NEON USER GUIDE TO REAERATION (DP1.20190.001) AND SALT-BASED DISCHARGE SAMPLING (DP1.20193.001)

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CHANGE RECORD

REVISION	DATE	DESCRIPTION OF CHANGE
A	08/16/2017	Initial Release
B	06/24/2020	Included general statement about usage of neonUtilities R package and statement about possible location changes. Updated language in Analytical Facility Data Quality section
C	03/08/2022	Updated section 4.4 Data Revision with latest information regarding data release
C.1	08/27/2024	Updated for information on the dataframe table for conductivity logger data and sites which are changing expected injection types and experiment frequencies.

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1 DESCRIPTION

1.1 Purpose

This document provides an overview of the data included in this NEON Level 1 (L1) data product, the quality controlled product generated from raw Level 0 (L0) data, and associated metadata. In the NEON data products framework, the raw data collected in the field, the specific conductance of water for example, are considered the lowest level, L0. 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 L1 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 and associated metadata from input data for Reaeration and Salt-based Discharge - which are components of a gas and salt tracer injection experiment. 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 Reaeration (DP1.20190.001) (AD[05]) and NEON Data Variables for Salt-based Discharge (DP1.20193.001) (AD[06]), 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 AOS Protocol and Procedure: Reaeration in Streams (AD[07]). The raw data that are processed in this document are detailed in the file, NEON Raw Data Validation for Reaeration and Salt-based Discharge (DP0.20190.001) (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., '20190') 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.001152	Aquatic Sampling Strategy
AD[03]	NEON.DOC.002652	NEON Data Products Catalog
AD[04]	Available with data download	Validation csv
AD[05]	Available with data download	Variables csv
AD[06]	Available with data download	Variables csv
AD[07]	NEON.DOC.000693	AOS Protocol and Procedure: Reaeration in Streams
AD[08]	NEON.DOC.000008	NEON Acronym List
AD[09]	NEON.DOC.000243	NEON Glossary of Terms
AD[10]	NEON.DOC.004825	NEON Algorithm Theoretical Basis Document: OS Generic Transitions
AD[11]	Available on NEON data portal	NEON Ingest Conversion Language Function Library
AD[12]	Available on NEON data portal	NEON Ingest Conversion Language
AD[13]	Available with data download	Categorical Codes csv

2.2 Acronyms

Acronym	**Definition**
SF6	Sulfur hexafluoride

3 DATA PRODUCT DESCRIPTION

The Reaeration field and lab collection (DP1.20190.001) data product provides data for four different injection types: "NaCl" and "NaBr", which are simultaneous inert gas, e.g. SF6, and conservative tracer, e.g. NaCl or NaBr, experiments and "model - slug" and "model - CRI", which are conservative tracer-only injections. The data packages include tracer concentrations in stream water, conductivity time series, wetted width measurements, and related injection information, e.g. start and end times and rates of tracer injection, collected using AOS Protocol and Procedure: Reaeration in Streams (AD[07]). From the data provided in the Reaeration field and lab collection data package, users can calculate reaeration rates, which may be an important component of stream metabolism estimates.

The Salt-based Discharge (DP1.20193.001) data product provides data for the four reaeration injection types along with "Discharge only" slugs and is comprised of the tracer injection information that includes only the field and external lab information related to salt tracer injection. In some of the smaller NEON streams, discharge calculated from the data provided by the Salt-based stream discharge data product may provide more accurate discharge estimates than those determined using a handheld unit that are published as part of the Stream discharge field collection (DP1.20048.001) data product.

Reaeration and salt-based discharge injections are only performed in wadeable streams. There are five different types of experiments: NaCl constant rate injection (NaCl), NaBr constant rate injection plus an NaCl slug (NaBr), NaBr or NaCl constant rate injection without inert gas injection (model - CRI), NaCl slug (model - slug), or NaCl slug for discharge measurements only, i.e. does not include wetted width measurements. An NaCl constant rate injection (conservative salt and inert, volatile gas) is the most common and takes place at streams with relatively low conductivity ($\leq$ 500 μS cm^{-1}) and low flows. At streams with high conductivity (> 500 μS cm^{-1}) and/or higher flows, lower concentrations of NaBr are used for the constant rate injection (conservative salt and inert, volatile gas) along with an NaCl slug that will register changes in conductivity with the data loggers so that travel times can be calculated. For high flow wadeable streams (>2000 L/s; e.g., BLUE - Blue River) and low slope, low reaeration streams (e.g., ARIK - Arikaree River) an NaCl slug (without a gas or salt constant rate injection) will be performed to enable reaeration modeling without field measured reaeration rates. When field challenges impact the ability to complete a planned NaCl or NaBr injection with inert gas, a partial record may be entered with injection type model - CRI. Injection type discharge only is used at sites where capturing discharge with the wading surveys is challenging.

