ALGORITHM THEORETICAL BASIS DOCUMENT (ATBD)

EDDY-COVARIANCE STORAGE EXCHANGE (PROFILE) ASSEMBLY RAW DATA PROCESSING

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Change Record

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1 DESCRIPTION

The Eddy Covariance Storage Exchange Assembly (hereafter referred to as the EC profile assembly) consists of a suite of sensors such as CO_2 and H_2O gas analyzer and isotopic CO_2 and H_2O analyzers (full details/descriptions can be found in AD[01]). The EC profile assembly is served to provide the measurements of CO_2 and H_2O concentration, the stable isotope of δ^{13}C in CO_2, δ^{18}O, and δ^{2}H in water vapor in the atmosphere at each tower measurement level. The vertical profile measurements of CO_2 and H_2O concentration will be used to calculate the storage fluxes which will be incorporated into the calculation of the net ecosystem exchange of CO_2 and H_2O.

1.1 Purpose

This document details the algorithms used for creating NEON preconditioned (L0p) data outputs from Level 0 (L0) DPs associated with the EC profile assembly and ancillary data as defined in this document (such as calibration data) obtained via instrumental measurements made by the EC profile assembly. It includes a detailed discussion of measurement theory and implementation, appropriate theoretical background, data product provenance, quality assurance and control methods used, approximations and/or assumptions made.

1.2 Scope

The theoretical background and entire algorithmic process used to derive preconditioned data from Level 0 data for the EC profile assembly is described in this document. The sensors defined in Table 1-1 are used for the EC profile assembly. This document does not provide computational implementation details, except for cases where these stem directly from algorithmic choices explained here.

Table 1-1. List of sensors used in the EC profile assembly, including NEON Data Generating Device (DGD) number based on NEON.DOC.001104.docx.

DGD Number	Sensor
0330600000	Sensor G2131-i Gas Analyzer for Isotopic CO2 240VAC, with 125 sccm internal orifice
0328050000	Sensor, L2130-i Analyzer for isotopic water vapor 90 to 240VAC 60HZ
CA07140000	Assembly, Pressure Transducer 0-100psi and Cable Small
CA07150000	Assembly, Pressure Transducer 0-3000psi and Cable Small
0347780000	Remote Thermometer Hygrometer Barometer with PoE
CD06640001	Harness, Grape Digital Out, 8 Solenoid Control
CD06640002	Harness, Grape Digital Out, 4 Solenoid Control

0341500000	Controller, Mass Flow, 5 SLPM, ID Eeprom
CD06640001	Harness, Grape Digital Out, 8 Solenoid Control
0341570000	Controller, Mass Flow, 5 SLPM, Whisper Series, EEPROM
CD08340000	Assembly, IRGA Sensor and EPROM DB9 Serial Adaptor
0341530000	Meter, Mass Flow, 20 SLPM, Whisper Series, ID EEPROM
CA08830000	Assembly, pressure transducer, 0-30 PSI, 4-20MA, enclosure
CD07150000	Assembly, 24VDC Pump and Control

Further detailed sensor info under each DGD is as following:

- Under DGD 0330600000, *Picarro G2131-i Gas Analyzer for Isotopic CO2* (NEON P/N 0330600000). It is used to make measurements of high precision CO2 concentration, H_2O concentration and isotopic CO_2 ($\delta^{13}C$) for air samples drawn from tower profile measurement levels. The reference document for the Picarro G2131-i Analyzer for Isotopic CO_2 is RD [03].
  - Operating System Software: Windows 7.
  - System Firmware: ver 1.5.0-n
  - Customized design with a critical orifice to allow 125 sccm flow rate through laser cavity
- Under DGD 0328050000, *Picarro L2130-i Analyzer for Isotopic Water Vapor* (NEON P/N 0328050000). It will be used in the measurements of $\delta^{18}O$, $\delta^{2}H$, and H_2O concentration for air samples drawn from tower profile measurement levels. The reference documents for the Picarro L2130-i Analyzer for Isotopic H2O are RD [04] and RD [05].
  - Operating System Software: Windows 7
  - System Firmware: ver 1.5.0-n
  - Other accessories:
    - A0211 Liquid Sample High Precision Vaporizer [NEON P/N: 0300280001]
    - A0325 HTC-xt Auto Sampler (NEON P/N 0328050001)
    - A0912 Switching valve and accompanying software (NEON P/N 0328050002)
- Under DGD CD08340000, LI840A CO2/H2O gas analyzer: LICOR P/N: LI840A-03 (NEON P/N: 0340570000). It will be used to measure the CO2 and water vapor (H2O) concentration for air samples drawn from tower profile measurement levels, which will be eventually used to determine the storage term of CO2 and H2O. The reference document is RD [08].

