NEON SCIENCE DATA QUALITY PLAN

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Change Record

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A	08/23/2018	ECO-05580	Initial release

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1 DESCRIPTION

1.1 Purpose

The purpose of this Data Quality Plan is to describe current and developing Quality Assurance and Quality Control (QA/QC) processes relevant to the collection and publication of data to the NEON Portal. This Data Quality Plan outlines the procedures for quality assurance and quality control activities supporting the management and dissemination of ecological data and information collected by the Observatory.

1.2 Scope

This Quality Plan applies to all of the NEON subsystems (IS, OS, AOP) producing data published to the NEON portal during the operations phase. It does not include details about the Commissioning processes executed as part of NEON Construction to ensure the completeness and quality of the initial versions of NEON data products (see RD [03]). The Data Quality Plan covers data workflow activities from planning and training through field sample and data collection, sample analyses, data verification, database operations, and publication on the NEON portal. It addresses requirements for training, sample collection, external laboratory data quality, data quality assurance, preventative maintenance, calibration and validation, data transitioning, and publication.

2 RELATED DOCUMENTS AND ACRONYMS

2.1 Applicable Documents

Applicable documents contain information that shall be applied in the current document. Examples are higher level requirements documents, standards, rules and regulations.

AD [01]	NEON.DOC.000001	NEON Observatory Design
AD [02]	NEON.DOC.050000	NEON Operations and Maintenance Plan
AD [03]	NEON.DOC.002651	NEON Data Product Numbering Convention
AD [04]	NEON.DOC.002652	NEON Level 1, Level 2 and Level 3 Data Products Catalog

2.2 Reference Documents

Reference documents contain information complementing, explaining, detailing, or otherwise supporting the information included in the current document.

RD [01]	NEON.DOC.000008	NEON Acronym List
RD [02]	NEON.DOC.000243	NEON Glossary of Terms
RD [03]	NEON.DOC.004321	NEON Science Commissioning Plan
RD [04]	NEON.DOC.050005	Field Operations Job Instruction Training Plan
RD [05]	NEON.DOC.002979	NEON Animal Care and Use Program Training Plan for Personnel Working with Live Vertebrate Animals
RD [06]	NEON.DOC.001271	AOS/TOS Data Management Protocol
RD [07]	NEON.DOC.004764	NEON Science Availability Plan
RD [08]	NEON.DOC.004825	OS Generic Transitions
RD [09]	NEON.DOC.001025	TOS Protocol and Procedure: Plot Establishment
RD [10]	NEON.DOC.003162	AOS Protocol and Procedure: Wadeable Stream Morphology
RD [11]	NEON.DOC.005512	Sensor Calibration, Validation System Design
RD [12]	NEON.DOC.004978	Instrumented Systems (IS) Algorithm Quality Assurance Document
RD [13]	NEON.DOC.011081	QA/QC Plausibility Testing
RD [14]	NEON.DOC.000783	Time Series Automatic Despiking for TIS Level 1 Data Products
RD [15]	NEON.DOC.001113	Quality Flags and Quality Metrics for TIS Data Products
RD [16]	NEON.DOC.000785	TIS Calibrated Measurements and Level 1 Data Products Uncertainty Budget Plan
RD [17]	NEON.DOC.001973	Flight Operator Training Procedure
RD [18]	NEON.DOC.001517	AOP Calibration Plan
RD [19]	NEON.DOC.004792	AOP Calibration Uncertainty Manual
RD [20]	NEON.DOC.004445	Imaging Spectrometer Calibration procedure
RD [21]	NEON.DOC.001515	AOP Flight Season Management Plan
RD [22]	NEON.DOC.001980	AOP Procedure: Flight Planning
RD [23]	NEON.DOC.001984	AOP Flight Plan Boundaries Design
RD [24]	NEON.DOC.002890	AOP Level 0 Data Quality Checks
RD [25]	NEON.DOC.004652	AOP Data Catalog Interface Control Document
RD [26]	NEON.DOC.004653	AOP Data Processing Pipeline Database Interface Control Document
RD [27]	NEON.DOC.003652	AOP Digital Camera Orthorectification Level 1 Processing Procedure

RD [28]	NEON.DOC.003314	NEON Imaging Spectrometer Level-1 Processing Procedure
RD [29]	NEON.DOC.003315	NEON NIS Level 1 Processing Procedure
RD [30]	NEON.DOC.003316	NEON Discrete LiDAR Level 1 Processing Procedure

2.3 External References

External references contain information pertinent to this document but are not NEON configuration-controlled. Examples include manuals, brochures, technical notes, and external websites.

ER [01]	Kelling S, Johnston A, Hochachka WM, Iliff M, Fink D, Gerbracht J, et al. (2015) Can Observation Skills of Citizen Scientists Be Estimated Using Species Accumulation Curves? PLoS ONE10(10): e0139600. https://doi.org/10.1371/journal.pone.0139600
ER [02]	Zhang J, Nielsen SE, Grainger TN, Kohler M, Chipchar T, Farr DR (2014) Sampling Plant Diversity and Rarity at Landscape Scales: Importance of Sampling Time in Species Detectability. PLoS ONE9(4): e95334. https://doi.org/10.1371/journal.pone.0095334
ER [03]	Rüger N, Berger U, Hubbell SP, Vieilledent G, Condit R (2011) Growth Strategies of Tropical Tree Species: Disentangling Light and Size Effects. PLoS ONE6(9): e25330. https://doi.org/10.1371/journal.pone.0025330
ER [04]	Joint Committee for Guides in Metrology. (2008) 100: Evaluation of measurement data – Guide to the expression of uncertainty in measurement.
ER [05]	Taylor, J. R. (1997) An introduction to error analysis: the study of uncertainties in physical measurements. 2nd ed. Sausalito, Calif.: University Science Books.
ER [06]	Taylor, B. N., and Kuyatt, C. E. (1994) Guidelines for evaluating and expressing the uncertainty of NIST measurement results. [Gaithersburg, Md.]: U.S. Department of Commerce, Technology Administration, National Institute of Standards and Technology.
ER [07]	Shiny from RStudio | https://shiny.rstudio.com/
ER [08]	GitHub | https://github.com/
ER [09]	http://help.ebird.org/customer/en/portal/articles/1055676-understanding-the-ebird-review-and-data-quality-process, accessed 18 October 2017.

2.4 Acronyms

AOP	Airborne Observation Platform
ATBD	Algorithm Theoretical Basis Document
CI-Dev	Cyberinfrastructure Development team
CLA	Collections and Laboratory Analysis
CVAL	Calibration, Validation and Audit Laboratory
DIWB	Data Ingest Workbook
FE	Permanent Field Ecologists
FT	Temporary Field Technician
HQ	NEON Headquarters
IACUC	Institutional Animal Care and Use Committee
IS	Instrumented Systems
NICL	NEON’s Ingest Conversion Language
OS	Observation Systems
PDR	Processed Data Repository
QA/QC	Quality Assurance and Quality Control

RFP	Request for Proposals
SCI	NEON HQ Science team
SOM	IS Science Operations Management
SOP	Standard Operating Procedure
UID	Unique identifier

2.5 Terminology

The use of common names for NEON software applications can vary across departments and domains. These applications have one technically accurate name, and at times one or more “common” names describing the same item. This section aims to clarify and associate “common” names with the technical names herein.

SYNONYMOUS AND COMMON NAME(S)	NEON TECHNICAL REFERENCE NAME
Fulcrum	Mobile Data Entry Application Platform
Magpie	Fulcrum Data QC Application
the Editor	OS L0 Data Editor
the Deleter	OS L0 Data Deleter

3 INTRODUCTION TO THE QA/QC FRAMEWORKS AND ASSURANCE PLANS

This Data Quality Plan describes the data frameworks that are currently in place, as well as the plans for additional development in the initial operations phase. The NEON subsystems are grouped based on the common QA/QC frameworks that they share. The three QA/QC frameworks described in this plan are:

1. Terrestrial and Aquatic Observation Systems (OS) Framework (Section 0)
2. Terrestrial and Aquatic Instrument Systems (IS) Framework (Section 0)
3. Airborne Observational Platform (AOP) Framework (Section 0)

Each of these sections includes a description of the existing quality framework, ongoing data QA/QC activities, and proposed data QA/QC improvements.

4 TERRESTRIAL AND AQUATIC OBSERVATIONAL SYSTEM (OS) QUALITY FRAMEWORK

The Terrestrial and Aquatic Observation Systems (OS) are reliant on detailed manual sampling of biological, chemical, and physical parameters in the NEON domains and subsequent analysis and/or curation and archiving of samples. Consequently, the primary source of errant or non-conforming data is human error, and thus quality control in the OS systems is focused on preventing errors at the front end, during data collection, entry, and ingest. The quality of OS data is highly dependent on training of field staff and assurance that OS protocols are executed consistently across the Observatory. In addition to training, data quality tools have been developed to limit the amount of errant data entering the data stream and to recognize errant data prior to final publication on the NEON data portal. Transitioning of the raw data (Level 0; L0 (AD[04])) is also an important quality process necessary to convert and ensure that "raw" observational data are published in a consistent format.

The major components of the OS Quality Framework (Figure 1) for OS data include:

1. Training
2. Vetting and auditing of external analytical laboratories
3. Data entry validation
4. Manual quality checking and data review
5. Automated data ingest validation
6. Data transitioning
7. Automated data QC
8. Data editing
9. Data revisioning

These components are described in Section 4 below. The OS training program and the data quality tools that are currently in place (Figure 1) include:

- Data entry validations (mobile applications developed in the Fulcrum platform [Spatial Networks, Inc.])
- Manual quality checks (performed by Field Science and Headquarters (HQ) Science staff)
- Data review (via custom Shiny (ER [07]) applications, known collectively as 'Magpie')
- Automated quality checks and validation (via the automated Cyberinfrastructure routines executed during the ingest of data, known as the 'Parser')
- Data processing (i.e., the transitioning of data from raw to higher level data products, as described in Algorithmic Theoretical Basis Documents (ATBDs; see Appendix 2))
- Publication processing of data for delivery on the NEON Data Portal

In addition, this section briefly outlines how NEON ensures and monitors the quality of data from external laboratory services. The end of Section 0 outlines future quality assurance improvements that are either currently under development or proposed solutions to fill in existing gaps in data quality process.

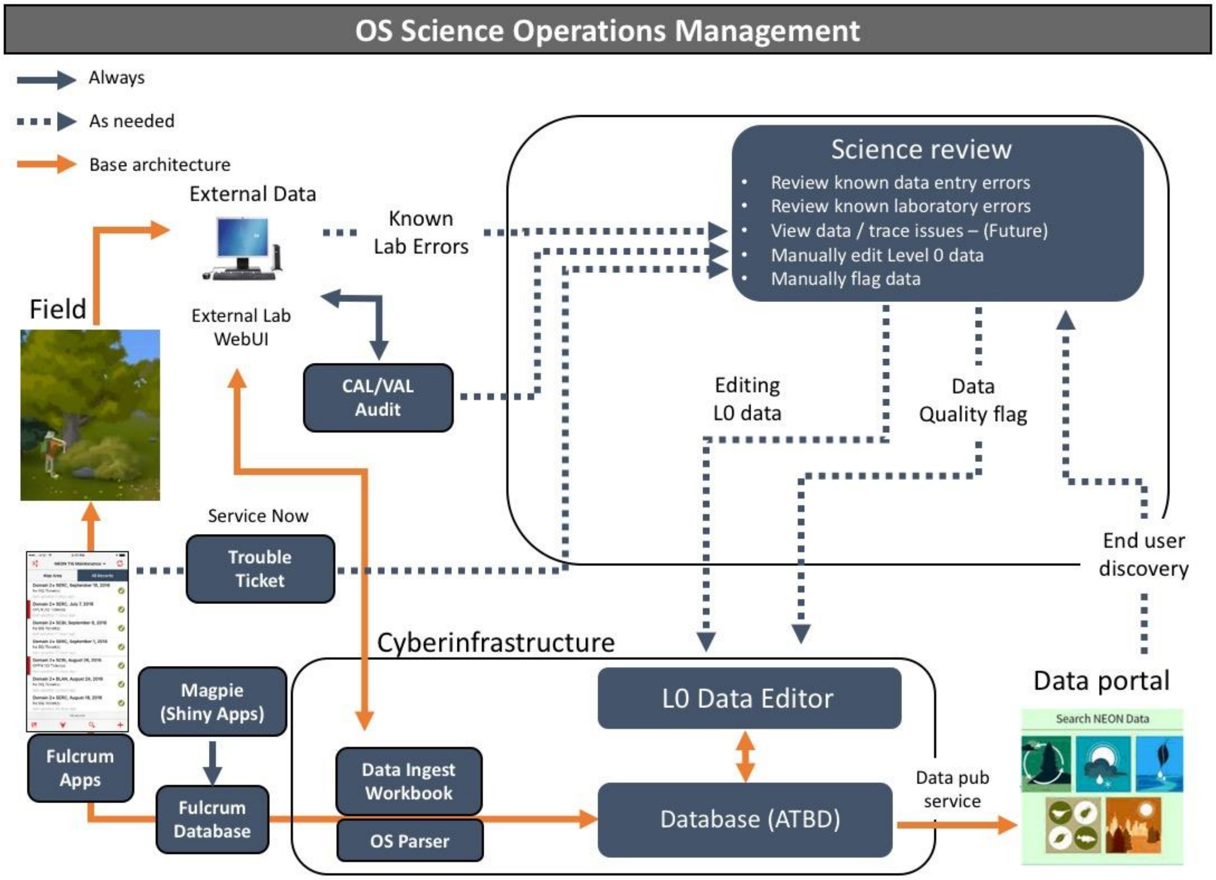

Figure 1. OS data QA/QC framework.

4.1 Training for TOS and AOS

Field staff are critical to OS data quality through manual sampling, analysis, and data entry. The Field Operations Job Instruction Training Plan ([RD [04]) describes the process used to design, develop, and deliver training for field staff responsible for (a) sampling as defined for the OS and (b) instrument maintenance as required for the Instrument Systems (IS). The Job Instruction Training Plan addresses the need for training temporary field technicians (FTs) and permanent field ecologists (FEs) on protocols and procedures associated with OS and IS subsystems. Field ecologists oversee all of the sampling and lead the crews of temporary field technicians. The training program for compliance with NEON's Institutional Animal Care and Use Committee (IACUC) is provided in the NEON Animal Care and Use Program Training Plan for Personnel Working with Live Vertebrate Animals (RD [05]).

4.1.1 OS Training Materials

The HQ Curriculum Designer initially developed the curricular materials for training on TOS protocols. The content is based on released protocols and discussions with the protocol author(s), the HQ staff scientist(s) with relevant subject matter expertise. Protocol authors review and approve all materials before field staff employ them. This includes PowerPoint presentations, graphics, instructional videos, lesson plans (which include a written quiz and answer sheet), and online recertification/refresher quizzes.

AOS training materials were initially developed at HQ by the aquatic science staff, using the same template and format as the TOS training materials. These materials were all designed to be instructor-led and provided broad descriptions of the procedure. More recently, the Curriculum Designer has developed self-guided training modules and online assessments that explore details of implementing protocols. In addition, an AOS Curriculum Guide provides directions for trainers on training new aquatic technicians.

