NEON USER GUIDE TO STABLE ISOTOPES IN PRECIPITATION (DP1.00038.001)

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CHANGE RECORD

REVISION	DATE	DESCRIPTION OF CHANGE
A	07/26/2017	Initial Release
B	07/06/2020	Included general statement about usage of neonUtilities R package and statement about possible location changes
C	03/16/2022	Updated section 4.3 Data Revision with latest information regarding data release
D	10/06/2022	Updated information pertaining to laboratory quality assurance and uncertainty, added sampling design changes
E	04/17/2025	Added information about the new neonUtilities Python package.
F	03/03/2026	Updated information about data quality analysis and the suspension of the data product.

TABLE OF CONTENTS

LIST OF TABLES AND FIGURES

1 DESCRIPTION

1.1 Purpose

This document provides an overview of the data included in this NEON Level 1 data product, the quality controlled product generated from raw Level 0 data, and associated metadata. In the NEON data products framework, the raw data collected in the field, for example, the dry weights of litter functional groups from a single collection event are considered the lowest level (Level 0). Raw data that have been quality checked via the steps detailed herein, as well as simple metrics that emerge from the raw data are considered Level 1 data products.

The text herein provides a discussion of measurement theory and implementation, data product provenance, quality assurance and control methods used, and approximations and/or assumptions made during L1 data creation.

1.2 Scope

This document describes the steps needed to generate the L1 data product Stable Isotopes in Precipitation - the isotopic ratios of deuterium and oxygen-18 in precipitation - and associated metadata from input data. This document also provides details relevant to the publication of the data products via the NEON data portal, with additional detail available in the file, NEON Data Variables for Stable Isotopes in Precipitation (DP1.00038.001) (AD[05]), provided in the download package for this data product.

This document describes the process for ingesting and performing automated quality assurance and control procedures on the data collected in the field pertaining to NEON Preventative Maintenance Procedure: Wet Deposition Collector (AD[05]). The raw data that are processed in this document are detailed in the files NEON Raw Field Data Ingest Workbook for Wet Deposition Chemical Analysis (DP0.00018.001) (AD[03]) and NEON Raw Laboratory Data Ingest Workbook for Stable Isotopes in Precipitation (DP0.20205.001) (AD[04]), provided in the download package for this data product. Please note that raw data products (denoted by ‘DP0’) may not always have the same numbers (e.g., ‘10033’) as the corresponding L1 data product.

2 RELATED DOCUMENTS AND ACRONYMS

2.1 Associated Documents

AD[01]	NEON.DOC.000001	NEON Observatory Design (NOD) Requirements
AD[02]	NEON.DOC.002652	NEON Data Products Catalog
AD[03]	Available with data download	NEON Raw Field Data Ingest Workbook for Wet Deposition Chemical Analysis (DP0.00018.001)
AD[04]	Available with data download	NEON Raw Laboratory Data Ingest Workbook for Stable Isotopes in Precipitation (DP0.20205.001)
AD[05]	Available with data download	Variables csv
AD[05]	NEON.DOC.003495	NEON Preventative Maintenance Procedure: Wet Deposition Collector
AD[06]	NEON.DOC.000008	NEON Acronym List
AD[07]	NEON.DOC.000243	NEON Glossary of Terms
AD[08]	Available on NEON data portal	NEON Ingest Conversion Language Function Library
AD[09]	NEON.DOC.004825	NEON Algorithm Theoretical Basis Document: OS Generic Transitions
AD[10]	Available on NEON data portal	NEON Ingest Conversion Language
AD[11]	Available with data download	Categorical Codes csv
AD[12]	NEON.DOC.005424	NEON Algorithm Theoretical Basis Document: OS Data Quality Control

3 DATA PRODUCT DESCRIPTION

All samples are collected via an automated wet deposition collector, which is simply an assembly comprising an enclosure with a retractable lid, two plastic collection bottles, thermometer, and an optical precipitation detector. The optical precipitation detector will open upon the onset of precipitation. This allows for all types of precipitation to enter the plastic collection bottles located within the enclosure. Once precipitation has ceased (as detected by the optical precipitation detector), the retractable lid will close until the next precipitation event occurs. Samples are then sent to an analytical facility for analysis of deuterium and oxygen-18 isotopic ratios.