As of the 2022 field season, an analysis with external review determined that a relationship with discharge was sufficient to change from NaCl or NaBr injections to model - slug injections at 12 sites. The following sites will now collect only model - slug injections that can be used to validate the existing gas exchange relationship with discharge: LEWI, POSE, GUIL, LECO, WALK, WLOU, COMO, PRIN, REDB, BIGC, OKSR, CARI. An additional site, BLDE, was moved to model - slug injections due to permitting restrictions. Additional sites will be re-evaluted at the end of 2024 to determine if additional experiments are needed or if they can also move to the slug - model injection type as well.

3.1 Spatial Sampling Design

Four stations downstream of the injection location (i.e. drip station) are sampled for analysis of salt tracer concentrations in the stream water (Figure 1) prior to tracer injection to capture background water concentrations. Once the injection is started and the tracers reach plateau, for NaCl and NaBr constant rate injections, samples are collected for gas and salt concenentration at each of the 4 stations prior to ending the tracer injection. A salt sample is also collected from the injection solution. At the most upstream station, station #1, and the most downstream sampling station, station #4, submersible data loggers are deployed that record conductivity, temperature, and specific conductance in the stream water throughout the injection experiments. A set of 30 (unless adverse conditions impacted data collection) wetted width measurements are also collected the same day as the tracer injection between station #1 and station #4.

As much as possible, sampling occurs in the same locations over the lifetime of the Observatory. However, over time some sampling locations may become impossible to sample, due to disturbance or other local changes. When this occurs, the location and its location ID are retired. A location may also shift to slightly different coordinates. Refer to the locations endpoint of the NEON API for details about locations that have been moved or retired: https://data.neonscience.org/data-api/endpoints/locations/

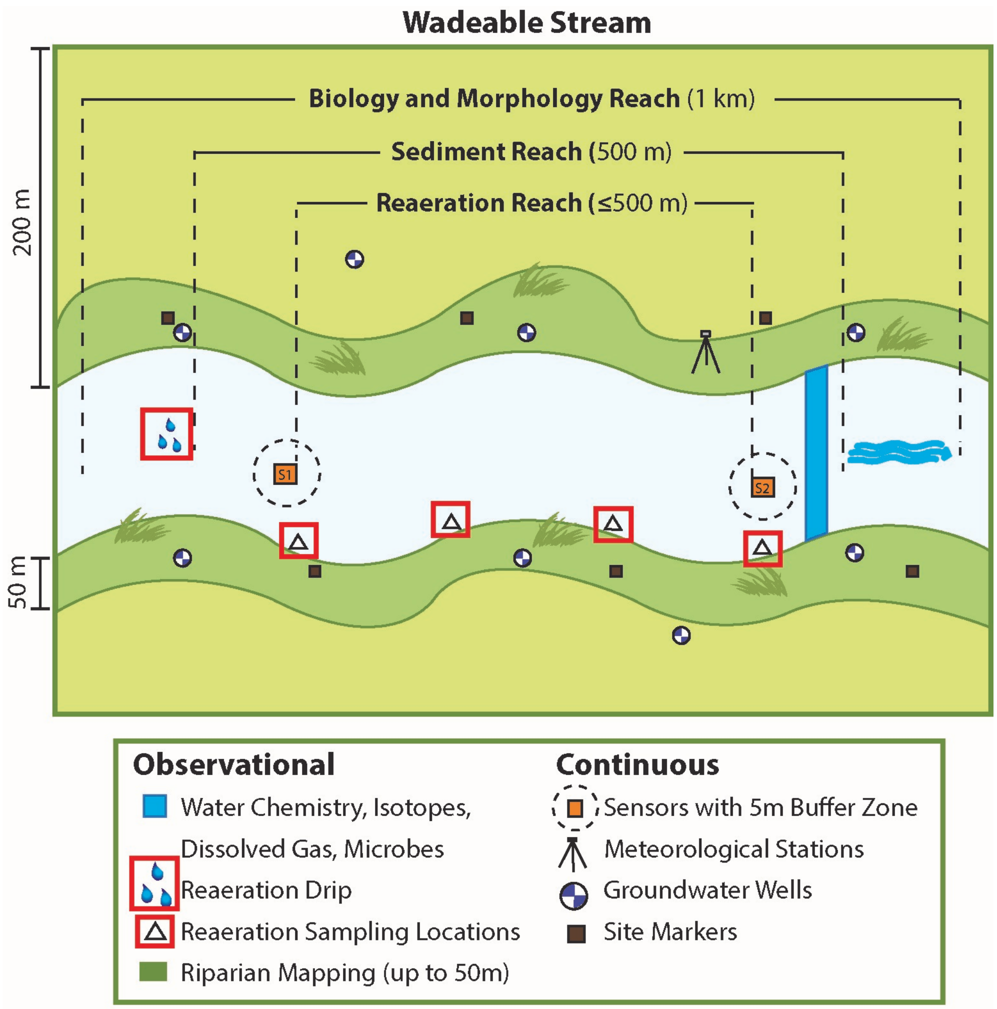

Figure 1: A generic wadeable stream site layout example with reaeration sampling stations.