Annual updates to the OS curriculum is a collaboration among the Curriculum Designer, field staff, and protocol authors. Curriculum revisers update materials, incorporate protocol revisions, and augment content with best practices and lessons learned in the field. After revisions are complete, the protocol author provides a final review and approval of all training materials.

NEON's intranet is used to distribute training materials to field staff. The materials are not included in NEON's document configuration system; however, a date and revision letter are used to track the versioning of the training materials. Materials also reference the corresponding version of the released document(s) on title pages of presentations and lesson plans. The Curriculum Designer is responsible for versioning, distributing new or revised training materials when they are available, and removing obsolete versions from circulation. All training materials are published in the 'Training Center' on the NEON intranet by the Curriculum Designer, following review by HQ Science staff. Records of review and approval are in development and are expected to be implemented in FY2018.

When new materials or versions of existing materials are uploaded to the Training Center, the designated Training Liaison at each Domain Support Facility is notified via the Training Liaison Bulletin Board. Liaisons are responsible for disseminating information to appropriate staff, although the Bulletin Board is visible to all field staff. In addition, the availability of new materials is announced at the weekly (TOS) or bi-weekly (AOS) Issue Resolution meetings and included in meeting notes. By design, master training materials can be copied and then modified by field staff to include domain- and site-specific content as needed. The Curriculum Designer is notified via email of any inadvertent changes to the master materials, so the master can be restored.

4.1.2 Training for OS

Experienced field ecologists and returning temporary field technicians are selected annually as designated trainers for each protocol within each domain. Trainers must take an online quiz and receive a score of 90 percent or higher before being certified to train others. In addition, at training events (see below), trainers must demonstrate competency by completing field and lab practicums under the observation of either protocol authors and/or fully trained colleagues.

Trainers are provided with a Curriculum Guide to training, an online presentation, and, for AOS trainers, a one-on-one remote session with the Curriculum Designer. The guide details the location of all training materials, how to use them, documentation procedures, and best practices for adult learning. Trainers also have access to the Curriculum Designer and protocol authors for questions, considerations, and feedback. When available, annual gatherings for large group trainings are held. These training events are primarily held for permanent staff and address best practices, including training components such as protocol implementation challenges.

Trainees are required to review self-guided training modules and the protocols prior to the hands-on training. Field staff designated as trainers provide hands-on training. Training is primarily domain-based. The training consists of classroom presentations and practicums in the field and laboratory. Following the completion of these components, newly trained field technicians work directly with experienced field staff on implementing protocols. Each TOS protocol has a lesson plan that provides the trainer with a framework for effective delivery of the curriculum. AOS lesson plans are thematically grouped based on target media of protocols: chemical, biological, or physical. Lesson plans include specific learning objectives, an estimate of the amount of time required for the lesson, material lists, directions for preparing for training, guidance on lesson development, and written quizzes for FTs to take as part of training. FEs and returning FTs are required to review protocols for updates and take an online refresher quiz to ensure they are up to date with recent protocol modifications.

4.1.3 Documentation of Completion of Training

A combination of written quizzes, online quizzes, and observation-based assessments (using checklists) are used to certify that field staff are qualified to conduct NEON procedures. Other than the online quizzes and training for procedures that must comply with NEON's IACUC, all records of completion are maintained by the Field Operations Manager and stored at the Domain Support Facility.

4.2 Field Data Planning and Tracking

4.2.1 Field Collection Planning

Planning of field data collection requires identification of protocols to be implemented at each field site in each year, timing of collection (e.g., growing season, peak green, peak biomass), and frequency of collection (e.g., bi-weekly, every 3 weeks, every 5 years). Detailed timing and frequency requirements for field collection, lab processing, and sample shipping for analysis are in configuration-controlled protocols. To aid in planning, estimated dates for annual onset and cessation of sampling are in configured protocols and aquatic site sampling design documents. For protocols that are conducted only once every 5 years, schedules are developed by balancing vegetation and climate regimes, staff availability, and coordination with AOP overflight schedules. In addition, each year Field Operations Managers create detailed schedules of all AOS and TOS sampling by site by day. Schedules are reviewed by protocol authors, and, following the implementation of any requested changes, annual schedules are posted on the NEON intranet for internal reference. Subsequently, any changes to the annual or inter-annual schedules are implemented only when approved by the Operations Integrated Product Team, which includes representatives from the Program Management Office, Science and Education, Field Science, Engineering, Finance, and Cyberinfrastructure.

4.2.2 Tracking and Reporting of Sample Collection Bouts

Field Operations Managers provide monthly status reports on the planned vs. completed bouts per protocol. Sampling deviations that result from protocol requirements (e.g., temperature threshold for sampling not met) or hazardous site conditions (e.g., stream flow exceeds safe wading limits) are noted, but these deviations are not included in percent completion metrics. Only sampling missed due to resource shortages or logistical issues can negatively impact the percent completion metric for a site. Throughout the month, potential or actual interruptions to data collection are reported via an internal incident reporting system. Beginning in 2019, HQ Science will also generate additional metrics of data quality and completeness, as described in the Science Availability plan (RD [07]).

4.2.3 OS Issue Tracking and Resolution

Field staff report field incidents through the internal incident reporting system. Generated incidence reports request protocol clarifications, report non-conforming sampling events, alert HQ Science about potential data quality issues, etc. Incident report recipients are responsible for resolving these issues. Resolutions may lead to protocol clarifications, protocol revisions, or changes to the training program. The internal incident reporting system can be queried for specific types of incidents.

4.3 Field Data Entry Validation and Review

4.3.1 Field Data Collection

Field staff capture information about the collection process as samples and data are collected. This includes all details on who, what, where, when, and how the samples and data are collected, along with pertinent observations and sample chain of custody information. Field staff are responsible for following all sampling requirements outlined within individual protocols and corresponding Standard Operating Procedures (SOPs). Field staff record data electronically on mobile devices using Fulcrum data applications whenever possible (see 4.3.3 below), but field staff always have paper datasheets available in case of hardware failure.

4.3.2 Transcription and Storage of Field and Lab Data Recorded with Paper Datasheets

Paper datasheets are change controlled documents made available for each relevant SOP of a sampling protocol. While technicians are required to use mobile data entry applications whenever possible, adverse field conditions or equipment failure may necessitate collecting data on paper. The OS Data Management Protocol (RD [06]) provides field staff with instructions on how to ensure that data collected on paper are properly handled from field collection to data entry. To summarize the protocol:

a) paper datasheets are scanned and saved as a digital copy upon return from the field
b) the data are entered into a data entry application
c) the digital data are reviewed (data quality check) to ensure that typos are not introduced into the final dataset
d) the paper copies stored at the Domain Support Facility are shipped at the end of the year to NEON headquarters for long-term reference

Data quality checks for manually recorded data involve reviewing a minimum of 10 or 10% (whichever is greater) of digital records against paper datasheets per sampling bout per protocol. Field staff randomly select the records to be checked and compare paper datasheet values against digital records. All data values are checked, and corrections made if there are deviations between paper and digital copies. If a single correction is made to a digital record, it is noted as an error. If the total errors detected exceeds 5% of the records checked, technicians must review an additional 10% of records to verify data quality. If the 5% threshold is exceeded for a third time, technicians are required to review every data record.

4.3.3 Data Entered Directly into Data Entry Applications

Digital data entry applications have been created for all OS sampling protocols using the Fulcrum platform (Spatial Networks, Inc.), and some AOS protocols also use the NEON Cyberinfrastructure (CI) spreadsheet uploader web interface. Fulcrum allows a developer to build and deploy a single application to many different operating systems simultaneously. Field staff can therefore collect data on a diversity of mobile devices, as well as enter data through a web browser on a desktop computer. In each case, the user interface has a consistent appearance, data validation rules, and workflow. Fulcrum applications implement quality control through several methods at the user interface level (Table 1). This means that data values are controlled and assessed at the time and point of capture. Data are prevented from entering the system, and moving on to data publication, if any validation rules are violated.

Table 1. Fulcrum application Quality Control method examples.

Method	Reason	Example(s)
Geographic Range Constraint	Field staff must select valid, geo-referenced locations for most protocols.	For collecting soil samples, technicians may only select plotID values that have the code "sls" associated with them.
Taxonomic Value Constraint	Field staff may only select animal or plant taxa that are known and that may exist within a domain's geographic boundaries.	For plant observations, technicians may only select taxonID codes published in the US Department of Agriculture's PLANT Database (plants.usda.gov) for a given domain.
Required Fields	Certain data fields are critical to a data product; field staff therefore cannot save and submit data unless a record includes values for these fields.	Data records are rejected if they are missing a valid sampling location, a sampling date, and/or username (i.e., who recorded the data).
List of Values (LOV) Constraint	Certain data fields have a limited set of acceptable values; field staff choose the value from a drop-down menu, rather than manually typing them, to prevent typos and ensure consistency.	The position of a plant's upper canopy, in relation to other plants, can only be described with five distinct values: "Open grown", "Full sun", "Partially shaded", "Mostly shaded", or "Full shade". Ticks must be identified as belonging to one growth stage: "larval", "nymph", or "adult".
Numeric Range	Most numeric data fields have established or reasonable minimum and	Soil pH values must be positive, recorded with

Constraint	maximum values. The sign of the numeric value is also important for interpretation.	decimals, and in the range [0, 14]. The diameter of a tree must be greater than 0 and less than 400 centimeters.
Conditional Validation	More complex scenarios necessitate comparing data values across different fields, and constraining the entry into one field based on the value entered into another field.	Male mammals can never be recorded as pregnant. The mass of a dried soil sample (i.e., after oven drying) must be less than the wet mass.

4.3.4 Data Review with the Fulcrum Data QC Application

Data entered directly onto mobile devices cannot be compared to a paper copy. With the large number of automatic, direct, and "in place" data validations made at time of entry (Table 1), field staff can instead focus on verifying higher-level data quality standards upon return from the field. These checks currently include verifying that data sets maintain referential integrity, the absence of duplicate records (within a table), orphan records (data that are missing a valid upstream parent sample), or "barren parent" records (parent samples missing required downstream child samples).

Fulcrum user interfaces are not designed to check or maintain referential integrity, therefore a separate QC application, code-named "Magpie", has been developed on a Shiny platform (ER [07]). The Magpie application is a user interface that allows field staff to query Fulcrum data tables for the presence of duplicate data records. Duplicate records are identified by information specified in the data ingest workbook (DIWB, see section 4.6.1 below for more details), and typically includes the combination of sampling location, date, and type to create a NEON unique identifier. If field staff find duplicate records, they first determine whether the record set consists of exact matches (i.e., every data value in the record set is identical) or inexact matches (i.e., one or more data values are not identical across the duplicate record set). Exact matches can be reported for deletion before data are ingested; inexact matches can either be corrected or reported for deletion, as appropriate. Additional functionality for Magpie is in development (see section 4.10 below).

4.4 External Laboratory Quality

4.4.1 External Laboratory Contracts and Audits

External laboratories conduct numerous analyses on samples collected by NEON field staff and return the resulting data to NEON HQ. The data quality requirements for external laboratory services flow down from NEON HQ Science and are detailed in the Request for Proposals (RFPs) and corresponding procurement contracts. The NEON Calibration, Validation and Audit Laboratory (CVAL) participates in the evaluation and selection of labs that bid on the RFPs. Once the selection is made, CVAL performs a pre-award document audit and, if necessary, an onsite audit to ensure the offeror's quality systems, equipment, and facilities will meet contractual needs. After awards are made, CVAL performs an annual audit of the laboratory (or more frequently, if quality comes into question). At a minimum, an annual audit ensures that the documentation is up to date and that data submission to NEON is proceeding according to plan. Annual audits can also include on-site audits or analysis audits where CVAL will send a known sample (blind, if possible) to ensure quality performance. Where external laboratory data quality does not meet data requirements, science stakeholders are made aware to discuss impact to data and potential data flagging needs. Further, if the laboratory is unable to remedy the relevant quality issues, the contract may be terminated and a new vendor sought.

4.4.2 Sample Tracking and External Laboratory Data Validation

Upon collection, field staff assign sample identifiers to each collected sample. Identifiers consist of a human-readable ID following a specified format, a barcode label, or both. Sample IDs are applied physically to the sample container and noted in the corresponding data record. At a minimum, these IDs are unique within each NEON protocol and domain combination. These sample IDs are critical to maintaining a chain of custody for each sample and for linking analytical data generated in the laboratory for a given sample to its associated field metadata.

At prescribed intervals throughout the field season, field staff package and ship field-collected samples to the designated analytical or archive facility. Associated with each shipment is a shipping manifest that captures all of the sample IDs contained within the shipment. A hard-copy of the manifest is included in the package, while a digital version is emailed to the receiving facility and NEON Collections and Laboratory Analysis (CLA) staff. Sample shipping manifests are generated manually or, more recently, via the shipping application developed in Fulcrum. Confirmation of receipt by the receiving facility is done through email and uploading of the receipt data into NEON's central Processed Data Repository (PDR) via the NEON CI spreadsheet upload interface. NEON CLA staff are responsible for maintaining digital copies of all shipping manifests.

External facilities upload analytical and/or custody data on a fixed schedule, as defined in the contract. Uploading of data is done through the CI spreadsheet uploader web interface. CLA and HQ Science are responsible for monitoring for deficiencies and resolving them with the contractors. CLA matches the number of samples invoiced with the number of samples in the returned data to inform invoice approval. If the number of samples shipped is small, CLA may manually match up samples shipped with data returned using data spreadsheets. The current process relies on the responsible staff scientist (typically the protocol author) to confirm that NEON is not charged twice for the same data.

4.5 Post-Collection Data Validation with the OS Parser (LO Data)

Once the data passes through the Fulcrum database or spreadsheet uploader, it enters the Parser (see section 4.6.1 below) and is quality assured through the instructions outlined in the Data Ingest Workbook, as described in section 4.6.1 below (see also Figure 1), prior to ingestion into the database.

Fulcrum HQ is the custom software that pulls data from Fulcrum and submits it to the OS Parser. Fulcrum HQ queries the Fulcrum cloud daily, and data that fall into a specific date range are automatically pulled from Fulcrum. Lag times for automatic ingest of Fulcrum data are defined per protocol to allow sufficient time for field staff to review and QC the data. When it pulls records, Fulcrum

HQ locks those records in Fulcrum, so field staff cannot modify data that have been posted to PDR. The data are then submitted to the Parser for further validation. If the Parser finds errors and rejects the data, Fulcrum HQ rolls back the transaction and unlocks the records, so data can be corrected by field or HQ science staff, as appropriate, before the next pull attempt.

4.6 Data Ingest Validation

4.6.1 OS Parser and Data Quality Control Ingest Workbook (DIWB)

All data ingested into the OS database tables are processed through the OS Parser, whether the data originate in Fulcrum applications or spreadsheets (Figure 1). See section 4.3.3 above for further details about Fulcrum applications. Data in spreadsheet format are uploaded via a custom NEON web-based interface. The OS Parser is an automated software system that reads and evaluates incoming data according to rules established in the DIWB. Parser validation rules are written in a standardized syntax called NEON's Ingest Conversion Language (NICL) that is interpreted and implemented in this software system (see NEON's Document Library – data.neonscience.org/documents – for a draft document explaining the language in greater detail: https://bit.ly/2pRAyAq). The Parser prevents data from entering the NEON database (PDR), if any rules defined by the DIWB are violated.