  - Equip 2 Swagelok fittings (Union, Bulkhead, SS, 0.25" OD Swagelok Part No.: SS-400-61) at the gas inlet and outlet of the sensor per NEON request.
  - Firmware version: 2.1.0
  - Power Requirements: Input Voltage 12-30 VDC
- Under DGD 0347780000, *Temperature sensor in the instrument hut*: Comet P/N: T7610. Remote Thermometer Hygrometer Barometer with Ethernet. POE Temp Sensor. NEON P/N: 0347780000
- Under DGD 0341530000, *Mass Flow Meter:* Alicat Scientific P/N: MW-20 SLPM-NEON. Meter, Mass Flow, 20 SLPM, Whisper Series, ID EEPROM, NEON P/N: 0341530000. The reference document for this sensor is RD [06]
- Under DGD 0341570000, *Mass Flow Controller* for Li840A IRGA: Alicat Scientific P/N: MCRW-5 SLPM-DS-NEON. Controller, Mass Flow, 5 SLPM, Whisper Series, EEPROM. NEON P/N: 0341570000. The reference document for this sensor is RD [07]
- Under DGD 0341500000, *Mass Flow Controller* for Validation Gas: Alicat Scientific P/N: MC-5 SLPM-NEON. Controller, Mass Flow, 5 SLPM, ID Eeprom. NEON P/N: 0341500000. The reference document for this sensor is RD [07]
- Under DGD CA07150000, *Cylinder Pressure Sensor:* Omega Engineering P/N: PX319-3KGI. Transducer, 0-3000 psi Gage Pressure (PT), 3000 psi Gage pressure range, DIN connection style. NEON P/N: 0335480000
- Under DGD CA07140000, *Delivery Pressure Sensor:* Omega Engineering P/N: PX319-100GI. Transducer, 0-100 psi Gage Pressure (PT), 100 psi Gage pressure range, DIN connection style. NEON P/N: 0335490000
- Under DGD CA08830000, *Inlet Pressure Sensor:* Omega Engineering P/N: PX319-030AI. 0-30 psi Absolute Pressure Transducer (PT) 30 psi absolute pressure range, DIN connection style. NEON P/N: 0335460000
- Under DGD CD07150000, *Sampling line vacuum pump,* Gast Manufacturing, Inc. P/N: 2032-101-G644. Pump, Rotary Vane Vacuum, 24V DC Brushless, 7.2 Amp, 3000 RPM, 0.13 HP, 0.10 KW, 9 Lbs. NEON P/N: 0334770000

Other important parts:

- *Solenoid Valve*: Components for Automation P/N: C9-211N105-41. Solenoid, 2-Way 24VDC .125 inch NPT Stainless Steel .0945 inch, Orifice Normally Closed. NEON P/N: 0309720000
- *Dehumidifier in the instrument hut:* General Electric P/N: ADEL50LR. Dehumidifier, 23 5/8 x 15 3/8 x 11 inches. NEON P/N: 0347810000

2 RELATED DOCUMENTS, ACRONYMS AND VARIABLE NOMENCLATURE

2.1 Applicable Documents

AD[01]	NEON.DOC.000465	Eddy Covariance Storage Exchange Assembly C^3
AD[02]	NEON.DOC.011081	ATBD QA/QC plausibility tests
AD[03]	NEON.DOC.000783	ATBD De-spiking and time series analyses
AD[04]	NEON.DOC.001069	Preprocessing for TIS Level 1 Data Products
AD[05]	NEON.DOC.000302	C^3 Single Aspirated Air Temperature
AD[06]	NEON.DOC.000723	Triple Point Temperature Calibration Fixture
AD[07]	NEON.DOC.000385	C^3 Triple Aspirated Air Temperature
AD[08]	NEON.DOC.002651	Data Product Naming Convention
AD[09]		
AD[10]		
AD[11]		
AD[12]		