3.1 Spatial Sampling Design

Stable Isotopes in Precipitation sampling is executed at 37 of NEON's 47 terrestrial sites and 7 of the 34 aquatic sites. These sites were selected to sample for Stable Isotopes in Precipitation in conjunction with Wet Deposition Chemical Analysis sampling. Sites for automated wet deposition sampling were selected based on the spatial distribution of the concentration of three chemical contaminants of interest: nitrate, ammonium, and sulfate. These areas of interest were identified using data from the National Atmospheric Deposition Program's National Trends Network. Areas of high and low deposition are distributed across the US (see figure 1), so the 44 instrumented sites selected for sample collection are meant to capture the full range of variability for these species. Sample collection occurs at a single point location at each site, in a double-chimney temperature controlled automated collector. Collectors are located at the top of terrestrial towers above the canopy or on the ground in a clearing to prevent throughfall collection.

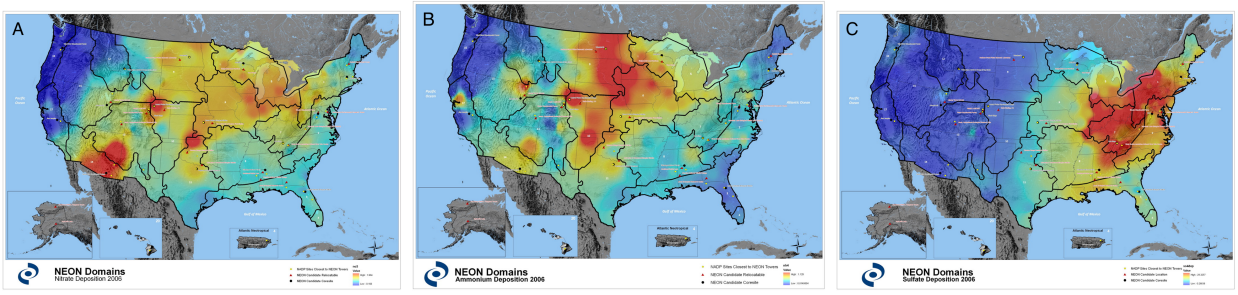

Figure 1: (A) Nitrate, (B) ammonium, and (C) sulfate concentrations in wet deposition accross the United States.

3.2 Temporal Sampling Design

Technicians service the instrument on a bi-weekly basis, and retrieve samples during instrument service. Sample retrieval is intended to occur every 14 days, however the schedules of field technicians can deviate from that schedule due to factors such as safety concerns or temporary lack of personnel. Additionally, technicians are instructed not to retrieve sample during precipitation events, which can delay sample collection. The maximum expected number of samples per site per year is 26, which for 44 sites results in a maximum expected number of samples across the entire observatory of 1144 samples annually.

The collector uses a precipitation sensor to perform wet-only collection, thus the sample collected at the

end of two weeks represents only the active precipitation events during that time.

Samples are collected in plastic bottles, and the isotope analysis subsample is filtered through a 2 micron filter into a 16 mL scintillation vial. The lids on the vials are secured with Parafilm to prevent sample loss during shipping. The subsample is then shipped to the laboratory for analysis, while any remaining sample is sent to the archive facility. In the case of no sample collected, the sample bottle will still be returned to the lab for cleaning, and the lab will also report no sample.

3.3 Theory of Measurement

Deuterium and oxygen stable isotopes in water are measured using cavity ringdown spectrometery. Isotopes are measured as the abundance ratio of a heavy, rare isotope (H) to a light, more common isotope (L), relative to those same ratios in a standard reference material.

$$\delta = [(R_{sample}/R_{standard} - 1)] \times 1000$$

where R = H/L. For all NEON aquatic stable isotope data, deuterium and $\delta^{18}O$ values are reported on the VSMOW-VSLAP scale.

3.4 Sampling Design Changes

2014 - 2018: During the first 4 years of sampling, vials containing water isotope samples were filled to 90% volume. Beginning in 2019, vials containing water isotope samples were filled to 80% volume to minimize the amount of samples that broke due to freezing during transport.

September - November 2021: The external laboratory responsible for H2O isotope analysis altered their analytical method and data return to measure and report a full propagation of measurement uncertainty rather than only the precision of replicate injections of the sample. The external laboratory stopped reporting the **d18OsdWater** and **d2HsdWater** fields in wdi_isoPerSample and started reporting the **d18OWaterUncert** and **d2HWaterUncert** fields. The date of this change will vary at a given site across the observatory, but any record after 2021-11-11 should only have the full propagation of uncertainty published.