The DIWB is a machine-readable spreadsheet that describes all the data fields collected for a given data product and defines the Parser validation rules for each field. The spreadsheet includes information that directs the Parser on:

a) where to post the incoming data in NEON's PDR
b) measurement units and data types
c) minimum/maximum data value ranges
d) conditional data validation rules (e.g., collection date must be after setup date)
e) valid values for categorical data (a.k.a., 'list of values')
f) valid names and geographic ranges of taxonomic identifications
g) which data fields are considered the unique identifier for a sample
h) referential integrity checks (e.g., "this unique sampleID must not already exist in PDR upon ingest" or "this sampleID must have a parent primary key in a related table").

The DIWB also contains instructions for simple calculations that can be conducted on incoming data to generate data quality flags or derived values using logical or arithmetic statements. Note that calculations are only possible using individual fields within a single data record; no summaries across records are calculated using this system.

Data ingest through the OS Parser is tested by a mockup data ingest workbook and corresponding mockup dataset, referred to as the 'Ingest Breaker'. The Ingest Breaker workbook contains several data product tables, across which there is at least one field validated or created by each available NICL function. The Ingest Breaker dataset consists of paired spreadsheets for each data product table: an input spreadsheet, to be uploaded to the Parser, and an output spreadsheet, containing the expected Level 0 data post to the database. For a subset of data product tables, there are also input data spreadsheets designed to be failed by the Parser for specified reasons; since these will not post to the database, they do not have corresponding output spreadsheets.

Data that enter the OS pipeline through the spreadsheet uploader or through Fulcrum are ingested by the Parser and their data values are checked against the rules and specifications described in the DIWB. Records that pass validation move on through the ingest process to populate the Level 0 database. Records that fail validation are rejected by the Parser, preventing ingest into the Level 0 database. Rejected records generate error messages that describe what caused the failure; these messages are sent to field staff and HQ Science staff, depending on the nature of the error and the source of the data (i.e., Fulcrum vs. external laboratory). In the spreadsheet-uploader user interface, the Parser operates two checkpoints, first running all non-sample-related validations. Error messages from this checkpoint are displayed to the user in real time. The user can correct the errors and re-submit, if possible. If data pass this first checkpoint, sample-related validations are then carried out. Errors at this stage are sent to NEON staff as described above. Staff can correct data errors or seek out the appropriate contacts to make corrections; if data are determined to be correct, or workflows are at fault, data collection applications or DIWBs may be modified to allow data ingest. The first batches of ingested L0 and processed L1 data for each data product are verified by the protocol author and a Data Products scientist using simple scripts to summarize and plot the data, facilitating the identification of unexpected or unreasonable values. Similar checks to be executed automatically against all processed data are in development to continually monitor quality.

4.7 OS Data Transitioning

All OS data products are transitioned (processed from incoming Level 0 values to Level 1 values posted on the public-facing data portal) via an Algorithm Theoretical Basis Document (ATBD; RD [08]). ATBDs describe (a) the process by which select incoming L0 fields are verified and copied to L1 for public consumption and metadata on geolocation and habitat attributes from definitional data tables maintained inside PDR are associated with incoming L0 data, and (b) the standardized routines for rectifying scientific names and higher taxonomically identified organisms, to include fuzzing or redaction of rare, threatened and endangered species (RT&E), as necessary.

Each datum stored in PDR is associated with a 'named location'; e.g., HARV_001.basePlot.div is one of the valid named locations for conducting plant diversity sampling. As part of the TOS plot establishment protocol (RD [09]), the AOS Rapid Habitat Assessment and Geomorphology protocol (RD [10]) and AIS sensor installation process, structured metadata about the location are collected either via field measurements (e.g., latitude, longitude, elevation) or from geodatabases (e.g., land cover, soil types). These data are uploaded to PDR separately (usually once, though updates are possible), through an independent process from the ongoing recording of repeat field measurements of individual data streams. The transition system joins information from the two data sources to deliver a complete data + metadata package on the portal.

4.7.1 Assigning Taxonomic information

For each type of taxonomic survey conducted by NEON (e.g., beetles, small mammals, fish), HQ science staff maintains a list of recognized names and synonyms, compiled from a variety of published or online sources (e.g., the Integrated Taxonomic Information Service - www.itis.gov). The taxon lists also include additional information on higher taxonomy (e.g., family, order, etc.) which field staff are not expected to know or return with the data. The transition system looks up taxa in incoming data streams by code or scientific name, determines the currently accepted scientific name for each datum, and returns the updated name plus associated higher taxonomy. For taxonomic identifications performed by NEON field staff, the end user receives only the de-synonymized names and associated higher taxonomy. For taxonomic identifications conducted by professional contractors, the end user will receive both the NEON-accepted taxonomy plus the original names and higher taxonomy applied by the taxonomist.

4.7.2 Fuzzing Taxonomy for RT&E

When a species of concern (Federally or State-listed taxa) is taxonomically identified as part of NEON's regular data collection, the ATBD fuzzes the taxonomic identifications as part of the L0->L1 processing (RD [08]). Fuzzing the taxonomic identifications consists of reassigning the taxonID code and associated scientificName from an identifying taxon (e.g., *Zapus hudonius preblei*) to a non-identifying taxonID code and scientificName (e.g., *Zapus sp*.). Where all species within a genus that are found in a domain are species of concern, NEON will fuzz taxonomy to the level of family (e.g., Dipodidae *sp.*). Note that genus sp. and family sp. taxonomic identifications are also regularly employed by technicians during regular sampling to designate individuals that were not identified to species (e.g., individuals missing pertinent morphological features required to key out the taxonomy to species). Thus, publication of a genus sp. or family sp. datum is not a definitive clue to locations of RT&E taxa. If full redaction is required for a site by species on request of the landowner (as is the case for the Great Smoky Mountains National Park site), the entire record of that taxon is redacted from the L1 output during processing.

4.7.3 Testing and Verification of Transition

The generic OS transition code is tested by Science using a mockup data ingest workbook, publication workbook, and corresponding data, referred to as the 'Transition Tester', as well as by CI staff employing standard unit testing and integration protocols. The Transition Tester publication workbook contains several data product tables, across which there is at least one field transitioned from L0 to L1 by each available data source. The Transition Tester data consists of paired spreadsheets for each data product table: an input spreadsheet, to be uploaded to the parser, and an output spreadsheet, containing the expected Level 1 data posted to the database after ingest and transition of the inputs. The Transition Tester is re-processed after any update to the transition code to ensure all functionality is retained and is version-controlled in a GitHub™ repository.

4.8 Data Publication

4.8.1 OS Publication Workbook

The OS Publication workbook serves a dual purpose:

a) to define the transition of data from L0 to L1 for a given product, and
b) to define the publication of L1 data to the data portal for a given product.

The workbook is machine-readable, and machine-read, for both purposes. Data transition is defined by fields in the publication workbook indicating:

a) the database location of L0 data to be transitioned
b) the type of transition for each datum: untransformed, location data, sample data, or taxonomic data
c) fixed inputs to the transition, such as which taxonomic data to search (plants, beetles, etc.)
d) the database location for the L1 data to be written to.

4.8.2 Publication of data to the NEON Portal

The publication process is shared for all OS data and IS data other than eddy covariance. The publication software extracts data from the database (PDR) and packages it for download, based on the criteria defined in the publication workbook. Publication criteria defined in the publication workbook include:

a) the database location of data to be published
b) field names, which are used both as identifiers in the database and as column headers in published data
c) data type, units, and measurement scale
d) data modifications to be made in publication process, such as rounding of numeric values and obfuscation of technician names
e) the spatial and temporal resolution for publication of each data table: are data specific to a site or to a laboratory, and how should user date query be interpreted?
f) basic vs. expanded data package designations.

Data products published by this process are published in a non-proprietary, tabular format (comma-delimited).

4.9 OS L0 Data Editor

Editing of L0 data is a critical component of OS data quality. As noted above, quality control in the OS subsystems is focused on avoiding errors at the points of entry and ingest. However, some low rate of error is expected to persist. When errors do occur and are discovered, L0 data editing allows for correction to be made as close to the point of origin as possible. Error discovery is currently opportunistic, but automated routines for error discovery are in development.

There are three interfaces involved in OS L0 data editing:

(1) the OS L0 Data Editor (the Editor)
(2) the OS L0 Data Deleter (the Deleter)
(3) the Sample Editor.

They serve different but complementary purposes, as described below.

4.9.1 The Editor

The Editor is a third point of entry into the OS Parser, in addition to Fulcrum and spreadsheet upload. L0 data are downloaded from the L0 Data Viewer, edited, and uploaded back to the Editor. The Editor uses the Parser to evaluate the changes that will be made to L0 data if the uploaded data are parsed, including edits to downstream data products not included in the upload. Spreadsheets of current data and pending edits are presented to the user for review and a submit button presented. If the user chooses to submit, the changes are processed by the Parser and posted to the database. This process ensures that all data edits are subject to the same rigorous validation processes as any other data.

4.9.2 The Deleter

In some cases, entire records or sets of records of OS data may need to be deleted from the database. The most common cause of this is accidental submission of duplicate data. The Parser is able to prevent duplicate submissions in certain circumstances, but not all.

Every record of OS L0 data in the database is numbered by a Unique identifier (UID). The Deleter is a simple interface that takes an input of a list of UIDs for deletion. Like the Editor, before posting to the database, it presents the user with a spreadsheet of changes that will be made if deletes are submitted.

4.9.3 The Sample Editor

Some edits to samples are made through the Editor, because they involve edits to the relationships between samples and data on a per-record basis, potentially resulting in the generation of new samples and re-assigning data to other samples. These types of changes need to pass through the full capabilities of the Parser. However, for the unique case of changing the identifier of a sample, but nothing else about the sample, the edit is made through the Sample Editor. The Sample Editor is a user interface that allows editing of a single sample identifier at a time; editable identifiers include sample tags, barcodes, and UIDs. The Sample Editor will change the value of a sample identifier in every instance where it appears in the database, retaining the underlying sample-data relationship. If an edit will result in changes to data or sample-data relationships, the Sample Editor rejects the edit and informs the user.

4.9.4 Post-Edit Transitions

After editing L0 data, the transition to L1 data must be re-run so that edits are reflected in published data. This is referred to as re-processing and is described below in section 5.9.3.

4.10 OS Quality Assurance Improvements under Development and Future Considerations

4.10.1 OS Training

Moving forward, updating of the OS training materials will become more integrated across teams, relying on the protocol authors (HQ Science), Field Science, and the curriculum designer. Current materials will be expanded upon to provide more details on how to implement protocols, according to lessons learned. Format for these materials will be self-guided and include online assessments. Best practices identified in the field will also be incorporated into the training materials where appropriate.

4.10.1.1 Long-term OS curriculum and training program plans

Annual turnover of field staff across the Observatory will remain a constant challenge to training and for ensuring consistency in protocol execution across all domains. Domain-centric training, while allowing focus on local flora and fauna identification, terrain and other domain-specific idiosyncrasies, lends to the divergence and persistence of potentially inconsistent or incomparable data. A training evaluation program should be developed and implemented. The training program should assess training effectiveness, trainers, trainee competencies, and facility operations. Due to the annual turnover of field staff, mentoring and additional in-field training may prove a more efficient use of time and resources than implementing individual or facility audits that only later inform the training program.

A learning management system that allows NEON to track completed training requirements and certifications would improve NEON's ability to manage work assignments and ensure proper staffing. NEON could also cross-reference data collection to training records to ensure staff has had sufficient experience prior to leading a data collection activity.

For OS, assessments or in field mentoring schemes are needed to ensure field technicians properly execute assigned protocols and perform all QA/QC procedures associated with data quality. Assessment tools are currently under development (see Appendix 1). However, the plan for executing assessments and facility audits will need to adapt based on the data quality issues identified over time. This will ensure that quality improvement efforts are focused on the areas with the greatest need for improvement.

4.10.2 Planning and Tracking of Field Collections

Development of the annual sampling plan for all sites is currently a manual process. It may be beneficial to automate scheduling and tracking execution against plan. This could improve the planning process among various stakeholders and potentially reduce the risk of introducing errors into the schedule, maximize sampling efficiency, and potentially reduce the number of missed data collection bouts. However, several protocols have schedules that are difficult to forecast. Changes in the number, and timing of expected sampling bouts due to fluctuating budgets or seasonality, etc., will continually challenge NEON's ability to automate sample bout scheduling.

The NEON Science Availability Plan (RD [07]) outlines the requirements for the availability of data on the NEON portal by site and subsystem. For example, a minimum of 80% of scheduled small mammal trapping nights should be completed at each site and the resulting data available to the end user. NEON reports monthly on performed fieldwork relative to plan, but does not follow the reporting through to the data available on the portal. The development of an automated means to track completed data collection bouts against data published to the portal would allow efficient calculation of availability metrics. Opportunities remain to identify root causes for missing data (missing sample collection, incomplete data, compromised sample integrity during shipment, lab analysis issues, lost samples, data not synchronized from data tablets, etc.). Monitoring of these metrics will facilitate corrective action.

4.10.3 External Laboratory Data Tracking

A Fulcrum sample tracking application automates shipping manifests and sample tracking by the field staff. This application enables all information pertaining to the chain of custody, including samples shipped, samples received, and data received, to be maintained in a database. Contractors can upload a sample receipt form, and the uploaded data are immediately validated or rejected if there are any deficiencies. The system is also planned to have a reporting capability that allows CLA to be notified of outstanding or missing data. Data can then be queried to determine if samples were shipped, received, and that data were analyzed and accepted by NEON's validation process. The system will output the number of samples that can be invoiced. The system is also planned to be updated to flag samples for which data were already received and invoiced to ensure duplicate payments are not made.

4.10.4 OS Data Versioning and Revision

See Section 5.9.3 Data Versioning under IS below, as it also pertains to OS data products.

4.10.5 Manual Flagging of Data

Each OS data product contains a placeholder field for manual entry of data quality flags. At present, these are generally used in only 3 scenarios: (1) To capture flagged data from external labs, using lab-specific routines; (2) To flag data from labs which have failed audits and (3) To flag legacy data which was imported into the CI system outside of the usual ingest pipeline and may therefore have not had all ingest QA/QC steps applied. Unlike the IS system, manual flagging occurs at the L0 data level and flags are copied to L1 during transition. This allows flags to be preserved when data are reprocessed.