3.2 Temporal Sampling Design

Reaeration measurements will be completed up to 10 times annually during NEON Site Characterization activities and up to 6 times annually during NEON Operations in wadeable stream locations until a relationship with discharge is developed. Sites that are high risk sites for flooding resulting in changes in stream morphology may be requested to continue to collect reaeration 10 times per year. Sampling events should be spread out throughout the year so as to collect a range of flows.

Timing of sampling is site specific and determined by rules developed using historical flow regime and environmental data. For example, streams with little or no flow during the summer dry-season are sampled more intensively during wet periods. Streams with snowmelt-dominated hydrographs are sampled more intensively during spring/summer-elevated flows than during winter snow-covered months.

3.3 Laboratory Quality Assurance and Uncertainty

NEON field procedures for collection of reaeration and salt-based discharge samples follow widely adopted community methods and all NEON technicians conducting this work receive proper training. For external laboratory analyses, facilities have been chosen for their use of analytical methods widely adopted by the aquatic chemistry community. Labs report the method detection limit, along with long-term analytical precision and uncertainty of standards analyzed as unknowns, for each gas or salt species in a summary file. This allows users to interpret and model the dissolved gas and salt data in the context of its uncertainty range. Contracted external facilities upload this summary file (rea_externalLabSummaryData) when they begin work for NEON, then again once per year or whenever their information changes (for example, a new instrument is acquired 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.

Occasionally, sample re-runs are requested following review of data returned from the external lab(s). For samples with salt concentrations less than the background concentrations measured for the same experiment, re-runs are requested. Another reason for salt or gas sample re-run requests is when a Dixon Q test flags a sample as an outlier compared to the other samples collected at the same station during plateau. In the case where the external lab re-runs a sample, the re-runs are ingested into the database and users can determine their preferred method for handling analytical duplicates.

3.4 Variables Reported

All variables reported from the field or laboratory technician (L0 data) are listed in the file, NEON Raw Data Validation for Reaeration and Salt-based Discharge (DP0.20190.001) (AD[04]). All variables reported in the published data (L1 data) are also provided separately in the file, NEON Data Variables for Reaeration (DP1.20190.001) (AD[05]) and NEON Data Variables for Salt-based Discharge (DP1.20193.001) (AD[06]).

Field names have been standardized with Darwin Core terms (http://rs.tdwg.org/dwc/; accessed 16 February 2014), the Global Biodiversity Information Facility vocabularies (http://rs.gbif.org/vocabulary/gbif/; accessed 16 February 2014), the VegCore data dictionary (https://projects.nceas.ucsb.edu/nceas/projects/bien/wiki/VegCore; accessed 16 February 2014), where applicable. NEON AOS 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 reaeration and salt-based discharge data are reported is a single water sample collected from a unique stationID. The namedLocation is the finest spatial resolution for the table and will be either stationID or siteID. All tables also contain a domainID and siteID field in addition to the namedLocation field. Overall, this results in a spatial hierarchy of:

sampleID (unique ID given to the individual sample) → **namedLocation** (ID of the sampling location) → **siteID** (ID of NEON site) → **domainID** (ID of a NEON domain).

The injection station (i.e. drip station) and four downstream sampling stations are predominantly stationary over time, and reaeration station #1 will always align with Sensor Set #1 while reaeration station #4 will always align with Sensor Set #2. However, differing flow conditions may necessitate shifting stations 2 or 3 either upstream or downstream. The exact geospatial location of these stations is less important for reaeration rate calculations than the distance the water flows between the stations. Users should use the downstream distances recorded in the data for each station as they could potentially be different for different dates (table: rea_backgroundFieldSaltData or sbd_backgroundFieldSaltData, field: stationToInjectionDistance).

Shapefiles of all NEON Aquatic Observation System sampling locations can be found in the Document Library: http://data.neonscience.org/documents. If users are interested in the geospatial locations of the data relative to a global coordinate system, those can be retrieved using the NEON data API using the **namedLocation** and the following:

1. The def.extr.geo.os.R function from the geoNEON package, available here: https://github.com/NEONScience/NEON-geolocation
2. The NEON API: http://data.neonscience.org/api

3.6 Temporal Resolution and Extent

The finest resolution at which reaeration and salt-based discharge temporal data are reported is the time of day. For field measurements and sample collections this is recorded to the nearest minute. For in situ conductivity logger measurements data is recorded to the nearest second. One injection experiment takes place on a single date. The total number of injection experiments per year is expected to be 6 - 10 per wadeable stream per site.