2.2 Reference Documents

RD[01]	NEON.DOC.000008 NEON Acronym List
RD[02]	NEON.DOC.000243 NEON Glossary of Terms
RD [03]	Picarro G2131-i Analyzer for Isotopic CO_2 - User's Guide Rev 03/06/12. Picarro, Inc. 3105 Patrick Henry Dr. Santa Clara California, 95054 USA.
RD [04]	Installation: L2130-i or L2120-i Analyzer and its Peripherals - User's Manual. Revision B, 8-7-2012. Picarro, Inc. 3105 Patrick Henry Dr. Santa Clara California, 95054 USA
RD [05]	Operation, Data Analysis, Maintenance, Troubleshooting | L2130-*i* or L2120-i analyzer and its Peripherals - - User's Manual. Revision 8-7-2012. Picarro, Inc. 3105 Patrick Henry Dr. Santa Clara California, 95054 USA
RD [06]	Precision Gas Mass Flow Meters Operating Manual. 1/10/2014 Rev. 28. DOC-ALIMAN16. Alicat Scientific. 7641 N Business Park Drive, Tucson, AZ 85743 USA
RD [07]	Precision Gas Mass Flow Controller Operating Manual. 09/18/2013 Rev. 29. DOC-ALIMAN16C. Alicat Scientific. 7641 N Business Park Drive, Tucson, AZ 85743 USA
RD [08]	LI-840A CO2/H2O gas analyzer instruction manual. Jan 2011. Publication Number 984-10690. LI-COR, Inc. 4421 Superior Street Lincoln, Nebraska 68504 USA

2.3 Acronyms

Acronym	Explanation
AIS	Aquatic Instrument System
ATBD	Algorithm Theoretical Basis Document
CI	NEON Cyberinfrastructure
CVAL	NEON Calibration, Validation, and Audit Laboratory
DAS	Data Acquisition System

DP	Data Product
FDAS	Field Data Acquisition System
GRAPE	Grouped Remote Analog Peripheral Equipment
Hz	Hertz
L0	Level 0
L0p	Level 0 prime
L1	Level 1
PRT	Platinum resistance thermometer
QA/QC	Quality assurance and quality control
SAATS	Single Aspirated Air Temperature
TRAATS	Triple Redundancy Aspirated Air Temperature

2.4 Variable Nomenclature

The symbols used to display the various inputs in the ATBD, e.g., calibration coefficients and uncertainty estimates, were chosen so that the equations can be easily interpreted by the reader. However, the symbols provided will not always reflect NEON's internal notation, which is relevant for CI's use, and or the notation that is used to present variables on NEON's data portal. Therefore a lookup table is provided in order to distinguish what symbols specific variables can be tied to in the following document.

Symbol	Internal Notation	Description
fdMoleCO2	CVALC0	Dry mole fraction of CO_2
d13CO2	CVALD0	Ratio of 13C:12C in CO_2
fdMole12CO2	CVALA0	Dry molar fraction of $12CO_2$
fdMole13CO2	CVALB0	Dry molar fraction of $13CO_2$
d2HWaterLow	CVALA1	δ^2H in water standard Low
d18OWaterLow	CVALB1	$\delta^{18}O$ in water standard Low
d2HWaterMed	CVALA2	δ^2H in water standard Med
d18OWaterMed	CVALB2	$\delta^{18}O$ in water standard Med
d2HWaterHigh	CVALA3	δ^2H in water standard High
d18OWaterHigh	CVALB3	$\delta^{18}O$ in water standard High
sd	U_CVALA2	Calibration coefficient. Standard deviation of the variable during the given time period
dfUcrtRaw	U_CVALD1	Calibration coefficients. Degrees of Freedom for calculating combined uncertainty using raw data
ucrtRaw	U_CVALA1	Calibration coefficients. Combined uncertainty calculated using raw data

