1 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.

8.2.1 Repeatability (natural variation)

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

$$u_{NAT}(\bar{X}) = \frac{s(X_i)}{\sqrt{n}} \tag{9}$$

where $s(X_i)$ is the experimental standard deviation of the soil water or salinity observations during the averaging period, and n represents the number of observations made over the same time period.

8.2.2 Calibration

Soil Moisture:

The uncertainty detailed here is similar to that described in Section 8.1.2. However, the relevant uncertainty for mean DPs, u_{A3}, does not consider individual sensor repeatability. This component of uncertainty estimates the uncertainty due to the accuracy of the measurements, a quantity which is not captured by the standard error (repeatability) of the mean. It is a constant value that will be applied to all L1 DPs.

Soil Salinity:

The manufacturer does not provide an uncertainty estimate of soil salinity measurements. The end-user should exercise caution when using these data, as the only metric of uncertainty provided is the standard error of the mean.

8.2.3 Combined Uncertainty

Soil Moisture:

$$u_c(\bar{G}) = \left(u_{A3}^2 + u_{NAT}^2(\bar{G})\right)^{\frac{1}{2}} \quad [\text{cm}^3 \text{ water cm}^{-3} \text{ soil}] \qquad (10)$$

Soil Salinity:

$$u_c(\bar{S}) = u_{NAT}(\bar{S}) \quad [\text{unitless}] \qquad (11)$$

8.2.4 Expanded Uncertainty

The expanded uncertainties are calculated as:

$$U_{95}(\bar{Y}) = \; k_{95} * u_c(\bar{Y}) \qquad (12)$$

Where:

$U_{95}(\bar{Y})$ = expanded uncertainty at 95% confidence

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

8.2.5 Communicated Precision

NEON calibrations revealed that the repeatability of soil water content measurements is significant to 0.000045 cm^3 cm^{-3}. As such, the communicated precision of L1, mean, soil water content data will be significant to four decimal places (i.e., 0.0001 cm^3 cm^{-3}).

8.3 Uncertainty Budget

The uncertainty budget is a visual aid detailing

i) quantifiable sources of uncertainty,
ii) ii) means by which they are derived, and
iii) 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 11. Uncertainty budget for individual soil water content and salinity measurements. Shaded rows denote the order of uncertainty propagation (from lightest to darkest).

Source of measurement uncertainty	**Measurement uncertainty component u(X_i)**	**Measurement uncertainty value**	$\frac{\partial f}{\partial x_i}$	$u_i(Y) \equiv \lvert c_i \rvert u(x_i)$ **[cm cm^{-3}]**
Soil $H_2$0 Content	$u_c(G)$	Eq. (7) [cm cm^{-3}]	n/a	n/a
Sensor/cal.	u_{A1}	AD[14] [cm cm^{-3}]	1	u_{A1}
Soil Salinity	n/a	n/a	n/a	n/a

Table 12. Uncertainty budget for L1 mean soil water content and salinity DPs. Shaded rows denote the order of uncertainty propagation (from lightest to darkest).

Source of uncertainty	**uncertainty component u(X_i)**	**Uncertainty value [cm cm^{-3}]**	$\frac{\partial f}{\partial x_i}$	$u_i(Y) \equiv \lvert c_i \rvert u(x_i)$ **[cm cm^{-3}]**
Soil $H_2$0 Content	$u_c(\bar{G})$	Eq. (10)	n/a	n/a
Natural variation	$u_{NAT}(\bar{G})$	Eq. (9)	1	$u_{NAT}(\bar{G})$
Sensor/cal.	u_{A3}	AD[14]	1	u_{A3}
Soil Salinity	$u_c(\bar{S})$	Eq. (9)	1	n/a

9 FUTURE PLANS AND MODIFICATIONS

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 soil water content profile measurements as an additional quality control check on the data.

Once depth information becomes available for the soil water content and soil temperature data products the default calibration test may be altered to use soil temperature data from the nearest temperature sensor or a soil temperature interpolation, rather than relying on the vertical index of the data product.

If a future experiment demonstrates a significant temperature effect on the normalization values of the TriSCAN sensor (i.e., similar to Paltineanu and Starr 1997) a correction may be added to account for the difference between the normalization temperature and the temperature in the field.

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

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