



<i>Title:</i> NEON User Guide to Wet Deposition Chemical Analysis (DP1.00013.001)	<i>Date:</i> 12/23/2020
<i>Author:</i> Robert Lee	<i>Revision:</i> B

# NEON USER GUIDE TO WET DEPOSITION CHEMICAL ANALYSIS (DP1.00013.001)

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## CHANGE RECORD

<b>REVISION</b>	<b>DATE</b>	<b>DESCRIPTION OF CHANGE</b>
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.



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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 Wet Deposition Chemical Analysis - the major ion concentrations, pH, and conductivity of 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 Wet Deposition Chemical Analysis (DP1.00013.001) (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[06]). 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 (DPO.00018.001) (AD[03]) and NEON Raw Laboratory Data Ingest Workbook for Wet Deposition Chemical Analysis (DPO.00019.001) (AD[04]), provided in the download package for this data product. Please note that raw data products (denoted by 'DPO') 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	Validation csv
AD[04]	Available with data download	Validation csv
AD[05]	Available with data download	Variables csv
AD[06]	NEON.DOC.003495	NEON Preventative Maintenance Procedure: Wet Deposition Collector
AD[07]	NEON.DOC.000008	NEON Acronym List
AD[08]	NEON.DOC.000243	NEON Glossary of Terms
AD[09]	Available on NEON data portal	NEON Ingest Conversion Language Function Library
AD[10]	NEON.DOC.004825	NEON Algorithm Theoretical Basis Document: OS Generic Transitions
AD[11]	Available on NEON data portal	NEON Ingest Conversion Language
AD[12]	Available with data download	Categorical Codes csv



### 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 major ion concentration, pH, and conductivity of the sample.

#### 3.1 Spatial Sampling Design

Wet Deposition Chemical Analysis sampling is executed at 37 of NEON's 47 terrestrial sites and 7 of the 34 aquatic sites. These sites were selected to sample areas with a range of wet deposition concentrations of three chemical contaminants: 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 of interest. 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.

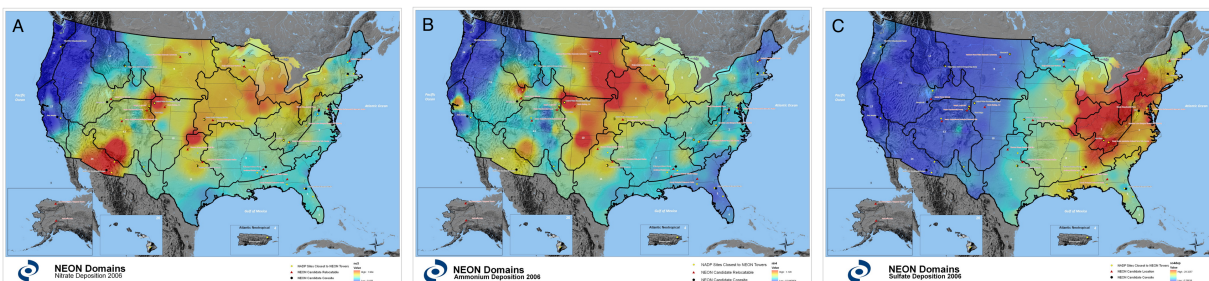


Figure 1: (A) Nitrate, (B) ammonium, and (C) sulfate concentrations in wet deposition across the United States.

#### 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 glass bottles, and are shipped directly to the laboratory for analysis and archiving upon retrieval. 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 Laboratory Quality Assurance and Uncertainty

Uncertainties reported for each analyte are the associated method detection limit of the analyte, as determined by an annual internal audit performed by the contract laboratory (Illinois State Water Survey). Chemical analyses are performed in accordance with practices defined by the National Atmospheric Deposition Program at the Central Analytical Laboratory. The Illinois State Water Survey and Central Analytical Laboratory generates annual quality assurance reports for wet deposition samples. Past reports are accessible at: <http://nadp.isws.illinois.edu/lib/qaReports.aspx#CAL>.

### 3.4 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 Wet Deposition Chemical Analysis (DP0.00019.001) (AD[04]). All variables reported in the published data (L1 data) are also provided separately in the file, NEON Data Variables for Wet Deposition Chemical Analysis (DP1.00013.001) (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.

### 3.5 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 meteorological 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.

### 3.6 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>

### 3.7 Associated Data Streams

The Stable Isotopes in Precipitation data product (DP1.00038.001) is closely related to Wet Deposition Chemical Analysis, as sampling for both products happens in the same instrument concurrently. Data for these products can be joined by the **sampleID** variable.

### 3.8 Product Instances

Collection of samples occurs on a bi-weekly basis, with an estimated maximum of 26 sampling events per year per site. Observatory-wide, the maximum number of records generated for this data product per year will be 1144. Factors such as periods without precipitation or delays in sample collection may limit the number of collection events.

### 3.9 Data Relationships

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

`wdp_collection` - > One record expected per **sampleID**, generates one child **chemSubsampleID**

`wdp_collectionChem` - > One record expected per **chemSubsampleID**

`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 `wdp_collection` table.

`wdp_chemLab` - > One record expected per **chemSubsampleID**, associated with chemistry measurements and uncertainties from the external laboratory

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

Data downloaded from the NEON Data Portal are provided in separate data files for each site and month requested. The `neonUtilities` R package contains functions to merge these files across sites and months into a single file for each table described above. The `neonUtilities` 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. For instructions on using `neonUtilities` 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[09]]).

### 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[10]).

### 4.3 Data Revision

All data are provisional until a numbered version is released; the first release of a static version of NEON data, annotated with a globally unique identifier, is planned to take place in 2020. 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 Change Log section of the data product readme, provided with every data download, 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.

Additionally, field-level data quality information is conveyed in the **wdp\_collection** and **wdp\_collectionChem** tables, in the **equipmentProblems** and **chemSubsampleCondition** fields. Entries in these fields will usually be accompanied by remarks explaining the specific conditions observed.

Records of land management activities, disturbances, and other incidents of ecological note that may have a potential impact are found in the Site Management and Event Reporting data product (DP1.10111.001)



#### 4.5 Analytical Facility Data Quality

The contract laboratory for Wet Deposition Chemistry communicates batch-level and record-level issues with samples and measurements, using the suite of quality flags described in the table below.

In addition, long-term analytical precision and accuracy of check-standard or secondary reference material analyses are reported for each analyte to allow users to interpret and analyze chemistry data in the context of their uncertainty ranges. The wdp\_chemLab data table, which is available in the data product basic packages, 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.

Data quality fields in **wdp\_chemLab**:

Table 1: Descriptions of the dataQF codes for quality flagging

<b>fieldNames</b>	<b>values</b>	<b>definition</b>
precipCalciumFlag precipMagnesiumFlag precipPotassiumFlag precipSodiumFlag precipAmmoniumFlag precipNitrateFlag precipSulfateFlag precipPhosphateFlag precipChlorideFlag precipBromideFlag	B H x	Below detection limit Artificially high measurement level Other issue (see the externalRemarks field).
labCondition	l c v i x	Lab error Contaminated sample Inadequate sample volume for analysis Incomplete chemical analysis Other