Symbol	Internal Notation	Description
ucrtAve	U_CVALA3	Calibration coefficients. Combined uncertainty calculated using average data
dfUcrtAve	U_CVALD3	Calibration coefficients. Degrees of Freedom for calculating combined uncertainty using averaged data
dfSd	U_CVALD2	Calibration coefficients. Degrees of Freedom for calculating repeatability (Standard deviation)

3 ANALYZER FOR CO2 AND H2O CONCENTRATION

3.1 Data Product Description

This section describes the processes to convert L0 DPs from the LI-COR LI-840A (hereafter referred to as IRGA) under the DGD 0353710000 into 1 Hz L0p DPs. The IRGA referred to as irgaStor in reference to DPs.

3.1.1 Variables Reported

The irgaStor L0p variables provided by the algorithms documented in this ATBD are displayed in Table Table 3-1.

Table 3-1: List of irgaStor-related L0p reported variables produced using this ATBD.

L0p DP	L0p fieldName	L0p DP Frequency	L0p Units	Input L0 fieldNames
CO_2 wet mole fraction	rtioMoleWetCo2	1 Hz	mol mol^{-1}	fwMoleCO2
H_2O wet mole fraction	rtioMoleWetH2o	1 Hz	mol mol^{-1}	fwMoleH2O
Cell Temperature	temp	1 Hz	K	tempCell
Cell Pressure	pres	1 Hz	Pa	presCell
CO_2 Absorption	asrpCo2	1 Hz	dimensionless	asrpCO2
H_2O Absorption	asrpH2o	1 Hz	dimensionless	asrpH2O
CO_2 dry mole fraction	rtioMoleDryCo2	1 Hz	mol mol^{-1}	rtioMoleWetCo2* rtioMoleWetH2o*
H_2O dry mole fraction	rtioMoleDryH2o	1 Hz	mol mol^{-1}	rtioMoleWetH2o*

*: These L0p DPs are used as inputs for CI to generate L0p DPs: rtioMoleDryCo2 and rtioMoleDryH2o.

3.1.2 Input Dependencies

Table 3-2 lists all irgaStor-related L0 DPs and specifies which L0 DPs will be used to produce L0p reported variables in this ATBD.

Table 3-2: A full list of irga-related L0 DPs.

L0 DP	L0 DP fieldName	Sample Frequency	L0 DP Units	Data Product Number	DPs that are used to produce L0p (Y/N)*
CO_2 wet mole fraction	fwMoleCO2	1 Hz	μmol mol^{-1}	NEON.DOM.SITE.DP0.00105.001.02316.700.000.000	Y
H_2O wet mole fraction	fwMoleH2O	1 Hz	mmol mol^{-1}	NEON.DOM.SITE.DP0.00105.001.02348.700.000.000	Y
Cell Temperature	tempCell	1 Hz	°C	NEON.DOM.SITE.DP0.00105.001.02349.700.000.000	Y
Cell Pressure	presCell	1 Hz	kPa	NEON.DOM.SITE.DP0.00105.001.02350.700.000.000	Y
CO_2 Absorption	asrpCO2	1 Hz	dimensionless	NEON.DOM.SITE.DP0.00105.001.02189.700.000.000	Y
H_2O Absorption	asrpH2O	1 Hz	dimensionless	NEON.DOM.SITE.DP0.00105.001.02184.700.000.000	Y

*: Only the L0 DPs in "Y" are selected to transform into L0p DPs reported in this ATBD.

3.1.3 Product Instances

All terrestrial sites across the NEON observatory have the IRGA analyzers; individual instances of all L0p data outputs from this analyzer are in Table 3-1.

3.1.4 Temporal Resolution and Extent

The temporal resolution of the reported L0p variables in Table 3-1 is 1 Hz.

3.1.5 Spatial Resolution and Extent

The IRGA analyzer will be located within the tower hut infrastructure. However, the analyzer's measurements reflect the points in space where the sample inlets are located on the tower infrastructure, which are site-specific.