During the initial deployment of each data product, one round of 'eyes-on' data checks was conducted to identify any systematic errors in the pipeline, but the data volume for OS during operations will far exceed that where humans can individually review all the data. The OS science staff envisions a system where a suite of automated tests would be developed through time to identify implausible data points for flagging and/or follow-up corrective action. Due to the heterogeneous nature of the OS data products, many of these tests will likely need to be data-product specific. A non-exhaustive list of possible analytical tests includes:

(1) Modeling observer effects to quantify systematic variation among technicians in quantities of interest. See Kelling et al. (2015; ER [01]) and Zhang et al. (2014; ER[02]) for examples of similar routines from other monitoring programs.

a. Flag data collected by technicians who consistently record implausible or outlier values
b. Follow-up with improved training practices to reduce inter-technician variation where it is high
c. Provide summary reports to end users to understand consistency of data collection

(2) Outlier detection.

a. Can be achieved through a variety of statistical methods, ranging from visual tests of summary statistics (currently employed by groups such as the Nutrient Network (NutNet)), to univariate analyses of individual measurement streams, to hierarchical models incorporating expected variation over space, time, and/or taxonomic groups, to more sophisticated hierarchical mixture models specifically designed to discriminate specific types of observational error (e.g., typos and mislabeled samples vs. routine measurement error); for an example of the latter, see Rüger et al. 2011 (ER[03]).
b. Outlier analysis may be conducted on raw data and/or derived quantities. For example, eBird checks included automated flagging of high total counts of individual species, individuals recorded out of season, or in unexpected geographic locations (ER [09]). Similarly, NEON should be able to take advantage of the repeated sampling central to the design to understand expected values and rates of temporal fluctuation for a variety of OS basic and derived data quantities.

(3) Crowd-sourcing error detection

a. The volume of external data users is expected to be much higher than the internal NEON staff as NEON moves into operations. Formalizing a feedback mechanism for external users to report data issues, HQ to staff to confirm and apply flags, is an additional venue for improved flagging and error detection.

Continued improvement of analytical routines to identify data quality problems and apply flags is expected throughout the life of the observatory. There is not a single accepted model for these types of quality checks in the ecological community, and it will likely be appropriate to solicit suggestions from the external community. This type of request for feedback could include surveys, technical working groups, workshops, or hackathons to develop a suite of best practices and code with extensive user-group buy-in.

5 AQUATIC AND TERRESTRIAL INSTRUMENT SYSTEMS (IS) QUALITY FRAMEWORK

NEON represents one of the largest and most diverse environmental sensor networks, streaming hundreds of gigabytes (GB) of sensor data per day. The quality of IS data is thus highly dependent on proper functioning of the sensors. To ensure data quality, NEON sensors are routinely calibrated, and field staff execute a robust preventative maintenance plan and remain vigilant when working around the sensors. Any measurement interference or visible problems observed in the field initiates a pathway to data flagging and resolution. The automated quality flagging of these data during the transition process to higher level data products (i.e., Level 1 and higher) is also an indispensable component of QA/QC. The details of the quality flagging for each data product can be found in its respective ATBD (see Appendix 2 for a complete list). However, the QC tests applied during the transition are largely limited to short time periods (< 4 hours) and data from a single sensor assembly at a time. Longer term and cross-sensor analyses are required to capture more complex sensor issues where the data are within plausibility limits but not representative of true environmental variation. A basic set of these analyses is operational, and more are in development. Finally, the results of quality tests and flagging are monitored, and recurring incidents diagnosed to trigger corrective action and verify that NEON scientific requirements are being met.

The major components of the IS Quality Framework (Figure 2) for IS data include:

1. Training
2. Sensor Preventive Maintenance
3. Sensor Calibration
4. Data Transitioning
5. Sensor Incident Tracking and Resolution
6. Continuous Data Monitoring
7. Data Revisioning

5.1 Training for IS

The IS training program is described in the Curriculum Guide for Instrument Systems Training. The guide describes the curriculum for training field staff on preventative maintenance of NEON's AIS and TIS and includes a summary of training responsibilities, prerequisites, and a description of the training materials. Training consists of independent study, on-the-job training and large group gatherings when available. Trainers provide training to new hires and use lesson plans within the Curriculum Guide to prepare for and deliver training. To date, field staff who have successfully maintained the NEON tower are identified as qualified trainers by Field Operations Managers and an Assistant Director for Field Operations. A new IS Training Curriculum is currently under development and will include requirements for trainers to be certified through a combination of a demonstration of technical proficiency, written assessment, participation in a training session, and a demonstration of training ability.

Development and updating of IS curricular materials follow a process similar to the OS curricular materials, described in Section 4.1. Initial training materials are developed from released maintenance documents. Once developed, training materials will be reviewed annually and updated when procedures

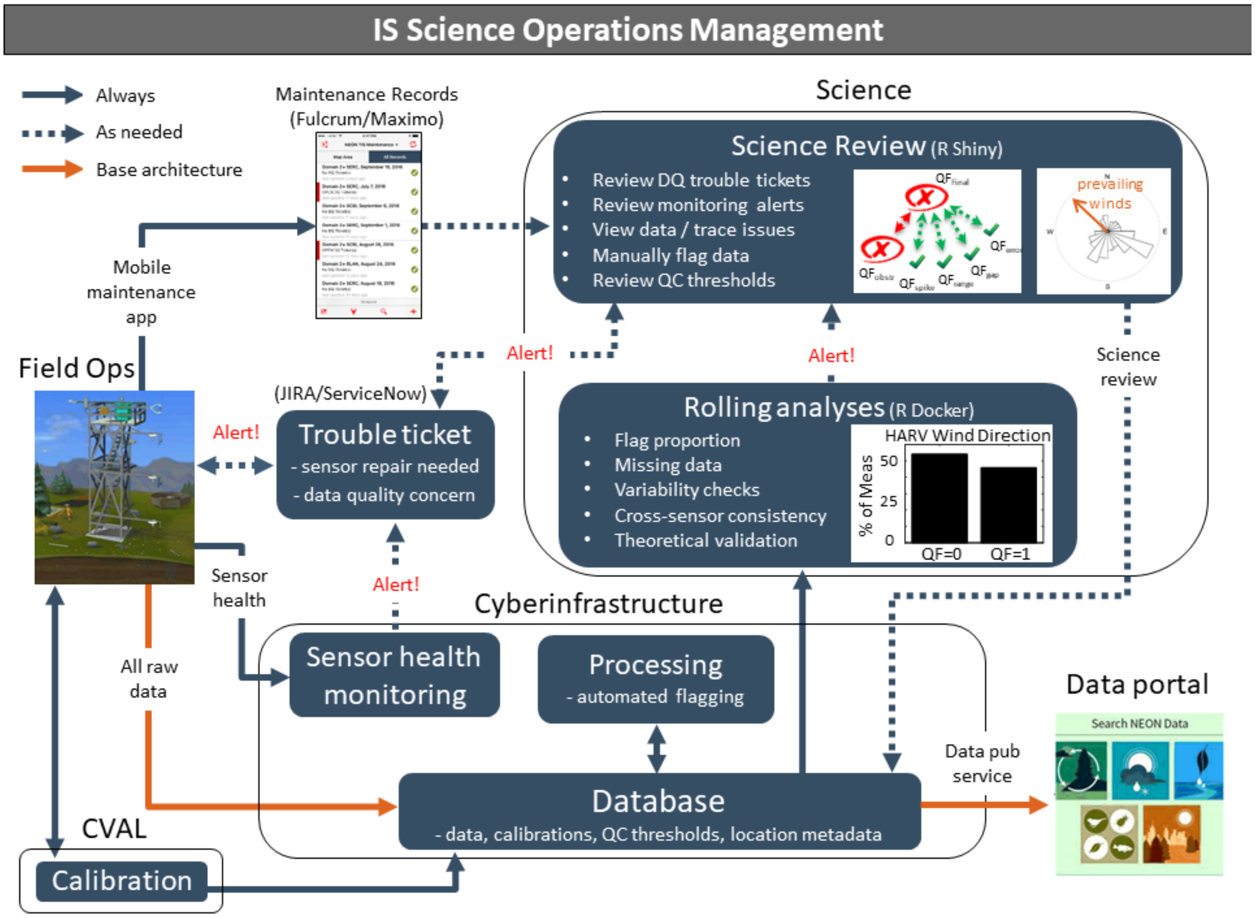

Figure 2. IS data QA/QC framework.

are revised. Wherever possible, best practices from the field are incorporated into the training materials as part of the revision process. Training materials are developed at HQ by the Instrument Training Content Developer, who works closely with the Curriculum Designer and science and engineering staff. Field and HQ science and engineering staff review all training materials prior to release.

5.2 Sensor Preventative Maintenance

Preventative maintenance is performed every other week (or as needed) for instrumented systems at NEON field sites. Complete instructions for performing preventative maintenance are within Preventative Maintenance Procedures (PMPs) specific to each instrument assembly as well as site infrastructure. These PMPs are change controlled and provided in electronic format, so they are easily accessible on field tablets while on site. Field technicians record all maintenance activities with a Fulcrum mobile application (Spatial Networks, Inc.). This application helps guide the workflow of preventative maintenance, has entries specific to each PMP, and includes tips and reminders for more complex tasks. The application also allows recording of time spent performing preventative maintenance for each subsystem, recording corrective maintenance tasks, and staging information to enter into the trouble-ticket management system and asset management system when returning to the lab.

5.3 Sensor Calibration Program

The sensor calibration system design document (RD [11]) details the calibration's traceability to national or international standards, including both documented and physical standards. Often, the physical standards' calibrations are outsourced to certified metrology facilities unless transfer of standards are maintained or acquired by CVAL. The frequency of calibration for each type of sensor has also been identified in RD [11]; these frequencies are based on the science requirements for sensor performance as captured in the NEON requirements database. However, current plans for monitoring the drift of calibration could modify the calibration frequency to be more or less frequent, depending on results and requirements. The sensor calibration system design (RD [11]) dictates that most instruments will be swapped out in the field annually with freshly calibrated sensors and returned to CVAL for re-calibration and deployment. In some instances, a sensor may return to the factory for factory calibrations, if more economical than developing the calibration capabilities in CVAL (e.g., DustTrak™, TSI, Inc.) or if a particular sensor fails CVAL validation (e.g., 3D Sonic Anemometer). Instrument metadata will be verified upon receiving the instrument back at NEON CVAL. In other cases, instruments may stay in the field and transfer standard/s will be used on-site to calibrate and validate the instruments, as per sensor-specific requirements (RD [11]). Comparisons with secondary transfer standards may be regularly scheduled or made on a case-by-case basis pending incident tracking reports. Specific Standard Operating Procedures for the calibration and operation of each type of sensor are captured in revision-controlled calibration documents. The product of calibrations are calibration messages. The calibration messages which include calibration information needed for transitions of data (as defined by ATBDs) are sent to the CI data pipeline and are then automatically incorporated into the data processing algorithms. The messages also contain sensor and calibration metadata for traceability to standards and conditions. Finally, messages provide a valid date range for when the calibration can be applied to a measurement stream as defined by RD [11] for frequency of calibrations, which is read into the data processing algorithm to generate quality flags if a sensor measurement stream goes outside the range.

5.4 Data Transitioning

All IS data products have an associated Algorithm Theoretical Basis Document (ATBD) which describes the processes necessary to convert "raw" sensor measurements into meaningful scientific units and their associated uncertainties. ATBDs include a detailed discussion of measurement theory and implementation, appropriate theoretical background, the linkage of the data stream(s) to the calibration file, data product provenance, specific quality assurance and control methods used, approximations and/or assumptions made, and a detailed exposition of uncertainty resulting in a cumulative reported uncertainty for the data product. A number of steps are involved in ensuring that the algorithms provided by Science in IS ATBDs are producing data as expected. An overview is provided here; additional details can be found in RD [12].

5.4.1 Algorithm Quality Assurance

The process of developing a data product detailed in this section is iterative in nature and involves numerous validation checkpoints between the Cyberinfrastructure Development team (CI-Dev) and Science (SCI) to ensure data quality. CVAL is also involved to ensure coefficient nomenclature, calibrated algorithms and stream identifications are properly captured. The amount of elapsed time from initial meetings between SCI and CI-Dev and the release of data products on the portal is a function of the complexity of the data and the algorithms within the ATBD. The framework below is broken down by deliverables and the team(s) responsible for their completion (Table 2). Many of the steps and deliverables have overlapping parts, and the entire process is dynamic. Active communication between CI-Dev and SCI is an important component of the framework which ensures the data products are completed in an efficient manner. The start of this process to the end release of the data products on the NEON data portal usually takes 3 to 6 months.

Table 2: Overview of team-specific deliverables for generating data products.

Deliverable	Description	Team
Command Control and Configuration Document (C^3)	A document that informs the configuration (e.g., output streams and reporting frequency) and command and control (e.g., heater controls) for a specific sensor type	SCI
Ingest Workbook	Contains details pertaining to L0 data products used in respective ATBD algorithms	SCI
Publication Workbook	Contains details pertaining to L1 data products produced via the algorithms within respective ATBD	SCI
Algorithm Theoretical Basis Document (ATBD)	Details the algorithms used for creating NEON Level 1 data products from Level 0 data, and ancillary data as defined in this document (such as calibration data) obtained via instrumental measurements made by a measurement assembly.	SCI
Constraint Thresholds	Informs the thresholds for QAQC tests performed during the transition from raw to processed data, as specified in the ATBD. The constraint files are structured such that specific constraints can be assigned to an individual instance of a sensor, e.g., ML1 SAAT can be assigned different QAQC constraints than other SAAT assemblies on the same tower.	SCI
Calibration Coefficients	An xml document containing applicable calibration coefficients for a specific sensor. These documents are traceable to a sensor's EPROM ID.	CVAL
Golden Dataset SCI	A .csv file containing L0' data for algorithm testing by SCI and CI. The term 'golden' infers that all data within this file should PASS all QAQC tests applicable to the sensor. The golden file produced by SCI is considered the reference dataset that the CI-Dev dataset will be compared to.	SCI
Tarnished Dataset SCI	A .csv file containing L0' data for algorithm testing by SCI and CI. The term 'tarnished' indicates that a majority of the data within this file should FAIL specified QAQC tests applicable to the sensor. Additionally, this file usually contains missing data and/or data gaps (consecutive missing data), which will inhibit certain QAQC	SCI

Deliverable	Description	Team
	tests from being run. The tarnished file produced by SCI is considered the reference dataset that the CI-Dev dataset will be compared to.	
Golden Dataset CI-Dev	A .csv file containing L0' data for algorithm testing by SCI and CI. The term 'golden' infers that all data within this file should PASS all QAQC tests applicable to the sensor. Used for comparison against the SCI golden dataset.	CI-Dev
Tarnished Dataset CI-Dev	A .csv file containing L0' data for algorithm testing by SCI and CI. The term 'tarnished' indicates that a majority of the data within this file should FAIL specified QAQC tests applicable to the sensor. Additionally, this file usually contains missing data and/or data gaps (consecutive missing data), which will inhibit certain QAQC tests from being run. Used for comparison against the SCI tarnished dataset.	CI-Dev
CERT Data	L1 data products produced by CI-Dev in the Certification (CERT) environment. These data are generated after SCI verifies that the SCI and CI golden / tarnished data are valid.	CI-Dev
PROD Data	L1 data products produced by CI-Dev in Production (PROD) environment. These data are generated after SCI verifies the L1 Data from CDS.	CI-Dev

5.4.1.1 Ingest and Publication Workbooks

These data product-specific deliverables, along with the ATBD, are interrelated and dependent on one another. The ingest workbook informs the raw (L0) data output by the sensor(s) to be used in the transition. Publication workbooks inform calibrated and quality controlled (L1) data products produced via the algorithms in the ATBD. The ATBD details the processes needed for converting the raw sensor data to calibrated and, in most cases, temporally aggregated data products. Ingest and publication workbooks can either be generated using spreadsheets or by using R scripts found in the *NEON-How to Make a Data Product* GitHub Repository. The creation of ingest workbooks is informed by the L0 data products listed within the respective sensor's Command Control and Configuration (C3) document. The data products outlined in the ingest workbook are used as inputs within the ATBD. As noted above, the complexity of an ATBD is a function of the underlying measurement theory and required algorithms. References to ingest and publication workbook are found within each ATBD to guide the CI-Dev team to these necessary components.