Data collection for Stable isotopes in precipitation was temporarily suspended as of 2026. Precipitation isotope samples were collected in the same mechanized system as wet deposition chemistry samples, and Wet deposition (DP1.00013.001) has been discontinued. NEON will be exploring options for a dedicated precipitation isotope collection assembly to resume sampling in the future.

3.5 Laboratory Quality Assurance and Uncertainty

External laboratory facilities have been chosen for their use of stable isotope analytical methods widely adopted by the scientific community. Labs report the long-term analytical precison and accuracy of standard reference materials analyzed as unknowns for each analyte in a summary file. This allows users to interpret and model the stable isotope data in the context of its uncertainty range. Contracted external facilities upload a summary file (asi_externalLabSummaryData) when they begin work for NEON, then again once per year or whenever their information changes (for example, a new instrument is aquired

or a change is detected in analytical precision). Additionally, NEON's Calibration/Validation department has regular procedures for auditing the quality assurance of external laboratories and their reports are available to data users.

Additionally, in the wdi_isoPerSample table, uncertainties in hydrogen (**d2HWaterUncert**) and oxygen (**d18OWaterUncert**) stable isotope ratio are reported for each record. These values represent a full propagation of uncertainty associated with an analysis, including the precision of replicate injections of the sample, precision of analyses of primary laboratory reference materials in the same analytical batch, and the uncertainty in the 'known' calibrated values of the primary laboratory reference materials.

3.6 Variables Reported

All variables reported from the field are listed in the file, NEON Raw Field Data Ingest Workbook for Wet Deposition Chemical Analysis (DP0.00018.001) (AD[03]) and all variables reported from the laboratory are listed in the file, NEON Raw Laboratory Data Ingest Workbook for Stable Isotopes in Precipitation (DP0.20205.001) (AD[04]). All variables reported in the published data (L1 data) are also provided separately in the file, NEON Data Variables for Stable Isotopes in Precipitation (DP1.00038.001) (AD[05]).

NEON spatial data employs the World Geodetic System 1984 (WGS84) for its fundamental reference datum and Geoid12A geoid model for its vertical reference surface. Latitudes and longitudes are denoted in decimal notation to six decimal places, with longitudes indicated as negative west of the Greenwich meridian.

Some variables described in this document may be for NEON internal use only and will not appear in downloaded data.

3.7 Spatial Resolution and Extent

The finest resolution at which spatial data are reported is the point location of the collector.

The basic spatial data included in the data downloaded include the latitude, longitude, and elevation of the collector, plus associated uncertainty due to GPS error. Sampling at terrestrial sites occurs at the tower top or on the ground in a clearing near a weighing gauge precipitation collector, while aquatic sampling occurs at a collector co-located with the meteorologic station at the site.

3.8 Temporal Resolution and Extent

The finest resolution at which temporal data are reported is the approximately bi-weekly range between **setDate** and **collectDate**.

The NEON Data Portal provides data in monthly files for query and download efficiency. Queries including any part of a month will return data from the entire month. Code to stack files across months is available here: https://github.com/NEONScience/NEON-utilities

3.9 Associated Data Streams

The Wet Deposition Chemical Analysis data product (DP1.00013.001) is closely related to Stable Isotopes in Precipitation, as sampling for both products happens in the same instrument concurrently. Data for

these products can be joined by the **sampleID** variable.

3.10 Product Instances

Collection of samples occurs on a bi-weekly basis, with an estimated maximum of 26 sampling events per year per site. Factors such as periods without precipitation or delays in sample collection may limit the number of collection events.

3.11 Data Relationships

The protocol dictates that each sample collection event corresponds to one record per unique **sampleID** in wdi_collection. This record will always have two child sampleIDs (**isoSubsampleID** and **isoTestSubsampleID**), even when no sample is collected. Thus, records where isotope analysis was impossible or only partly completed will still have an associated laboratory analysis table available.

wdi_collection - > One record expected per **sampleID**, generates two child samples, one **isoSubsampleID** and one **isoTestSubsampleID**

wdi_collectionIso - > One record expected per **isoSubsampleID**

wdi_collectionIsoTest -> One record expected per **isoTestSubsampleID**

wdp_sensor - > All sensor data from the collector will be output for the month selected. Sensor data can be subset to the date range of sample collection by subsetting the **date** variable between the **setDate** and **collectDate** variable reported in records in the wdi_collection table.

wdp_isoPerSample - > One record expected per **isoTestSubsampleID**, associated with water isotope analyses from an external laboratory

asi_externalLabSummaryData -> One record expected per laboratoryName x analyte x method x labSpecificStartDate combination. Used to associate sample data with relevant uncertainty values

Each **sampleID** will have one child **isoSubsampleID** in wdi_collectionIso, and one child **chemSubsampleID** in the Wet Deposition Chemistry Analysis data product. Thus **sampleID** can be used to join records for Wet Deposition Chemistry Analysis and Stable Isotopes in Precipitation.