The NEON Data Portal currently provides data in monthly files for query and download efficiency. Queries including any part of a month will return data from the entire month. All queries, regardless of the date range specified, will include a copy of rea_externalLabSummaryData which provides summary information from the external lab about the method detection limits, the equipment used, and precision and accuracy. Code to stack files across months is available here: https://github.com/NEONScience/NEON-utilities

3.7 Associated Data Streams

There are no directly associated data streams for Reaeration field and lab collection and Salt-based discharge. The protocol for these two data products is only performed on a day when other activities are not taking place in order to prevent disturbing the stream during the injection experiment.

3.8 Product Instances

The NEON Observatory contains 24 wadeable streams.

Reaeration and salt-based discharge sampling yields a set of background samples and a set of plateau samples per sampling event. There will be 6 complete sampling events per year in wadeable streams and may be some additional incomplete records for experiments that experience field challenges. The background set of samples consist of one sample collected from each of the four sampling stations and an injectate solution sample (5 total salt samples). It is assumed that the gas used for the injection, usually SF6, is not present in the water naturally, and therefore background samples are not needed. The plateau samples consist of 5 replicates at each of the 4 sampling stations once the most downstream station, station #4, has reached a constant, maximum conductivity (20 total salt and 20 total gas). Observatory-wide, this will yield a total of 4320 to 7200 wetted width records and 3600 to 6000 salt concentration records and 2880 to 4800 gas concentration records for reaeration and salt-based discharge per year.

3.9 Data Relationships for Reaeration

The protocol dictates that the tracer injection will take place at each siteID per event (one record expected per siteID and collectDate combination in rea_fieldData). A record from rea_fieldData will usually have 4 child records in rea_backgroundFieldSaltData and rea_plateauMeasurementFieldData (one for each sampling station), two child records in rea_backgroundFieldCondData (one for the upstream, station #1 and downstream, station #4 stations where conductivity loggers are deployed), many child records in rea_conductivityFieldData (logger conductivity data is collected and a record is created every 10 seconds during the duration of the injection experiment). 30 records are created in rea_widthFieldData (one for each wetted width measurement) for each injection experiment. Each record from rea_plateauMeasurementFieldData is expected to have 5 child records in rea_plateauSampleFieldData (one fore each replicate collected at the station). Each record from rea_backgroundFieldSaltData (background samples), rea_plateauMeasurementFieldData (plateau samples), and rea_fieldData (injectate sample) is expected to have one child record in rea_externalLabDataSalt with the salt tracer concentration. Each record from rea_plateauMeasurementFieldData is expected to have one child record in rea_externalLabDataGas with the gas tracer concentration. However, duplicates and/or missing data may exist where protocol and/or data entry aberrations have occurred; *users should check data carefully for anomalies before joining tables*. Below, the data relationships are also summarized in a bulleted list. Records with an injection type of “model - slug” and “model - CRI” may contain fewer records and/or tables than described below.

- rea_fieldData has one record per injection experiment (unique siteID and collectDate combination)
- rea_backgroundFieldSaltData has one record per injection experiment per station (4 children of rea_fieldData)
- rea_plateauMeasurementFieldData has one record per injection experiment per station (4 children of rea_fieldData)

- rea_backgroundFieldCondData has one record per injection experiment per upstream, station #1, and downstream, station #4, station (2 children of rea_fieldData)
- rea_widthFieldData has 30 records per injection experiment (unique siteID and collectDate combination)
- rea_plateauSampleFieldData has one record per sample collected per station per experiment (5 children of rea_plateauMeasurementFieldData)
- rea_externalLabDataSalt contains external lab records for background samples (4 **saltBackgroundSampleID** samples in rea_backgroundFieldSaltData per collectDate), tracer injectate samples (one **injectateSampleID** sample in rea_fieldData per collectDate), and plateau samples (20 **saltTracerSampleID** samples in rea_plateauSampleFieldData per collectDate)
- rea_externalLabDataGas has one external lab record per sample in rea_plateauSampleFieldData **gasSampleID**
- rea_externalLabSummaryData has one record expected per laboratoryName x analyte x method x labSpecificStartDate combination. Can use corresponding variables in externalLabData tables to associate sample data with relevant uncertainty values and method detection limits

RELEASE-2023 and earlier

- rea_conductivityFieldData has one record per 10 second interval per injection experiment. The set of records that take place over time for a station and injection experiment date can be linked using the **hoboSampleID** which is a field in each record of both rea_conductivityFieldData and rea_backgroundFieldCondData tables.