Once completed, ingest and publication workbooks are validated via NEON's DPS Data Product App. The back end of this application is the definitive database of identifiers and controlled terms for all NEON data products. The application will check for errors within the respective workbook and provide a breakdown of terms, units, and descriptions. If no errors exist in the respective workbook, the responsible scientist alerts a member of NEON's Data Products (DPS) group and uploads the workbook(s) to the appropriate version-controlled GitHub Repository. The workbooks are then assigned unique data product numbers and accessible for CI-Dev use. If the workbooks need to be updated at any time, the scientist is responsible for making these updates and repeating this process until no errors in the workbook exist.

5.4.1.2 ATBDs

Active communication among SCI, CVAL and CI-Dev is critical to delivering a robust ATBD. An initial draft of the ATBD is delivered to CVAL and CI-Dev early in data product development, to allow teams to begin analyzing the algorithm and check for inconsistencies between the data fields listed within the ATBDs and those found in the respective ingest, calibration files and publication workbooks. This also provides an opportunity for CI-Dev to request any necessary clarifications on equations and/or quality control processes detailed in the ATBD. During the time CI-Dev is reviewing the ATBD, the scientist(s) typically begin generating the threshold files (detailed in the section below). After analyzing the ATBD, the member(s) of CI-Dev responsible for coding the algorithms will provide a list of comments and questions to the scientist. This process is iterative and usually takes approximately 6 rounds of editing to ensure that SCI and CI-Dev have the same understanding of the data product details.

5.4.1.3 Constraint Thresholds

The constraint thresholds contain the parameter values needed to apply the quality control (QC) algorithms within the ATBD. For all IS sensors, a nominal suite of QC tests is applied to inform the validity of the data (these can be found in RD [13]RD [11]). In most cases, a single file of constraint thresholds is needed for a sensor assembly. However, there are some instances where multiple constraint files are needed. For instance, some sensor assemblies (e.g., 2D wind) require additional QC tests that are sensor-specific and not applicable to all sensors within the suite of IS measurement systems. In some instances, communication among SCI, CI-Dev, and NEON's System Integration and Verification team is necessary to ensure certain algorithm parameters (e.g., boom direction) are properly documented for CI-Dev to implement in their code.

Constraint thresholds are typically generated using data-driven methods, scientific judgment, and/or applicable resources from the World Meteorological Organization (WMO), National Oceanic and Atmospheric Administration (NOAA), other governing body, and information from NEON's CVAL. All constraint thresholds will be refined over time on a site-by-site or measurement level-by-measurement level basis using historical climatological data or NEON data when enough have been gathered for robust analysis. Site- or measurement level-specific thresholds are maintained in constraint files by SCI in a GitHub repository. CI transfers this information into PDR for use during data processing. CI is currently developing an application that will allow SCI to upload the constraint thresholds directly to PDR so that constraint information exists in only one location.

5.4.1.4 Calibration Coefficients

In many cases, raw sensor data (L0) are calibrated to meaningful scientific units, e.g., from V to W m^{-2}, via calibration coefficients provided by CVAL. Only a select few sensors throughout the NEON Observatory do not utilize calibration coefficients because their raw data are already calibrated internally within the sensor. Whether or not calibration coefficients are needed for a specific sensor-type is indicated in the ATBD. However, even when calibration coefficients are not applied, CI must still store and link the calibration information to carry the traceability from the calibration through to the data product and to ensure the calibration frequency policy (see section 5.3 above) is maintained for flagging purposes. The calibration coefficients are provided by CVAL and stored in the CI data store (a local repository managed by CI), and then provided to the data users by CI.

5.4.1.5 Golden and Tarnished Datasets

Two types of datasets are independently generated by SCI and CI-Dev to test the validity of the algorithms specified in the ATBD. Golden and tarnished datasets cannot be generated until the ATBD, ingest workbook, publication workbook, constraint file(s), and calibration (if applicable) files are finalized. In both cases, SCI and CI-Dev start with the same input (L0) data and aim to produce identical output, i.e., the L0' data and QC flags (see section 5.4.2 below) detailed within the ATBD. Coding these algorithms independently and in different programming languages tests the robustness of the algorithm to convert raw and uncalibrated data to calibrated data and the effectiveness of the communication between SCI and CI. The first dataset comprises 'golden' data needed to generate the temporally aggregated L1 data products derived from the ATBD. The term 'golden' infers that all L0 and/or L1 input data *pass* all the QC tests within the dataset. The second dataset comprises tarnished data, i.e., it includes data that will fail one or more QC test. Taken together, these tarnished data must represent the spectrum of possible failures for all QC tests specified in the ATBD. These datasets are typically created for only a single site and include at least one- to two-days' worth of data in these files.

After SCI submits the golden and tarnished data to CI-Dev, the CI-Dev team reviews SCI's datasets and also creates their own. Once complete, the CI-Dev team will compare their data to that prepared by SCI. If the data within the respective files do not match, CI and SCI collaborate to resolve discrepancies. SCI is responsible for the final verification of the golden and tarnished datasets.

5.4.1.6 CERT and PROD Data

Once SCI has verified the output of the golden and tarnished data, the CI-Dev team generates L1 Data Products in their Certification (CERT) environment. These data are sent to SCI for verification of data signatures and data quality. If issues are discovered, CI and SCI collaborate to resolve them. Once issues are resolved, CI-Dev processes the data in the Production (PROD) environment. A final check is done by comparing the PROD and CERT data to ensure consistency, and then the CI-Dev team delivers the data product to the Cyberinfrastructure-Operations (CI-Ops) team for deployment to the Data Portal.

5.4.2 Automated Data Quality Control

Each ATBD specifies the automated quality control algorithms and procedures that applied to the data transitioned into usable data products. As described in RD [13] and RD [14], these include a standard suite of plausibility tests applied to individual calibrated raw measurements that evaluate whether data are present and whether the measurements are within acceptable limits for range and variability. In addition, each ATBD specifies relevant sensor-specific quality tests, such as evaluating status codes reported directly from the sensor or evaluating the adequacy of airflow through the assembly.

Using data-driven methods, the HQ Science team specifies thresholds for quality control tests that determine if data are acceptable. Quality thresholds are maintained in a version-controlled library. When insufficient data are available to determine appropriate test thresholds, historical values or expert knowledge are used to set test limits until enough data are available. Test thresholds will be re-evaluated at regular (e.g., annual) intervals or when continuous data monitoring procedures (see below) identify the need for adjustment.

The results of automated quality control algorithms applied to calibrated raw measurements are aggregated into corresponding Quality Metrics that summarize the proportion of raw values that passed, failed, or could not be evaluated over the aggregation interval of the data product (e.g., for each 30-minute average value). The Quality Metrics for individual quality tests are then aggregated further into a Final Quality Flag for each output value, representing a use/do-not-use indicator. The Final Quality Flag is included with the basic download package of the data product, and the results of the individual Quality Metrics are provided in the expanded download package. The detailed procedure for determining Quality Metrics and the Final Quality Flag is described in RD [15].

5.4.3 Uncertainty Estimation

The objective of a measurement is to estimate the value of a particular quantity known as the measurand. Because uncertainty of measurement is inevitable, measurements should be accompanied by a statement of their uncertainty for completeness (JCGM 2008 (ER[04]); Taylor 1997 (ER[05])). Quantifying the uncertainty of IS measurements provides a measure of the reliability and applicability of individual measurements and their associated IS data products. The IS Calibrated Measurements and Level 1 Data Products Uncertainty Budget Plan (RD [16]) describes the philosophy and rationale for assuring that estimates of IS measurement uncertainties are traceable to nationally and internationally accepted standards. This document serves as a guideline for quantifying measurement uncertainties of in-situ, sensor-based measurements throughout the Observatory.

The basis of this overarching philosophy spawns from the Guide to the Expression of Uncertainty in Measurement (commonly referred to as the Guide or GUM; JCGM 100:2008, ISO 1995; ER[04]). The purpose of the GUM is to promote information regarding the quantification of measurement uncertainties and to provide a basis for the international comparison of measurement results (ISO 1995). The National Institute of Standards and Technology (NIST) follows the principles set forth in the Guide and provides further suggestions for correct quantification of measurement uncertainties (Taylor and Kuyatt 1994; ER[06]). The JCGM (100: 2008) GUM is as updated version of ISO's (1995) version, and is the most up to date reference.

For all purposes, the processes by which NEON evaluates and quantifies measurement uncertainties emulates those proposed by JCGM (2008). This approach ensures that NEON's IS data products are traceable to accepted standards. Additionally, all methods are transparent to the end-user via ATBDs provided with each data product.

5.5 Data Publication

As in data transitioning, the process detailed in this section is iterative and involves numerous validation checkpoints between CI-Ops and SCI, before the final data are released on the Data Portal. The phases of the IS Workflow outlined below may require repeating tasks and re-starting the process from various checkpoints. The IS Workflow is broken down by publication testing environments and the team(s) responsible for their completion. Communication and completion of tasks by SCI and CI-Ops is coordinated by a SCI data products team member. Table 3 provides definitions of the critical deliverables and resources that inform IS Algorithm Quality Assurance during the publication phase.

Table 3. Overview of terms associated with releasing a data product to the Data Portal

Terms	Description
L1 Test Data	A subset of an L1 data product from one NEON site over a limited time-frame. These test data represent exactly what will be published on the Data Portal.
CERT-Portal	A certification development version of the production infrastructure that is useful for testing functionality and operations prior to performing them in the PROD-Portal.
PROD-Portal	The production environment used for managing science data and operations for data product publication.
ReadMe File	A .txt file that contains high level information about the data product (i.e. sensor information, study area, etc.) and is automatically generated during the publication process and is included in the published data packages.
Change Log	Part of the Data Product ReadMe file. Contains high level descriptions of issues and resolutions (i.e. manual flagging for data at a given site location and/or date range).
Variables File	A .csv file that is automatically generated during the publication process from the Publication Workbook, and contains variable definitions, including data type and units. Included in the published data packages.

5.5.1 Preparation for Publication

SCI reviews and updates the readMe Collector, a document containing specific data products information made available on the NEON Data Portal and in the readme .txt file in the downloaded data packages. The readme Collector includes the data product name, data product ID, science team, data product short name, keywords, data product abstract, data product design description, study area, sensor information, document list, basic description, expanded description, data product catalog remarks, derived data products, source data products, and related data products. Once the readMe Collector is updated, SCI informs the CI-Ops Data Product Portal team, whereupon they verify all updated information and update the Data Product Catalog, if needed.

As an additional quality control measure, SCI reviews all of the documentation again to evaluate the consistency in reported data streams and quality test constraints between the ATBD, Publication Workbook, and Constraint files. As part of this review, SCI also ensures that the appropriate plausibility tests are applied to the data product in the ATBD (RD [13]). If discrepancies exist, SCI updates the documentation and communicates to CI-Dev for re-coding and re-ingesting before the L1 test data are published to the CERT Portal. SCI once again validates the Publication Workbook via NEON's DPS Data

Product App to check for revised terms. In the event that SCI amends the publication workbook, SCI notifies the CI-Ops Data Products Portal Team that new data product terms and numbers need to be assigned. CI-Ops communicates that term assignments are complete, and the Publication Workbook is uploaded by SCI to the CERT Portal in preparation for publishing.

5.5.2 Publication of L1 Test Data to CERT Portal

The scientist responsible for assisting in the development of the data product determines an appropriate site and date range for validation of publication data. After the finalized Publication Workbook has been uploaded to the CERT Portal, these parameters are used by CI-Ops to run L0 to L1 data transitions for the test dataset. Once publication of the L1 test data is successful, CI-Ops notifies SCI to review and validate the data on the CERT Portal.

A series of data quality assurance checks are performed by the scientist who assisted in developing the data product (see RD [12]). SCI reviews the downloaded package to verify the presence of: basic and expanded data packages, the most up-to-date associated documents, the correct number of data files (.csv format) for applicable temporal aggregation periods, appropriate data columns, and attached ReadMe and Variables files. When an unexpected attribute or file is present or an expected attribute or file is missing from the downloaded data packages, the data product requires modification from SCI and republishing from CI-Ops.

During the data check, SCI completes two tasks. First, SCI verifies that all of the expected data files are in the downloaded package. Next, SCI reviews the data and metadata for validity. During the time series data check, the data are scrutinized by SCI for accuracy and realistic fluctuations of the measured environmental phenomenon. SCI also reviews the results of the QC flags. If too many flags are thrown (i.e., not equal to 0) this may indicate a need for adjustments in the QAQC thresholds/constraint files.

After SCI completes the IS Data Product Checklist (RD [12]) and approves the validity of the L1 Test Data on the CERT Portal, SCI uploads the Publication Workbook to the PROD Portal (NEON Data Portal). SCI then confirms to CI-Ops that the L1 Test Data are approved for publication to the PROD Portal.

5.5.3 Publication of L1 Test Data to PROD NEON Data Portal

Upon completion of the test data validation, CI-Ops publishes the L1 Test Data to the PROD Data Portal. Once the L1 Test Data has been successfully published to the PROD Portal, SCI performs the same IS Data Product Checklist that was conducted in the CERT testing environment for the PROD NEON Data Portal with the addition of a metadata review that includes the ReadMe file and Variables file checks. For the ReadMe file check, SCI verifies the following information: the data product name and number are correct, the correct sensor and manufacturer are listed, the correct associated documents are listed, there is a statement on data quality and data citation, and the change log is accurate. During the Variables file check, SCI ensures there is a line for each column in the data file for the smallest applicable temporal aggregation period. A row should be present for every unique row in the Publication Workbook.

In some cases, there will be a need to repeat investigation, coding, ingesting, and/or publishing of the data product. If quality issues are identified at any point in the process, then the workflow tasks are repeated at the appropriate checkpoints. If no additional data quality issues are discovered, SCI notifies CI-Ops that the data product is approved for global deployment and all available sites can be published for that data product. CI-Ops turns on all L0 to L1 transitions for the data product.

5.6 Sensor Problem Tracking and Resolution

NEON field sites host a suite of scientific instruments that stream data continuously to NEON headquarters (HQ) for processing into data products. Many of the instrument systems report status information either directly from the sensor or the status information is derived from logic executed by the location controller (LC). Proper handling and timely routing of sensor health status information is important for: (1) avoidance or correction of instrument problems/errors, and (2) quality control (flagging) of data products when the instrument is in an error state.

While the status information used for (1) and (2) may be similar or identical, the allowable latency period is different. For the purposes of data quality control, sensor status information need only be processed into quality flags sometime prior to publishing the data on the NEON Data Portal, currently about one month after collection of raw sensor measurements. On the other hand, fulfilling NEON's operational availability requirements necessitates near-immediate awareness of sensor malfunction so that appropriate personnel can be notified and corrective actions taken, as subsequent delays in incident resolution are likely unavoidable due to the ordering of replacement parts and/or the frequency of site visits.