Data downloaded from the NEON Data Portal are provided in separate data files for each site and month requested. The neonUtilities package in R and the neonutilities package in Python contain functions to merge these files across sites and months into a single file for each table. The neonUtilities R package is available from the Comprehensive R Archive Network (CRAN; https://cran.r-project.org/web/packages/neonUtilities/index.html) and can be installed using the install.packages() function in R. The neonutilities package in Python is available on the Python Package Index (PyPi; https://pypi.org/project/neonutilities/) and can be installed using pip. For instructions on using the package in either language to merge NEON data files, see the Download and Explore NEON Data tutorial on the NEON website: https://www.neonscience.org/download-explore-neon-data.

4 DATA QUALITY

4.1 Data Entry Constraint and Validation

Many quality control measures are implemented at the point of data entry within a mobile data entry application or web user interface (UI). For example, data formats are constrained and data values controlled through the provision of dropdown options, which reduces the number of processing steps necessary to prepare the raw data for publication. An additional set of constraints are implemented during the process of ingest into the NEON database. The product-specific data constraint and validation requirements built into data entry applications and database ingest are described in the document NEON Raw Field Data Ingest Workbook for Wet Deposition Chemical Analysis (DP0.00018.001), provided with every download of this data product. Contained within this file is a field named 'entryValidationRulesForm', which describes syntactically the validation rules for each field built into the data entry application. Data entry constraints are described in Nicl syntax in the validation file provided with every data download, and the Nicl language is described in NEON's Ingest Conversion Language (NICL) specifications ([AD[08])

4.2 Automated Data Processing Steps

Following data entry into a mobile application or web user interface, the steps used to process the data through to publication on the NEON Data Portal are detailed in the NEON Algorithm Theoretical Basis Document: OS Generic Transitions (AD[09]).

Published data are reviewed for completeness, timeliness, and validity using an internal set of tests and metrics, as detailed in the NEON Algorithm Theoretical Basis Document: OS Data Quality Control (AD[12]). These quality tests are used to guide process improvements, audits of analytical facilities, and data updates, but do not generate quality flags in published data.

4.3 Data Revision

All data are provisional until a numbered version is released. Annually, NEON releases a static version of all or almost all data products, annotated with digital object identifiers (DOIs). The first data Release was made in 2021. During the provisional period, QA/QC is an active process, as opposed to a discrete activity performed once, and records are updated on a rolling basis as a result of scheduled tests or feedback from data users. The Issue Log section of the data product landing page contains a history of major known errors and revisions.

4.4 Quality Flagging

The **dataQF** field in each record is a quality flag for known issues applying to the record, added by NEON Science upon data review. At present, there are no dataQF entries for the surface water and groundwater stable isotope data products.

Additionally, field-level data quality information is conveyed in the **wdi_collection** and **wdp_collectionIso** tables, in the **equipmentProblems** and **isoSubsampleCondition** fields. Entries in these fields will usually be accompanied by remarks explaining the specific conditions observed.

4.5 Analytical Facility Data Quality

Analytical labs that generate aquatic stable isotope data calibrate each run of NEON samples with primary reference materials, and include secondary reference materials alongside NEON samples in order to gauge run acceptability. Labs communicate issues with sample measurements using the suite of quality flags described below. In general, an entry of 0 in a quality flag field means there is no issue to report.

In addition, long-term analytical precision and accuracy of secondary reference material analyses are reported for each lab to allow users to interpret and analyze aquatic stable isotope data in the context of their uncertainty ranges. The data tables asi_externalLabSummaryData and apl_externalLabSummaryData, which are available in the data product expanded package, contain the long-term precision and accuracy of lab analyses.

For further information about individual laboratory QA procedures, refer to the lab-specific SOPs found in the NEON Data Portal document library (http://data.neonscience.org/documents), External Lab Protocols section. NEON's Calibration/Validation department has regular procedures for auditing the quality assurance of external laboratories and their reports are also available to data users.