RELEASE-2024 and later

- rea_conductivityFieldData will contain a single record for each hoboSampleID, of which there are usually two per sampling event. The 0.1 Hz conductivity data are in the expanded data package, stored in one file per hoboSampleID. The neonUtilities R package (>=2.4.0), using either stackByTable() or loadByProduct(), stacks the conductivity data files and names the resulting table rea_conductivityRawData. To produce the equivalent of the previous xxx_conductivityFieldData table, join the rea_conductivityFieldData to the rea_conductivityRawData, joining on the hoboSampleID.

3.10 Data Relationships for Salt-based Discharge

The Salt-based Discharge (DP1.20193.001) data product is a subset of the tracer injection information that includes only the field and external lab information related to the salt tracer injection. This section describes the tables that are part of the salt-based discharge publication package. The protocol dictates that the tracer injection will take place at each siteID per event (one record expected per siteID and collectDate combination in sbd_fieldData). A record from sbd_fieldData will usually have 4 child records in sbd_backgroundFieldSaltData and sbd_plateauMeasurementFieldData (one fore each sampling station), two child records in sbd_backgroundFieldCondData (one for the upstream, station #1 and downstream, station #4 stations where conductivity loggers are deployed), many child records in sbd_conductivityFieldData (logger conductivity data is collected and a record is created every 10 seconds during the duration of the injection experiment). Each record from sbd_plateauMeasurementFieldData is expected to have 5 child records in sbd_plateauSampleFieldData (one fore each replicate collected at the station). Each record from sbd_backgroundFieldSaltData (background samples), sbd_plateauMeasurementFieldData (plateau samples), and sbd_fieldData (injectate sample) is expected to have one child record in sbd_externalLabDataSalt with the salt tracer concentration. However, duplicates and/or missing data may exist where protocol and/or data entry aberrations have occurred; *users should check data carefully for anomalies before joining tables*. Below, the data relationships are also summarized in a bulleted list. Records with an injection type of "model - slug", "model - CRI", or "Discharge only" may contain fewer records and/or tables than described below.

- sbd_fieldData has one record per injection experiment (unique siteID and collectDate combination)
- sbd_backgroundFieldSaltData has one record per injection experiment per station (4 children of sbd_fieldData)
- sbd_plateauMeasurementFieldData has one record per injection experiment per station (4 children of sbd_fieldData)
- sbd_backgroundFieldCondData has one record per injection experiment per upstream, station #1, and downstream, station #4, station (2 children of sbd_fieldData)
- sbd_plateauSampleFieldData has one record per sample collected per station per experiment (5 children of sbd_plateauMeasurementFieldData)
- sbd_externalLabDataSalt contains external lab records for background samples (4 **saltBackgroundSampleID** samples in sbd_backgroundFieldSaltData per collectDate), tracer injectate samples (one **injectateSampleID** sample in sbd_fieldData per collectDate), and plateau samples (20 **saltTracerSampleID** samples in sbd_plateauSampleFieldData per collectDate)
- rea_externalLabSummaryData has one record expected per laboratoryName x analyte x method x labSpecificStartDate combination. Can use corresponding variables in externalLabData tables to associate sample data with relevant uncertainty values and method detection limits

RELEASE-2023 and earlier

- sbd_conductivityFieldData has one record per 10 second interval per injection experiment, the set of records that take place over time for a station and injection experiment date can be linked using the **hoboSampleID** which is a field in each record of both sbd_conductivityFieldData and sbd_backgroundFieldCondData tables.

RELEASE-2024 and later

- sbd_conductivityFieldData will contain a single record for each hoboSampleID, of which there are usually two per sampling event. The 0.1 Hz conductivity data are in the expanded data package, stored in one file per hoboSampleID. The neonUtilities R package (>=2.4.0), using either stackByTable() or loadByProduct(), stacks the conductivity data files and names the resulting table sbd_conductivityRawData. To produce the equivalent of the previous xxx_conductivityFieldData table, join the sbd_conductivityFieldData to the sbd_conductivityRawData, joining on the hoboSampleID.

3.11 Special Considerations

The equations needed to calculate reaeration rates and salt-based discharge from the data available in this downloaded package are detailed and referenced in the appendix. The information provided there is outside of the scope of basic QA/QC of L0 data used to create this L1 data product. However, the field and laboratory methods chosen were designed to enable these calculations by data users, thus a discussion of them is provided. NEON does maintain the reaRate R package, that can be found in the NEON-reaeration GitHub repository (https://github.com/NEONScience/NEON-reaeration) that contains functions to make some of the calculations outlined in the appendix.