Status monitoring of Instrumented Systems occurs at the site level. Information on sensor health status and field reports are sent to HQ where incident reports will be generated and applicable quality flagging will be applied to the data. Two categories of incident tracking differentiate the information source/type as well as downstream handling:

1. Sensor health status warning/error
2. Field-identified measurement interference

5.6.1 Sensor Health Status Warnings and Errors

In addition to reporting scientific measurements, many sensors report their health status. Most often this is in the form of status codes that correspond to normal vs. error conditions. Alternatively, ancillary measurement streams may be used to warn of impending error status, such as when the tank pressure of a calibration gas is low. Sensor health status is continuously monitored so that appropriate action can be taken to avoid or resume normal sensor operation.

The location controller (LC) at each site monitors the health status of each sensor assembly, as specified in the Command, Control, and Configuration (C3) document for each sensor assembly. The Science and Engineering departments have identified the IS sensor or configuration data to be monitored by the LC as part of the Problem Tracking and Resolution system, including the conditions that indicate current or imminent error status, and the information to be reported to the trouble ticket management system.

Currently, field staff use software to manually connect to the LC to discover whether any sensor systems are in error status. If error status is present, the staff either corrects the error immediately or creates an incident report for system for tracking and resolution.

The NEON enterprise incident management system currently in development (ServiceNow™) includes a “knowledge database” that will document solutions to commonly encountered problems. These solutions and corrective maintenance procedures will then be available to those reporting similar issues in the future.

Sensor status information reported directly from the sensor is typically a Level 0 (raw) data product, and appropriate quality flagging occurs during normal processing. In the few cases where quality flagging does not occur in normal processing, the incident report is also sent to HQ Science staff to manually flag downstream data products (see below).

5.6.2 Field-Identified Measurement Interference

NEON measurement assemblies are in the natural environment rather than in a controlled setting. As a result, field staff often encounter the interference of a measurement assembly by some known or unknown cause in which the sensor continues to operate normally but data are adversely affected for a period before, during, or after identification of the problem. For example, in early July of 2016, field staff visited the Smithsonian Environmental Research Center site and found several throughfall precipitation collectors clogged by leaves and animal nests. Thus, the sensors were operating normally but recording no rainfall events. Field staff cleared the blockages, but the throughfall precipitation data between the previous site visit and the date the blockages were cleared needed to be quality flagged. There will also be cases where the problem cannot be resolved immediately, therefore requiring additional tracking and further action to resolve the issue.

Using the incident management system, field staff can tag an issue as a “Data Quality Trouble Ticket”. This alerts HQ Science (SCI) staff to review the issue. Each trouble ticket typically includes the following information:

a) Site
b) Observer
c) Date
d) Issue title and summary
e) Affected sensor and their location
f) NEON asset tag (if available)
g) Photos of the problem
h) Action taken in the field

Upon receipt of an incident report, Science staff reviews data relevant to the quality concern and interacts with field staff via the incident management system to discuss the concern. If warranted, Science manually flags the affected data (see below).

5.7 Continuous Data Monitoring and Resolution

Central to an efficient and robust science operations management framework is the application of algorithms that monitor data quality as data are processed. If too much data are flagged, it could indicate that quality test thresholds need adjustment or that a sensor needs attention. Post-processing tests can also be used to apply more complex analyses useful in detecting data that are within plausibility limits but do not reflect true environmental variation. For example, soil temperature at progressive depths should be correlated. If not, one or more temperature sensors likely need replacement.

The IS Science Operations Management (SOM) tool employs several continuously monitored post-processing tests (“rolling analyses”) that will allow Science staff to monitor data quality and will alert them to potential quality issues needing review. Monitoring algorithms were developed in a version-controlled GitHub repository and verified for accuracy by manually checking random samples of data. The NEON Operations Plan includes a dedicated set of Science staff that will receive and address alerts from this system (AD[02]). "Eyes on the data" is an important component of QA/QC, but it is not feasible to have human eyes on every data product all the time. By providing summary statistics and alerts for human review, eyes on the data can be efficiently targeted where needed.

The following is a non-exhaustive list of rolling analyses being implemented within IS SOM.

- Quality flag duration/proportion (large amounts of data flagged) (Implemented)
- Complete time-series check (missing time stamps) (Implemented)
- Time-frequency analysis (Under Development), to capture changes in:
  - Underlying data frequency
  - Measurement noise
  - Diel and seasonal patterns
- Consistency tests (Implemented)
  - Within-product (correlated profiles or systems)
  - Cross-product (different sensors measuring fundamentally similar quantities)
- Validation of science requirements
  - Observatory-wide (Implemented)
    - Operational availability meets or exceeds defined thresholds (RD [07])
  - Data product-specific (Under Development)
    - E.g., Wind coordinate rotation angle of 3D sonic within design limits
    - E.g., Energy balance closure of Eddy Covariance Turbulent Exchange System
    - E.g., SUNA Nitrate analyzer sensor data validated with nitrate samples collected from water grab samples analyzed at external lab

5.8 Manual Flagging

Science staff with the relevant expertise review reports of measurement interference by field staff (Data Quality Trouble Tickets, see above) as well as alerts from data quality monitoring algorithms within the IS SOM system (see above). It is also likely that public users of NEON data will alert NEON of additional data quality concerns. The Science Review Flag acts as a catch-all for communicating quality issues not captured by the automated quality flagging applied in the standard data processing pipeline (as specified in the ATBD for each data product).

The Science Review Flag is used to modify the Final Quality Flag accompanying all Level 1 and higher (L1+) IS data products. The Final Quality Flag aggregates results from individual quality tests performed on raw, Level 0 data to communicate a binary use/do-not-use indicator for each mean value of a L1+ data product and is published in the basic download package. When users download the basic data package, they receive the data along with its associated Final Quality Flag. If, after review, Science reviews a potential data quality issue not captured by automated flagging and determines that the Final Quality Flag does not correctly indicate suspect data, data are suspect, the Science Review Flag is raised for the affected data product and time-period is raised, which in turn raises the Final Quality Flag regardless of its previous value. Users may determine the reason the Final Quality Flag was raised by downloading the expanded download data package, which includes the results from of each individual quality test, as well as the Science Review Flag. The reason for raising the Science Review Flag for a given data product and time-period is be documented in the readme information downloaded with each data product.

5.9 IS Quality Assurance Improvements under Development and Future Considerations

5.9.1 IS Training Program

New IS curriculum is currently under development and includes self-guided training materials. Training videos describing complex maintenance tasks are in production, the Sampling Support Library – the online intranet database of all training materials, protocols, SOPs, and related resources to support NEON's field staff - is being updated to facilitate integration with the independent study modules, and quizzes and knowledge checks for assessing trainee improvement are under development.

The new IS training materials will also outline usage of the Fulcrum Instrument Preventive Maintenance Application and include a dedicated section with information on how to access the application, open an account, and begin using the application. The IS training materials will focus on how to integrate the Fulcrum application into the maintenance bout and detail what reporting is required.

5.9.1.1 Long-term IS Curriculum and Training Program Plans

The IS training program must continually adapt to changes that will occur over the lifetime of the Observatory. Changes to training may be required for site specific adaptations, changes in instrumentation resulting from discontinuations or upgrades, or due to the discovery of data quality issues. To date, the IS training program has been continually evolving and, as such, strict document control of IS training materials across the Observatory has not been practical (note that Standard Operating Procedures are controlled documents). Instead, updated training materials are posted on the NEON SharePoint by the Curriculum Designer where training staff and trainees can easily access the most current versions of all materials.

Development of additional supplemental training materials should be considered. These would include table-top or field training exercises designed to challenge the ability of trainees to critically assess and react to real-life situations encountered in the field. Currently, trainees mostly learn by rote, which is not optimal when the annual turnover rate of field technicians is a factor. This will remain a challenge for all training programs.

The training program must develop and implement tools to assess the training program, trainers, trainee competencies, and facility operations. For IS, tools to assess the ability of field technicians to properly perform instrument preventative maintenance bouts and to properly implement the Fulcrum Preventative Maintenance application would help to identify individuals in need of supplemental training or mentoring. These types of documented assessments would provide the end user with increased confidence in data quality and reduce the amount of aberrant data entering the data stream.

5.9.2 Sensor Health Status Warnings and Errors

In the future (in development), the LC will send a health status message directly to the incident management system. It is planned that health status messages will be sent directly after an error status is found, but these messages may be sent at a lower frequency (maximum latency of 1 day) if the LC cannot handle immediate sending. Note that sensor status information reported directly from the sensor is typically a Level 0 data product and may also be sent within a standard data message to the CI data pipeline (for standard processing). The processing of health status messages is independent of standard data processing. Each health status message will include sufficient details to identify the affected system and the error encountered.

5.9.3 Data Reprocessing and Versioning

The NEON CI architecture enables multiple types of data reprocessing for both the IS and OS subsystems. Data are reprocessed when the science team or external data user has identified and corrected issues, such as errors in data entry in the OS system, corrected by the Data Editor, or errors in calibration in the IS system, corrected by updating calibration factors. Corrections are incorporated into data published on the data portal by re-running the transitions from L0 to L1; i.e., reprocessing. Reprocessing is conducted so that corrected data can be made available to the community quickly, without the necessity of waiting for the next Version. All OS and IS data files on the NEON Data Portal include a time stamp in the file name indicating the date and time of file generation; reprocessed data can be identified as such by the new time stamp. The science user interface and frequency of reprocessing will be tailored for each system.

Reprocessing will also occur to create annual “versions” of NEON results. These reprocessing events occur 18 months after period of collection to allow for compilation of varied sources. The NEON CI is designed to support and provide the necessary capacity for reprocessing during the period of Initial Operations. Data of all levels will be periodically reprocessed as part of a formal Versioning and Revision system. The goals of this system are to:

a) create data traceability by providing a historical record of data and algorithm changes (based on community best practices),
b) classify and communicate the implications of changes in data and associated algorithms, and
c) strike a reasonable balance between minimizing data latency, maximizing data improvements and quality control, and limiting overhead associated with processing and storing multiple data iterations.

The three iterations of data reprocessing that NEON CI will support are:

- **Provisional**: Provisional data are data that have been recorded since the most recent Version. These data are dynamic and can be updated at any time, without guarantee of reproducibility. Provisional data allow for near-immediate availability of data on the Data Portal, while retaining the ability to make corrections or additions as they are identified.
- **Version**: Versioned data provide a consistently processed dataset over the entirety of data within the same Revision of the data product (see below). Versioning occurs at yearly intervals and each Version includes data up to 18 months previous from the versioning date to allow sufficient time for all additions, corrections, and back-calibrations, etc. to be applied. (For example, Version 2020 produced on Jan 1, 2020 would include data up to June 30, 2018).
    - Data or processing changes between Versions are of a minor nature such that successive Versions are considered directly comparable except for minor corrections or the inclusion of additional data. Released data Versions will be static (unchanging), stored, and accessible for the lifetime of NEON. Versions will be assigned a Digital Object Identifier (DOI) that can be used to access the data and for citation.
    - The default download from the Data Portal will include the most recent Version plus all available Provisional data. Downloaded data files will be tagged with the version ID. The full Version history will be available from the Data Product Catalog. Each Version will be annotated with a summary of changes made between the current Version and preceding Version.
- **Revision**: A data product Revision occurs upon a sensor or processing change so significant that data from different Revisions of the same data product are not directly comparable and should be used with caution when combining for use or analysis. Upon a data product Revision, the REV Field of the data product ID (NEON.DOM.SITE.DPL.PRNUM.REV.TERMS.HOR.VER.TMI) will be incremented, indicating the significant nature of the change (AD[03]). Each Revision will be annotated with a summary of changes made between the current Revision and preceding Revision.

When a data product Revision occurs, it may not be possible to apply the new Revision to previous data, or to continue producing previous Revisions with new data (for example, if a new sensor is introduced). In these cases, a period of overlap will occur between subsequent Revisions so that differences between Revisions can be accounted for in long-term analyses. A science review panel will decide the necessary period of overlap.

6 AIRBORNE OBSERVATIONAL PLATFORM (AOP) QUALITY FRAMEWORK

The AOP consists of aircraft-mounted remote sensing instruments that will provide long-term, quantitative information on land use, vegetation structure, and biophysical and biochemical properties over the NEON sites, in addition to supporting Principle Investigator directed research and targets of opportunity over regional scales. The remote sensing payload consists of three primary sensors integrated into a common frame along with the associated support equipment required for operation and data collection. The AOP payload consists of the NEON Imaging Spectrometer (NIS), Waveform and Discrete LiDAR, and a high-resolution Digital Camera. The payload also includes two Global Position system (GPS)/Inertial Measurement Units (IMUs); a high-quality unit required for the NEON rigorous orthorectification and an additional unit that is used for the NEON Imaging Spectrometer (NIS) timestamp.

The quality of AOP data is highly dependent on proper payload operation, maintenance, and calibration. This begins in the AOP Sensor Test Facility with the maintenance and calibration of the payload and associated instrumentation. Airborne Sensor Operators are thoroughly trained on the operating the instrumentation as well as flight collection decision-making. Since weather is a critical aspect of the overall data quality, it is imperative that the data is collected under the required weather conditions with full weather documentation recorded and included in the metadata.

Data quality continues with extraction and backup of the data from the flight disks. During this process, L0 data quality assurance and quality checks are performed for each sensor and later after ingest into the NEON Data Center, L1+ QA/QC checks are performed which include automatically generated reports that are reviewed by Science staff. The AOP quality framework discussed in this document includes a description of the AOP training program and a description of the quality processes currently in place. These processes include L0 data quality checks, payload maintenance and calibration, data management, and L1+ QA/QC.

6.1 Training for AOP Personnel

The flight operations crew consists of the pilot and co-pilot, and a team of three Airborne Sensor Operators (ASO) who rotate through defined duties on a daily rotation. The first ASO operates the NEON imaging spectrometer, the second operates the LiDAR/camera system, and the third provides ground coordination and support at the Fixed-base operator (FBO) in addition to monitoring the GPS units and providing data download support. The pilots are Twin Otter International (TOI) employees and are managed by Twin Otter. NEON relies on TOI to verify their qualifications, certifications, and insurance for both the pilots and the aircraft. The AOP training described in this plan refers only to the Airborne Sensor Operators (ASOs) and their Instructors.

Airborne Sensor Operator Instructors are selected based on their experience and qualifications. The NEON Lead designates the Primary Instructors (PI). Instructors must have completed the qualification standards they are authorized to sign off. These qualification standards are outlined in the Flight Operator Training Procedure (RD [17]) and include all the procedures to operate all aspects of the AOP payload safely and effectively.

6.1.1 ASO Classroom Training

Prior to hands-on training with the flight hardware, the ASO's receive classroom consisting of self-guided reading material and lectures. This begins with the written procedures for payload operation and daily support activities as guided by the overall training plan (RD [17]). Training materials include a mixture of online (Dropbox™) maintained documents and an AOP Apache Subversion™ versioned repository of all training materials and procedures. These are synchronized with the latest official versions released through the NEON Agile software environment but are maintained separately for ease of access while the ASOs are deployed.

AOP Science staff also trains the ASOs through a series of lectures on the purpose and methodology of the nominal flight collection and instrument operations to improve ASO understanding of the overall collection philosophy.