3.2 Scientific context

The balance of carbon, water and heat exchange over ecosystems are important research fields to understand and forecast climate change. Eddy-covariance is one of the most direct methods for evaluating CO_2, H_2O and heat exchanges (i.e., fluxes) between ecosystems and the atmosphere. Principally, the net exchange can be calculated from a mass balance consisting of transport into or out of a control volume, and enrichment or depletion in the volume. The latter term is also called storage flux, and can have large contributions to the net exchange over short time scales (minutes to hours), particularly within a closed forest with a tall canopy (Ohkubo et al., 2008): Ecosystems can be highly variable from the ground surface to the canopy top and above, and vertical profiling is a very important method for evaluating storage fluxes and understanding the process of gas exchange (Ohkubo et al., 2008). The H_2O and CO_2 vertical profiles and storage flux can be estimated by measuring their concentration at multiple vertical levels. At each NEON site, a LI-840A CO_2/H_2O Gas Analyzer will be used to measure CO_2 and H_2O concentration in air samples from multiple heights (varies from 4 to 8 levels, depending on the canopy height at individual site).

3.2.1 Theory of Measurement

The LI-840A CO_2/H_2O is an absolute, non-dispersive, infrared (NDIR) gas analyzer based upon a single path, dual wavelength, infrared detection system. The CO_2 and H_2O measurements are a function of the absorbed energy in the IR as it travels through the optical path. Concentration measurements are based on the difference ratio in the IR absorption band between a reference and sample signal. Reference and sample channels measure infrared gas absorption in a single path through the use of narrow band optical filters with appropriately selected bands. The CO_2 sample channel uses an optical filter centered at 4.26 micrometers, corresponding to an absorption band for CO_2. The reference channel for CO_2 has an optical filter centered at 3.95 micrometers, which has no absorption due to CO_2. The H_2O sample channel uses an optical filter centered at 2.595 micrometers, corresponding to an absorption band of H_2O. The reference channel for H_2O has an optical filter centered at 2.35 micrometers, which is a non-absorbing region for H_2O.

The LI-840A CO_2/H_2O Gas Analyzer optical path is a thermostatically controlled IR detection system. The optical bench operation is based upon a broad band IR source and a pyroelectric detector. The source is mounted in a parabolic reflector to collimate the light and increase energy throughput down the optical path to the detector. The reflector and optical path are gold plated to further increase energy transmission. The detectors are pyroelectric devices that operate based on thermal energy received. The narrowband optical filters allow only the wavebands of interest to illuminate the detector, allowing for the determination of CO_2 and H_2O concentrations in the presence of other infrared absorbing gases.

The detectors respond to thermal energy, so it is necessary to precisely regulate the detectors' temperature. This allows for differentiation of thermal gradient noise from the received signals from the optical path. The detection system is shown in Figure 1 below.

