NEON USER GUIDE TO STABLE ISOTOPES IN PRECIPITATION (NEON.DP1.00038)

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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 concentrations 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 (NEON.DP1.00038) (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 (NEON.DP0.00018) (AD[03]) and NEON Raw Laboratory Data Ingest Workbook for Stable Isotopes in Precipitation (NEON.DP0.20205) (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 Level 1, Level 2 and Level 3 Data Products Catalog
AD[03]	NEON.DP0.00018.001 _dataValidation.csv	NEON Raw Field Data Ingest Workbook for Wet Deposition Chemical Analysis (NEON.DP0.00018)
AD[04]	NEON.DP0.20205.001 _dataValidation.csv	NEON Raw Laboratory Data Ingest Workbook for Stable Isotopes in Precipitation (NEON.DP0.20205)
AD[05]	NEON.DP1.00038.001 _variables.csv	NEON Data Variables for Stable Isotopes in Precipitation (NEON.DP1.00038)
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]		NEON's Ingest Conversion Language (NICL) specifications

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 glass 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 glass 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 concentrations.

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 contaiminants 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 43 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 at aquatic sites to prevent throughfall collection.

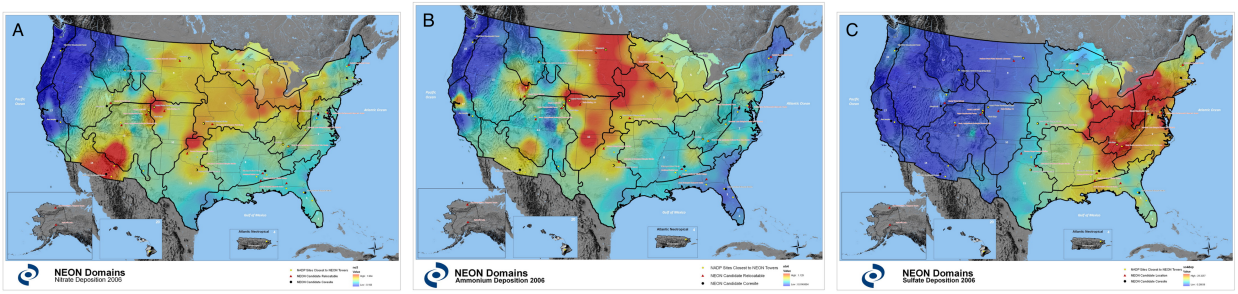

Figure 1: (A) Nitrate, (B) ammonium, and (C) sulfate concentrations in wet deposition accross the United States.

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 precpitation events, which can delay sample collection. The maximium 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 glass bottles, and the isotope analysis subsample is filtered through a 2 micron filter into a 20 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 remiaining 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 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 uncertainty 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.

3.5 Variables Reported

All variables reported from the field are listed in the file, NEON Raw Field Data Ingest Workbook for Wet Deposition Chemical Analysis (NEON.DP0.00018) (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 (NEON.DP0.20205) (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 (NEON.DP1.00038) (AD[05]).

NEON spatial data employs the World Geodetic System 1984 (WGS84) for its fundamental reference datum and Earth Gravitational Model 96 (EGM96) for its reference gravitational ellipsoid. 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.

3.6 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 always occurs at the tower top, while aquatic sampling occurs at a collector co-located with the meterologic station at the site.

During NEON construction, spatial data may not be available yet for some locations, and the spatial fields in downloaded data may be blank.

3.7 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

3.8 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.

3.9 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.

3.10 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 labSpecificStart-Date 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 Isotope Concentrations in Precipitation.

4 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 (NEON.DP0.00018), 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[09]).