6.1.2 ASO Sensor Test Facility and Payload Installation Facility Hardware training

After classroom training, ASOs operate the full payload in the AOP Sensor Test Facility (hereafter to referred to as the Lab) under guidance from senior ASO and Lab personnel. This training utilizes current procedures and covers the full operation of the payload. This reduces the in-flight training required and reduces the overall training cost. Typically, this is done in conjunction with the checkout of the payload from the lab for scheduled flight operations but may also occur independently if needed.

NIS training consists (but is not limited to) of operating the NIS including controlling the NIS environmental health, connecting and hooking up various components including external vacuum components, collecting prototypical Science data, and recording and storing full metadata that will be collected. LiDAR training consists of the operation of the discrete and waveform LiDAR systems, the operation of the digital camera systems, operation of the GPS/IMU system, and projecting the planned flight lines to the TOI pilots.

The final component covered is the operation of the Hotel Kit. The Hotel Kit automates the extraction and L0 QA/QC of the flight data. Typically flight disks are saved from the previous flight season to enable extraction and QA/QC of actual flight data, but, if these are not available, various Lab datasets may be used for partial training.

6.1.3 ASO Flight Training

The final training step consists of flight training on the AOP instrumentation. At this point, the ASO trainee should be fully versed in operating the full payload and support equipment in the lab as integrated system. Typically, subsequent to installation of the checked-out payload into the Twin Otter, the ASO trainees operate the payload in the aircraft. This enables them to test the full installation as well as gain an understanding of the conditions and subtleties of payload operation in the aircraft. It also enables full operation of the power system, including transfer from 'ground' power to 'survey' power, which is used for flight operations.

Flight Operation training initially consists of the ASO Trainee observing the ASO Trainer while the ASO Trainer is conducting one of the three ASO positions. The next step is for the ASO trainee to conduct those same activities with the ASO Trainer supervising the ASO Trainee. After the ASO Trainer is confident in the ASO Trainee's ability to operate the AOP instrumentation under flight conditions, the ASO Trainer signs off on the ASO Trainee as being certified to operate the AOP Payload during flights.

Annual re-certification is required for subsequent years and is conducted by the Flight Operations Trainers. The Trainers are recertified by each other, as they are considered the experts at conducting the required flight operations, including operating the AOP instrumentation.

6.2 Integrated System (Payload) and Sensor Maintenance

The AOP Payload is the primarily the responsibility of the AOP Sensor Test Facility. While the payload is stationed in the Sensor Test Facility during the offseason, routine maintenance and calibration of the sensors are conducted. After the payload has been fully vetted, it may be checked out by the Flight Operations team for the flight season. After completion of the flight season, the payload is returned to the lab and checked back into the lab where offseason maintenance will be conducted. Calibration of the NIS and LiDAR sensors are also conducted during the off-season in the Sensor Test Facility and may be completed once after check-in and once shortly before checkout if needed. Prior to the next flight season, the payload is integrated and tested as a system and the NIS calibration is verified. The payload is then checked out of the Lab by Lab personnel with ASOs verifying the payload operation and status. During the deployment, ASOs may support Lab personnel in resolving any issues that arise, but the Lab retains primary responsibility for maintaining the payload in operating condition.

6.2.1 Sensor Test Facility Off-Season Maintenance

The offseason maintenance of the AOP Payloads begins with the return of the payload to the Sensor Test Facility. During the check-in, any issues with operating the sensors and integrated payload are noted. These are prioritized and scheduled for repair during offseason. After the payload is checked in and potential issues that prevent operation are repaired, the various sensors are calibrated as discussed in the next section. Maintenance of the payload consists of testing and verifying the performance of payload and replacing components that have fallen below specifications. In addition, components approaching end-of-life are replaced. These changes are tracked to ensure components are replaced as required. Typically, Lab personnel conduct all maintenance required by the NIS and Support systems. The LiDAR system maintenance is conducted by the vendor, although some aspects relating to integrating the LiDAR system may be conducted by the AOP team.

6.2.2 Issue Resolution During Deployed Flight Campaigns

Issues encountered during the flight season are reported in the daily flight logs. These logs are routinely tracked by all AOP personnel and provide the most reliable method for raising issues impacting collection. In addition, issues may be recorded in NEON's incident management reporting system, as this provides a long-term record of the issue and the steps taken to resolve it. These reports may be used to identify systemic issues and address those issues between flight seasons.

Hardware issues are typically routed directly to Lab personnel. Troubleshooting occurs with the Lab personnel guiding ASOs through the relevant steps required to isolate the issue. If remote trouble shooting is unsuccessful, Lab personnel will be deployed along with support equipment as needed. If the payload (or sensor) is unable to be repaired while deployed, the aircraft and installed payload will be returned to the Boulder Hangar for additional troubleshooting. If necessary, the payload will be de-installed and returned to the Lab for serious issues and will likely result in missing a large portion of the scheduled flight season.

Data quality issues identified by the L0 QA/QC checks, the L1+ QA/QC checks or by manual inspection by AOP Scientists are typically routed through the Science Subject Matter Expert (SME). The SME attempts to determine if it is a processing error or was initiated with a hardware error. Fully identifying the cause of the issue may require combined consultations between the AOP Science, Lab, and Flight Operations staff.

6.3 Sensor Calibration Program

The AOP Calibration Plan (RD [18]) defines the plan for calibration of the sensors included on the NEON payloads. The calibration plan includes the determination of the baseline calibration in the NEON AOP Sensor Test Facility (STF). The STF is traceable to first principles or to the National Institute of Standards and Technology (NIST). The uncertainty of the calibration is discussed in the AOP Calibration Uncertainty Manual (RD [19]). Independently, the STF sensor calibration is verified through a series of engineering and calibration flights occurring prior to deployed flight operations, as well as the long-term verification of the sensor calibration in the field. This document also includes a discussion of the calibration methods employed and how the calibration results will be verified.

This Calibration Plan describes the expected methods of calibrating the airborne sensors utilized by the Airborne Operations Platform (AOP) team. The primary emphasis of this document is on the calibration of the imaging spectrometer. However, the calibration activities supporting the LiDAR sensor and the Digital Camera are also included. A brief overview of these systems is presented as it applicable in describing the calibration plan. A broad overview of the calibration process is described including the laboratory calibration and verification of the calibration. Pre-deployment calibration flights that are used to determine the geolocation/orthorectification calibration for the sensors are included.

The Calibration Plan emphasizes a description of the methods required to determine the NIS radiometric and spectral calibration as well as further sensor characterization such as a) dynamic range and linearity, or b) signal-to-noise. The test sets used in the calibration process are described, and expected uncertainty given, when determined. Independent methods to verify the calibration determined in the laboratory calibration are discussed. Operationally, the collected imagery will also be verified to ensure that the instrument is operating as expected and producing high-quality data.

The NEON Imaging Spectrometer Calibration procedure (RD [20]) describes the systematic procedure for the user to follow in creating a NIS calibration cube. It also includes a procedure for verify the radiometric calibration through vicarious methods after installation of the payload in the aircraft.

6.3.1 Sensor Test Facility Calibration

The AOP Sensors are calibrated in the STF during the offseason after Lab personnel have checked-in the payload. Typically, the NIS sensor is calibrated both before and after the flight season if time permits. NIS calibration consists of three main components, the characterization of the NIS Focal Plane Array (FPA), the spectral calibration of the NIS, and the radiometric calibration. While collection of the calibration data may occur in any order, it is important to characterize the FPA prior to processing the spectral calibration, and to complete spectral calibration before completing the radiometric calibration.

Specific Test sets in the AOP Sensor Test Facility are utilized to collect the required calibration data. In addition, NIS On-Board Calibration (OBC) data is collected during these calibration collections on the AOP Test Sets. The OBC system is part of the overall NIS sensor package and is used to monitor changes in the sensor performance between the calibration work in the AOP Sensor Test Facility and the flight data collected during deployment. The OBC data is heavily used during the L0 QA/QC process and may also be used to dynamically adjust the NIS calibration to account for sensor changes from the lab calibration.

The AOP STF Test Sets are designed to be traceable to the National Institute of Standards and Technology (NIST) or to first principles. For the spectral calibration, emission and laser lines are used that are very well defined. For the radiometric calibration, a NIST FEL lamp is used as the primary source with an included stated uncertainty. The uncertainty in the calibration is used to propagate the NIS calibration uncertainty throughout the AOP data products.

The vendor calibrates the LiDAR system. This work required that the subframe be de-integrated from the PIM frame. This is scheduled with the vendor, typically takes one to two weeks, and is typically conducted in December. At the time of LiDAR calibration, the vendor also performs any required maintenance on the LiDAR and digital camera system. When AOP and vendor are satisfied the LiDAR system has completed the maintenance and calibration, the subframe is integrated back into the PIM and full payload testing may be conducted prior to payload checkout.

6.3.2 Flight Calibration

AOP also requires a series of calibration flights after installation of the payload into the aircraft. These flights are designed to verify the Lab calibration in an independent manner, verify LiDAR performance after calibration by the vendor, and to determine calibration parameters that are not able to be determined in the lab.

A vicarious in-situ calibration flight is conducted to verify the radiometric performance of the NIS. This requires collecting reflectance data of a well characterized area, modeling the atmosphere, and predicting how much light is propagated to the NIS. This is compared to the reported radiance to verify agreement.

The LiDAR performance is verified through a planned flight over the Boulder runway. High-quality GPS data has been collected across the runway such that the overall runway surface is very well known. The

LiDAR is cycled through the various collection setting to ensure vertical data quality across the range of nominal operating conditions. In addition, a flight is conducted over NEON HQ. The NEON HQ buildings have been surveyed and the corners are very well known. These known building edge and corner points are compared to the reported LiDAR locations of the same features. This ensures horizontal quality of the collected data.

Finally, two other flights are flown to determine the geolocation/orthorectification of the LiDAR and NIS data. The first of these is to verify the timestamps assigned to the LiDAR and NIS data. It is important to understand any difference that may stem from hardware or software differences between the sensors to ensure accurate co-registration of the independent data streams. The second flight is used to determine the roll, pitch, and yaw of the installed sensors to relative to the GPS/IMU.

6.4 AOP Flight Season Management Plan

While AOP may be thought of as an instrumented system in that the payload primarily consists of remote sensing instrumentation, it also contains an aspect of the Observation based systems in that specific collection times are determined by the ASOs within required constraints. These constraints dictate the quality of the AOP data through determining when the AOP data may be collected, daily temporal periods for a specific deployment period to limit solar illumination geometry, and general weather conditions to minimize weather impact on the collected data.

The purpose of the Flight Season Management Plan (RD [21]) is to define the framework and associated guidelines for conducting AOP flight operations acquiring airborne remote sensing data across all NEON domains on an annual basis through deployment of two science payloads. The Flight Season Management Plan focuses primarily on Flight Campaign Planning, including:

1) the basic criteria for defining the AOP survey area over each NEON terrestrial and aquatic site
2) creation of flight plans and supporting documentation used during airborne surveys
3) scheduling of the annual airborne campaign for each payload
4) FBO selection
5) permitting and FAA requirements.

Flight planning is also critical to the overall quality of the collected AOP data. It is important that the planned flight lines adequately cover the survey area with enough overlap between adjacent lines to minimize coverage gaps. In addition, local topographic variations may result in large variation in coverage width and must be accounted for in the planning process. In addition, the flight plans include instrument parameters that are specific to the flight plan. Under ideal conditions, the entire survey area would be collected under optimal conditions; however, AOP prioritizes both sites within a NEON Domain as well as areas within the survey area for each site. This enables the Flight Operations team to concentrate on the highest priority areas while striving to collect the entire survey area.

The purpose of the Flight Plan Procedure document (RD [22]) is to provide systematic guidance on the creation of standard ALTM-NAV flight plans for use with Optech Gemini LiDAR systems deployed on AOP flight campaigns over NEON sites including the definition of the instrument parameters that align with the planned flight lines.

This document covers creation of flight plans for NEON core and relocatable terrestrial and aquatic sites based on the flight survey area designs defined in RD [23]. The procedure document assumes that the user has access to NEON-specific data sets, including tower shapefiles, TOS boundary shapefiles, and AOP flight survey boundary box shapefiles for all NEON sites. It guides the prioritization of the NEON sites and survey areas within the sites. The result of the flight planning process are the flight plans for the season along with summary documents utilized by the ASOs to implement the flight plans according to the scientific goals behind the collection philosophy.

6.5 AOP Data Management

AOP Data Management begins with the collection of the data during Flight Operations implementing the flight plans for a site. The collected data is recorded onto independent hard-drives with a hard-drive (or a series of Raided hard-drives) allocated to each AOP instrument or collection component. After the flight is completed, the flight disks are removed from the flight instrumentation and stored in Pelican cases and taken to the Hotel Kit. The Hotel Kit is used to automatically extract the flight data, implement the L0 QA/QC algorithms, and augment data included in the AOP flight data bases. After the data has been backed-up, it is exported to an external RAID set. One RAID disk is maintained in the field while the other is shipped to the NEON Data Center where the data is ingested into the Elastic Cloud Storage (ECS) system. Data is then pulled from the ECS by AOP Scientists and processed through the AOP Pipeline where additional metadata are generated. During the processing, L1+ QA/QC reports are automatically generated that are reviewed by AOP Scientists to ensure the data are of the expected quality. If the data are acceptable, the data are published to the Data Portal for download by external users.

6.5.1 L0 Data Ingest and QA/QC

The L0 Data QA/QC procedures are documented in the AOP Level 0 Data Quality Checks document (RD [24]). The purpose of this document is to describe the L0 raw quality assurance and quality checks to be performed for each sensor on the NEON AOP. The quality checks determine, to the extent possible, that the raw data is within range and acceptable for producing higher-level data products. The document also guides AOP personnel through the procedure of implementing the code used to perform these checks.

In the field, the data must be extracted from the sensor systems prior to the implementation of L0 quality checks. Currently, this is performed through the Hotel Kit, with a custom algorithm. In an operational scenario, the airborne sensor operators (ASOs) will extract the L0 data and perform the quality checks in-field at the end of each day of acquisition. The extraction of L0 data and associated quality checks must be completed prior to the beginning of the following day’s acquisition, imposing a maximum time for data extraction and execution of quality checks of 12 hrs.

The document describes the quality checks for each individual sensor systems including 1) the GPS / IMU, 2) the spectrometer, 3) the waveform LiDAR, 4) the digital camera, followed by a section 5) assessment of spatial coverage for the LiDAR, camera and spectrometer. Detailed within each section are the in-range criteria imposed for success, raw data required for verification, algorithm design, and, if required, potential limitations and future improvements.

6.5.2 L1+ Data QA/QC

The AOP data are processed through the AOP Data Processing Pipeline. This automates a series of processing steps, particularly for the NIS; it also interacts and continues from manual processing steps required for creation of the Smoothed Best Estimate of Trajectory (SBET) detailing the plane's location throughout the flight and manual processing through COTS software of the LiDAR data. The manual and automated processing steps are detailed in a series of documents (RD[25-30]). During the Pipeline processing steps, a series of L1+ QA/QC reports are generated. The reports provide information on processing decisions and quality of the resulting data. They also provide an easy mechanism for AOP Science Staff to review metrics relating to the data quality of the relevant data product. These reports are typically emailed out to the SME and to the person guiding the processing. They are also maintained with the completed data and serve to inform the external user of the decisions that were made in the processing workflow.