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 drop-down 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 Data Validation for Reaeration and Salt-based Discharge (DP0.20190.001), 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[11]).

A schematic of the data entry application design is depicted in Figure 2 located at the end of this document.

Data collected prior to 2017 were processed using a paper-based workflow that did not implement the full suite of quality control features associated with the interactive digital workflow.

4.2 Calculations made on data ingest

Specific conductance, conductivity normalized to 25 ◦C, is calculated during data ingest for **lowRangeHobo** and **fullRangeHobo** using Equation 1 specified by *Standard Methods for the Examination of Water and Waterwater*. **lowRangeSpCondLinear** and **fullRangeSpCondLinear** are calculated using an r value of 0.0191, which is the value for a pure potassium chloride solution. **lowRangeSpCondNonlinear** and **full-**

RangeSpCondNonlinear are calculated using a non-linear r value calculated according to **??** derived from the Practical Salinity Scale 1978 (PSS-78) equations. S is assumed to be 0 for all NEON sites since conductivity has been measured below 1500 microSiemens.

$$SC = \frac{AC}{1 + r(T - 25)} \tag{1}$$

Where:

SC is Specific Conductance at 25 degrees Celsius in microSiemens per cm

AC is the measured conductivity of the sample in microSiemens per cm

r is the temperature correction coefficient for the sample

T is the temperature of the sample in Celsius

$$r = A + B \cdot T + C \cdot S + D \cdot T^2 + E \cdot S^2 + F \cdot T \cdot S \tag{2}$$

Where:

r is the temperature correction coefficient for the sample

S is the salinity of the sample

T is the temperature of the sample in Celsius

A = 1.86221444

B = 0.00799141780

C = -0.00204882760

D = -0.0000479386353

E = 0.0000167997158

F = -0.0000155721008

4.3 Automated Data Processing Steps

Following data entry into a mobile application of 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]).

4.4 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.

4.5 Quality Flagging

The **dataQF** field in each data record is a quality flag for known errors applying to the record. Please see the *Special Considerations* section of this document for a list of known errors that may be present in the data, and below for an explanation of **dataQF** codes specific to this product.

Table 1: Descriptions of the dataQF codes for quality flagging

fieldName	value	definition
dataQF	legacyData	Data recorded using a paper-based workflow that did not implement the full suite of quality control features associated with the interactive digital workflow

\end{table}

In the rea_fieldData table, the **incompleteExperimentQF** quality flag is used to indicate that a reaeration experiment is incomplete in some way, e.g. a field discharge measurement was not collected. Often this is a result of an unplanned mishap during data collection, i.e. an equipment malfunction. This flag is populated on a semi-annual basis following science review. An external lab data flag in this table indicates that there will not be any external lab data returned for any samples for the indicated type of analysis. For example, an externalLabSaltDataNA flag indicates that no salt concentrations will be returned from the external lab at all. If more than one flag is applicable, the appropriate flags with be concatenated with a pipe "|" delimiter.

Table 2: Descriptions of the dataQF codes for quality flagging field data

fieldName	value	definition
incompleteExperimentQF	HOBO_S1_dataNA	HOBO file for station 1 not available for reaeration experiment
incompleteExperimentQF	HOBO_S4_dataNA	HOBO file for station 4 not available for reaeration experiment
incompleteExperimentQF	fieldDischargeDataNA	Wading survey discharge data not available for reaeration experiment
incompleteExperimentQF	externalLabSaltDataNA	External lab salt data not available for reaeration experiment
incompleteExperimentQF	externalLabGasDataNA	External lab gas data not available for reaeration experiment

\end{table}

In the rea_backgroundFieldSaltData_in and rea_plateauSampleFieldData_in tables, the **incompleteExperimentQF** quality flag is used to indicate that External lab data will not be returned for one or more samples in the specific record. This flag is populated on a semi-annual basis following science review. For example, an externalLabSaltSampleDataNA flag indicates that no salt concentrations will be returned from the external lab for the saltTracerSampleID, but external lab gas data may be returned for the gas sample in the same record and external lab salt data may be returned for other salt samples collected during the respective reaeration experiment. If more than one flag is applicable, the appropriate flags with be concatenated with a pipe "|" delimiter.

Table 3: Descriptions of the dataQF codes for quality flagging external lab data

fieldName	value	definition
incompleteExperimentQF	externalLabSaltSampleDataNA	External lab salt data not available for sample
incompleteExperimentQF	externalLabGasSampleDataNA	External lab gas data not available for sample

\end{table}

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)

4.6 Analytical Facility Data Quality

Data analyses conducted for reaeration conform to the current data quality standards used by practitioners. On at least an annual basis a QAQC summary file is reported that contains a description of the method, method detection limit, precision, and measurement uncertainty associated with a specific time range and analyte. This is published in the **rea_externalLabSummaryData** or **sbd_externalLabSummaryFile** table in the expanded download package.