6.6 AOP Quality Assurance Improvements under Development and Future Considerations

6.6.1 Data Review

AOP Science Staff are currently responsible for reviewing the processed data. This is facilitated through the creation of the L1+ QA/QC reports. However, quantitative tolerances are not set for each data product (and may not be able to be defined for all data products). It would be ideal to automatically flag suspect data for review (rather than review all data) and automatically reprocess when desired.

APPENDIX 1. APPROACH AND RATIONALE FOR SELECT OS QUALITY ASSESSMENT TOOLS

During the operational phase, NEON will conduct annual assessments of the Observational Data Systems. These assessments will eventually become part of a larger Observatory Audit Plan which will be wider in scope. The primary purpose of these annual assessments is to help identify quality issues, address errors, and improve practice before an error occurs. Specifically, quality issues may be addressed through further or improved training, or through the improvement of standard operating procedures and processes.

As the Observatory moves from the construction phase to the operational phase, much about the quality of OS data products remains to be learned. Over time, internal data quality observations and feedback from the user community will allow evidence-based decisions to drive the types of assessments that are performed in any given year. This prioritization of field assessments and quality metrics will ensure that the most significant data quality issues are addressed first.

This preliminary plan to assess various quality aspects of the OS subsystems is primarily based on observations from the Field Ecologists, observations by the HQ Science team, and the results of commissioning tests performed during construction. Initially, the assessments will include a combination of protocol-specific evaluation tools or checklists and select commissioning tests. The basic approach is to evaluate areas known to require improvement and areas expected to be satisfactory, with the intent of monitoring to verify that the processes are done correctly and to successfully track improvement.

Although a number of protocol-specific assessment tools have been developed to-date, efforts will be made to ensure that further development is consistent with specific quality issues as they arise. Tailoring of the quality assessment tools will also be partially dependent on who ultimately conducts the assessment, senior Field Ecologists, HQ Science staff, dedicated trainers, or a combination thereof. Ultimately, the number and types of assessments performed in any given year must be based on need. However, implementation will likely be influenced by budgetary, scheduling, and human resource restrictions. These details will be thoroughly addressed during the operation phase.

An initial list of TOS and AOS protocols to be assessed through field audits and desktop, commissioning-style tests is below (Tables 4 and 5). These protocols and tests are representative of areas where quality issues are currently expected to be satisfactory or suspect. The rationale for their selection and evidence, where available, is indicative of the currently available means by which assessments are prioritized. Implementation of field assessments will be further developed during operations.

Table 4. Initial selection of observational protocols selected for audit during operations.

Subsystem/ Protocol	Rationale	Evidence (+/-)
AOS/Discharge	This protocol measures the underlying driver of all physical, chemical, and biological dynamics in stream and river systems. It is the foundation of several L4 data products and higher-level calculations performed by the user community. Accurate measures of discharge and the quantification of the uncertainty associated with these measurements is therefore critical to user data.	Evidence of errors include (1) recording incorrect stage values associated with the measurement; (2) incorrect locations of where each vertical is located on the meter tape and (3) incorrect individual rod depths.
AOS/Microbes (benthic and surface)	This protocol requires special sterilization techniques, which will likely benefit from an eyes-on check.	There is currently no evidence of quality issues with these data. However, contamination cannot be distinguished from the data.
AOS/Algae Sampling	This protocol is a combination of field and domain lab work. Proper homogenization and filtering techniques in the lab must be ensured across domains.	External lab data indicate a potential lack of homogenization as evidenced by wide variability around replicate filters.
AOS/Reaeration	This protocol has a large amount of equipment and includes adding tracers to the stream to sample. While this protocol appears complex, implementation of the protocol is straightforward as long as the execution is well-organized.	Field staff appears to have consistently and successfully implemented this protocol, as evidenced by the lack of errors to date in the Fulcrum data entry application. The application helps ensure all necessary data are collected.
AOS/Macro-invertebrates	This protocol is relatively simple and straightforward, with minimal equipment involved. It represents a good opportunity for process development and a demonstration of success.	Field staff appears to have consistently and successfully implemented this protocol, as evidence by the ease of legacy data processing and minimal problem tickets.
TOS/Vegetation Structure	This protocol is complex, as its implementation varies with the diversity of species and growth forms across NEON sites. It also requires mapping of individuals, which requires making measurements in often challenging conditions (e.g., dense brush). Data entry is also more complicated than most protocols, as there are complex contingencies for required fields based on growth Form. These data are critical for scaling up with the AOP data.	This protocol has consistently generated the most problem tickets over the years, and the recent attempts to ingest the data into the new pipeline revealed numerous and ubiquitous errors in the data.
TOS/N	This protocol is unique among TOS protocols	Early analytical data indicate

Subsystem/ Protocol	Rationale	Evidence (+/-)
transformations	in that it involves precise analytics and high attention to detail around washing, glove wearing, and other sterile techniques. The Field staff is generally inexperienced in these techniques.	widespread contamination and associated issues.
TOS/Sampling locations	This assessment is proposed as a cross-protocol assessment to ensure that the appropriate sampling locations are being sampled and recorded, from the resolution of plotIDs to subplotIDs to clipIDs. Hot checks can be conducted in the field for a variety of protocols to ensure that the correct locations are being sampled, and that the correct locations are then entered into the corresponding Fulcrum application.	Numerous reports of sampling location errors have been reported across protocols and across sites.
TOS/Small mammal	This protocol is complex, time intensive, equipment intensive, and involves animal care. With several potential sources of error, this protocol should be monitored for consistent practices across the observatory.	IACUC audits and commissioning tests have revealed high rates of success across domains in the implementation of this protocol over the years.
TOS/Litter	This protocol is relatively simple and straightforward, with minimal equipment involved. It represents a good opportunity for process development and a demonstration of success.	Field staff appears to have consistently and successfully implemented this protocol, as evidence by the ease of legacy data processing and minimal problem tickets.

Table 5. Initial observational desktop, commissioning-style tests selected for audit during operations.

Subsystem/ Protocol	Rationale	Evidence
AOS/Surface Water Chemistry Process Quality	This test is designed to test the quality of water chemistry sample, by evaluating timing of sample processing, timing of sample shipping, and shipment condition.	Approximately 15% of domains have failed some part of this test, which led to a change in shipment equipment and packing strategies in some domains.
AOS/Aquatic Sediment Chemistry Process Quality	This test is designed to test the quality of water chemistry sample, by evaluating timing of sample processing, timing of sample shipping, and shipment condition.	Domains in recent years have mostly passed this test.
AOS/Riparian Process Quality	This test evaluates sample timing, sampling location, and sample completeness.	Domains in recent years have mostly passed this test.
AOS/Macroinvertebrates and	This test evaluates sample timing, sampling location, and sample completeness, for 2	Approximately 20% of domains have failed to ship samples on

Subsystem/ Protocol	Rationale	Evidence
Zooplankton Process Quality	consecutive bouts.	time, which has resulted in additional oversight of the shipping timeline.
AOS/All Bio Bouts Process Quality	This test evaluates sample timing, sampling location, and sample completeness.	Domains in recent years have mostly passed this test.
AOS/Surface Water Chemistry Data Quality	This test evaluates replicates of alkalinity measurements completed in the domain labs. Domains will continue to collect replicate data on ~10% of samples in Operations to quantify the analysis uncertainty.	Domains in recent years have mostly passed this test.
AOS/Stream Discharge Data Quality - modified	Includes the addition of tests to quantify how many measured values are outside the flowmeter's measurement range and how many subsections within the entire discharge cross-section contained a flow >10% of total.	No data analyses have been conducted to date to inform the prevalence of this issue, but the risk is sufficiently high to warrant testing.
TOS/Plant diversity process quality test	Plant diversity sampling must be conducted a) in full, b) in the designated locations, and c) at the right time of year to adequately estimate site-level diversity.	Domains in recent years have mostly passed this test.
TOS/Soil Biogeochemistry process quality test	Soil biogeochemistry must be conducted a) in full, b) in the designated locations, and c) at the right time of year to adequately estimate site-level biogeochemistry parameters.	Domains in recent years have mostly passed this test.
TOS/Plant Phenology process quality test	Plant phenology sampling must be conducted according to the specified schedule to be able to characterize the timing of phenophases with adequate precision. This test checks that phenology sampling happened each year according to the site-specific schedule.	Plant phenology sampling occurs at varying frequency throughout the year and, at its peak, may be required 3x per week. This protocol presents a particular challenge for field staff due to the uncertainty in scheduling, and therefore warrants continued attention.
TOS/Digital hemispherical photos (DHP) process quality test	DHP photos must all be taken in a standardized manner, with the correct camera settings, and with the files named and organized consistently for the photos to be properly processed in the CI pipeline.	Multiple domains have failed to correctly setup the DSLR for acquiring photos, and many domains experienced DHP organization issues, which prevent the ingest and publication of the photos.
TOS/Small mammal taxonomic classification process quality test	Small mammal sampling requires a sufficient number of bouts to yield robust data for density estimation and population dynamics. This test checks that a minimum of 80% of scheduled bouts occurred.	All domains have passed this test in construction. If we have to reduce sampling due to budget constraints, however, it will become more pressing as the risk of insufficient sampling

Subsystem/ Protocol	Rationale	Evidence
		will be increased.
TOS/Ground beetle taxonomic classification process quality test	The integrity of the ground beetle samples relies on rapid removal of vertebrate bycatch from the invertebrates and rinsing with ethanol. The subsequent sorting and accurate identification of beetles from the sample relies on adequate preservation of the sample. This test checks that these steps are conducted according to the protocol.	Domains in recent years have mostly passed this test.
TOS/Small mammal taxonomic classification	This test is a desktop assessment of repeatability in classifying recaptured individuals to genus, species, and sex, key parameters for small mammal diversity and demography.	A number of sites failed at least one of the tests in construction; therefore, continued testing is warranted.
TOS/Ground beetle taxonomic classification data quality test	This test is a desktop assessment of accuracy of field staff identifications of carabids, a key parameter for ground beetle abundance and diversity.	Domains in recent years have mostly passed this test, so this provides a great opportunity to demonstrate success.
TOS/Contamination test of microbial soil samples	A test that looks for contaminants in the microbial taxa being detected in the TOS soil samples is of high importance. Handling of samples can inadvertently introduce microbial taxa into the soil, which, unless specifically targeted, may go unnoticed and result in inflated estimates of microbial diversity and abundance.	No data analyses have been conducted to date to inform the prevalence of this issue, but the risk is sufficiently high to warrant testing.

APPENDIX 2. COMPLETE LIST OF ALGORITHM THEORETICAL BASIS DOCUMENTS (ATBDS)

Subsystem	Number	Document Title
AOP	NEON.DOC.001210	NEON ATBD - NEON Imaging Spectrometer Level 1B Calibrated Radiance
AOP	NEON.DOC.001211	NEON ATBD - AOP Digital Camera Image Orthorectification
AOP	NEON.DOC.001288	NEON ATBD - Imaging Spectrometer Radiance to Reflectance
AOP	NEON.DOC.001290	NEON ATBD - Imaging Spectrometer Geolocation Processing
AOP	NEON.DOC.001292	NEON ATBD - L0-to-L1 Discrete Return LiDAR
AOP	NEON.DOC.001293	NEON ATBD - L0-to-L1 Waveform Lidar
AOP	NEON.DOC.001455	NEON ATBD - Spectral Photometer
AOP	NEON.DOC.002387	NEON ATBD - Lidar Ecosystem Structure Level-2 Data Product
AOP	NEON.DOC.002390	NEON ATBD - Elevation (DTM and DSM)
AOP	NEON.DOC.002391	NEON ATBD - Vegetation Indices
AOP	NEON.DOC.003791	NEON ATBD - Elevation (Slope and Aspect)
AOP	NEON.DOC.003839	NEON ATBD - AOP Leaf Area Index
AOP	NEON.DOC.003840	NEON ATBD - AOP fPAR
AOP	NEON.DOC.004326	NEON ATBD - AOP Surface Albedo
AOP	NEON.DOC.004363	NEON ATBD - AOP Total Biomass
AOP	NEON.DOC.004364	NEON ATBD - AOP Water Indices
AOP	NEON.DOC.004365	NEON ATBD - AOP Spectrometer Mosaic
AOP	NEON.DOC.005052	NEON ATBD - AOP Digital Camera - Mosaicing
IS	NEON.DOC.000007	NEON ATBD - TIS Soil Water Content and Water Salinity
IS	NEON.DOC.000646	NEON ATBD - Single Aspirated Air Temperature
IS	NEON.DOC.000651	NEON ATBD - Atmospheric Properties and Units
IS	NEON.DOC.000652	NEON ATBD - Biological Temperature
IS	NEON.DOC.000653	NEON ATBD - Barometric Pressure
IS	NEON.DOC.000654	NEON ATBD - Triple Aspirated Air Temperature
IS	NEON.DOC.000780	NEON ATBD - 2D Wind Speed and Direction
IS	NEON.DOC.000781	NEON ATBD - Photosynthetically Active Radiation
IS	NEON.DOC.000809	NEON ATBD - Net Radiometer
IS	NEON.DOC.000810	NEON ATBD - Primary Pyranometer
IS	NEON.DOC.000813	NEON ATBD - Quantum Line Sensor
IS	NEON.DOC.000814	NEON ATBD - TIS Soil Heat Flux Plate
IS	NEON.DOC.000815	NEON ATBD - Global, Direct and Diffuse Pyranometer
IS	NEON.DOC.000816	NEON ATBD - Secondary Precipitation and Throughfall (tipping bucket)
IS	NEON.DOC.000851	NEON ATBD - Humidity and Temperature Sensor
IS	NEON.DOC.000898	NEON ATBD - Primary Precipitation (DFIR)
IS	NEON.DOC.001198	NEON ATBD - Surface Water Elevation
IS	NEON.DOC.001316	NEON ATBD - Surface Water Temperature
IS	NEON.DOC.001328	NEON ATBD - Groundwater Level, Temperature, and Specific Conductivity
IS	NEON.DOC.001571	NEON ATBD - TIS Soil Temperature
IS	NEON.DOC.001624	NEON ATBD - Homogeneity and Stationarity
IS	NEON.DOC.001789	NEON ATBD - Above Canopy and Understory/Snowpack Phenology Camera
IS	NEON.DOC.002181	NEON ATBD - Nitrate
IS	NEON.DOC.004388	NEON ATBD - Temperature at Specific Depths in Surface Water

Subsystem	Number	Document Title
IS	NEON.DOC.004571	NEON ATBD - Eddy-Covariance Data Products Composite
IS	NEON.DOC.004737	NEON ATBD - Summary Weather Statistics
IS	NEON.DOC.004738	NEON ATBD - Buoy 2D Wind Speed and Direction
IS	NEON.DOC.004931	NEON ATBD - Water Quality
IS	NEON.DOC.004968	NEON ATBD - Eddy-Covariance Storage Exchange (Profile) Assembly Raw Data
IS	NEON.DOC.011081	NEON ATBD - QA/QC Plausibility Testing
IS	NEON.DOC.011083	NEON ATBD - Soil CO2 profile
OS	NEON.DOC.004825	NEON ATBD - OS Generic Transitions