As of 07/01/20, analytical replicate values ran in the lab as a process check are recorded in the appropriate analyticalReplicate column. Samples that were run multiple times by the lab are recorded as additional rows. Prior to 07/01/20, sample replicate values can be pulled from the remarks field. In all cases where NEON has asked for samples to be re-run following data return, sample data is submitted as a new row and all data published to allow user to evaluate data.

5 REFERENCES

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6 APPENDIX

6.1 Calculating salt-based discharge from a constant rate injection

$$Q = \left[\frac{C_1 - C_b}{C_2 - C_b}\right] q$$

where

Q is the discharge of the stream

q is the rate of flow of the injected tracer solution (table: fieldData, fields: dripRateStart & dripRateEnd, there will be one pair of records per site per injection experiment date)

C_b is the background concentration of the stream (table: externalLabDataSalt where saltSamplID = saltBackgroundSampleID, there will be one record for each station)

C_1 is the concentration of the tracer solution injected into the stream (table: externalLabDataSalt where saltSamplID = injectateSampleID, there will be one record per site per injection experiment date)

C_2 is the measured concentration of the plateau of the concentration-time curve (table: externalLabDataSalt where saltSamplID = saltTracerSampleID, there will be 5 replicates for each station)

Adapted from Rantz et al. U.S. Geological Survey, Water Supply Paper 2175, chapter 7.

6.2 Calculating salt-based discharge from a slug injection

$$Q = \frac{V_1 \cdot C_1}{\int_0^\infty (C - C_b)dt}$$

where

Q is the discharge of the stream

V_1 is the volume of the tracer solution introduced into the stream (calculate as the difference between the dripEndTime and dripStartTime multiplied by drapRateStart and/or dripRateEnd, all found in fieldData table, there will be one set of records per site per injection experiment date)

C_1 is the concentration of the tracer solution injected into the stream (table: externalLabDataSalt where saltSamplID = injectateSampleID, there will be one record per site per injection experiment date)

C is the measured concentration at a given time at thge downstream sampling site (the conductivityFieldData table contains conductivity measurements recorded at stations #1 and #4 every 10 seconds during the tracer injection; users should not include data collected prior to the dripStartTime in their calculations)

C_b is the background concentration of the stream (table: externalLabDataSalt where saltSamplID = saltBackgroundSampleID, there will be one record for each station)

The term $\int_0^\infty (C - C_b)dt$ can be approximated by the term

$$\Sigma_{i=1}^{N} \frac{(C_i - C_b)(t_{i+1} - t_{i-1})}{2}$$

where

i is the sequence number of a sample (table: conductivityFieldData, field: measurementNumber)

N is the total number of samples (measurement number of the last measurementNumber used minus measurementNumber for dateTimeLogger ~ dripStartTime)

t_i is time when sample, C_i, is obtained (table: conductivityFieldData, field: dateTimeLogger)

Adapted from Rantz et al. U.S. Geological Survey, Water Supply Paper 2175, chapter 7.

6.3 Calculating reaeration rates

6.3.1 Calculating Tracer Gas (SF6) Loss Rate

1. Background correct the salt (NaCl or NaBr) plateau samples.
2. Divide SF6 concentrations by the background corrected salt plateau samples for the site
3. LR_{SF6} is the slope of the relationship between LN(salt corrected SF6 concentration)(y-axis) and distance downstream (x-axis)

6.3.2 Calculating travel times and velocity

$$Vr = downstreamDistance/traveltime$$

The time difference between the station #1 and #4 peak of the slug or time of arrival of 50 % of the relative concentration for a constant rate injection is the travel time. There are some other methods of estimating travel time using the initial rise, center of mass, or harmonic mean for a slug injection, which could also be used (Calkins and Dunne, 1970; Waldon, 2004).

6.3.3 Calculating Tracer Gas Reaeration Rate

$$k_{SF6} = LR_{SF6} \cdot V_r$$

where

LR_{SF6} is the SF6 loss rate

V_r is the water velocity

6.3.4 Calculating Gas Transfer Velocity for O_2

$$k_2 = k_{SF6} \cdot 1.34$$

where

k_{SF6} is the SF6 reaeration rate coefficient

1.34 is from Wanninkhof (1992)

$$k_{O_2} = k_2 \cdot z$$

where

k_2 is the O_2 reaeration rate coefficient

z is the mean depth (Q/Wavg/Vr) (table: conductivityFieldData, field: waterTemp)

6.3.5 Normalize O_2 Gas Transfer Velocity to schmidt number of 600 (Jahne et al. 1987, Wanninkhof 1992, Raymond et al. 2012)

$$k_{600} = \left(\frac{600}{S_{CO_2}}\right)^{-0.5} \cdot k_{O_2}$$

$$S_{CO_2} = A - BT + CT^2 - DT^3 = 1800.6 - 120.10 \cdot T + 3.7818 \cdot T^2 - 0.047608 \cdot T^3$$

where

T is the mean temperature in degrees Celsius (table: conductivityFieldData, field: waterTemp)

6.3.6 k_{600} can be used to calculate the k of any gas at any temperature using (Jahne et al. 1987, Wanninkhof 1992)

$$k = \left(\frac{S_{CO_2}}{600}\right)^{-0.5} \cdot k_{600}$$

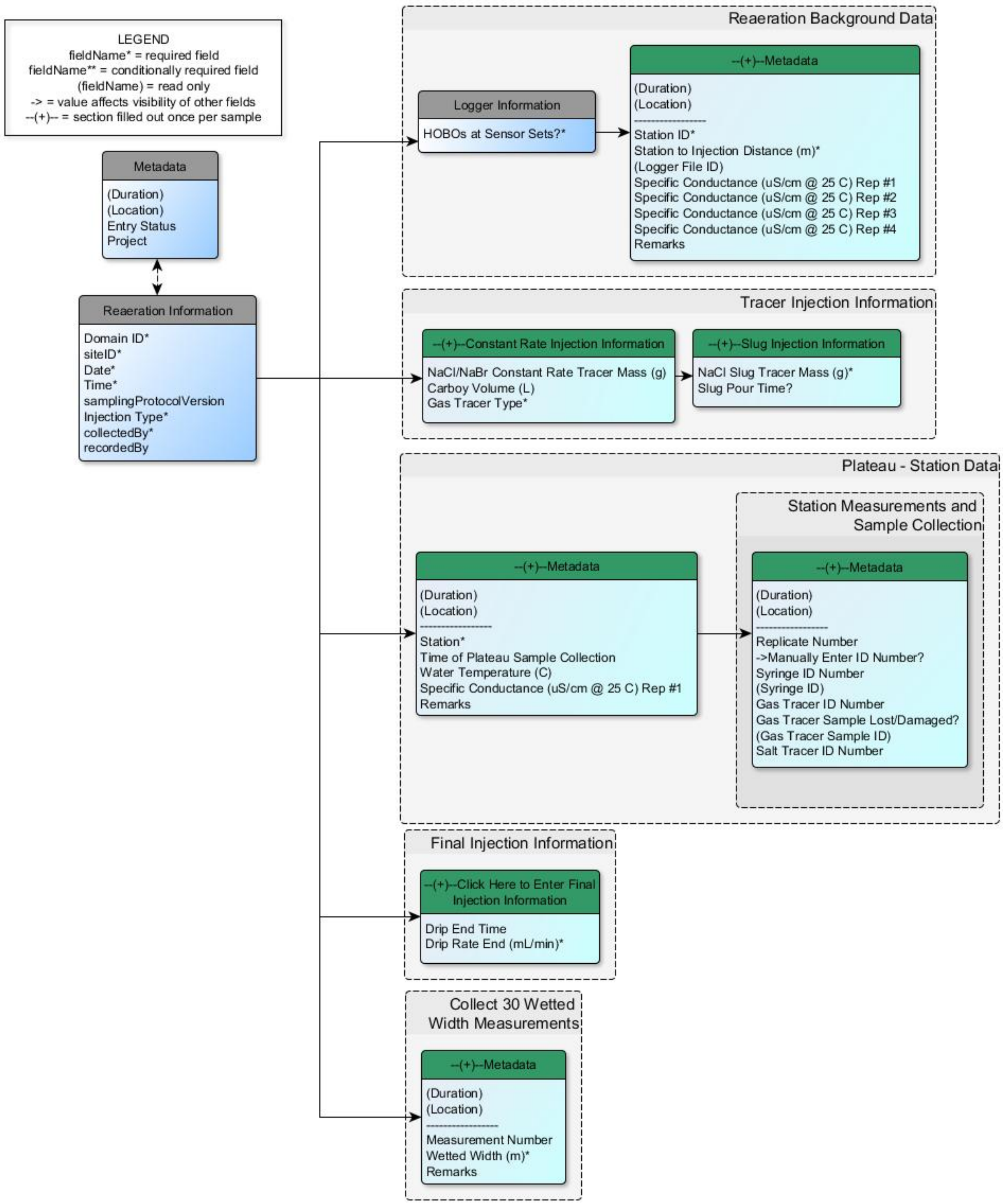

Figure 2: Schematic of the applications used by field technicians to enter reaeration and salt-based discharge data