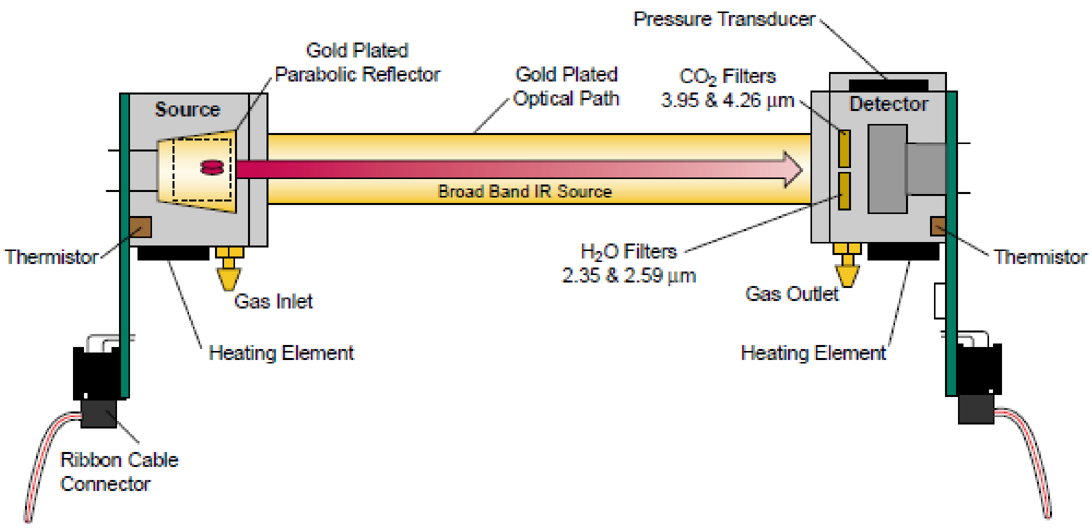

Figure 1. Schematic diagram of the LI-840A optical bench. Source: https://www.licor.com/documents/y10gor2jal2p3t8ev4hm

The instrument uses digital signal processing techniques to determine the temperature and pressure corrected CO_2 and H_2O concentrations based on the optical bench signals using a radiometric computation. The data are passed through a double rectangular hyperbola (CO_2) or 3rd order polynomial (H_2O) that performs linearization of the detector signal to a mole fraction in air given in µmol CO_2 per mole of air (ppm), and mmol H_2O per mole of air (ppt) as NEON L0 DPs.

3.2.2 Theory of Algorithm

The LI-840A computes CO_2 and H_2O concentrations using an equation of the general form

$$c = f(\alpha g(\alpha, P))S(\alpha))T \tag{3.1}$$

where c is concentration, $f()$ is the calibration function, α is the absorptance, g (α,P) is the pressure correction, S(α) is the span, and T is the temperature (Kelvin) of the gas in the cell, typically 324.65 Kelvin (51.5 °C). Absorptance is computed from

$$a = (1 - \frac{V}{V_0} Z) \tag{3.2}$$

where V and V_O are the raw detector sample and reference readings, and Z is the zeroing parameter. Span is a linear function of absorptance.

$$S(\alpha) = S_0 + S_1\alpha \tag{3.3}$$

For the detailed equations to calculate H_2O concentration, they can be found on page B-2 of RD[08].

For the detailed equations to calculate CO_2 concentration, they can be found on page B-3 to B-7 2 of RD[08].

3.3 Algorithm Implementation

Data flow for L0p signal processing is outlined in the following order.

1. Select L0 data streams for further data processing. See Table 3-2.
2. Regularize time stamp as described in section 3.3.1. Generate a complete 1 Hz L0p data set (fill in NAs) by converting L0 DPs under LI-840A in accordance with AD[04].
3. Convert fwMoleCO2 (μmol mol-1 , L0 DP) to rtioMoleWetCo2 (mol mol-1 , L0p DP) according to Eq. (3.4);
4. Convert fwMoleH2O (mmol mol-1 , L0 DP) to rtioMoleWetH2o (mol mol-1 , L0p DP) according to Eq. (3.5);
5. Calculate rtioMoleDryCo2 (mol mol-1) from rtioMoleWetCo2 (mol mol-1) and rtioMoleWetH2o (mol mol-1) according to Eq. (3.6);
6. Calculate rtioMoleDryH2o (mol mol-1) from rtioMoleWetH2o (mol mol-1) according to Eq. (3.7);
7. Convert tempCell (°C) to temp (K) according to Eq. (3.8);
8. Convert presCell (kPa) to pres (Pa) according to Eq. (3.9). See info below in section 3.3.2.

3.3.1 Time regularization

Data collected from IRGA is at ~1 Hz. To generate a complete L0p dataset with respect to 1 Hz frequency, missing timestamps and the corresponding data values will be filled with NaN (not NA) following the procedures detailed in AD[04]. In this case we will use the default options with a windowing approach described by Eq. 3 in AD[04], and when multiple data values fall within a single window we will use the closest value determined by minimum absolute deviation, option 1 in AD[04].

3.3.2 Unit conversion

Measurements (L0 DPs) output from the IRGA analyzers are provided in their standard units using their own internal propriety algorithm. We need to convert some of them to NEON standard units. See below:

fwMoleCo2 (μmol mol-1 , L0 DP) is total wet mole fraction of CO_2 in the air. It will be converted to rtioMoleWetCo2 (mol mol-1 , L0p DP) below:

$$\mathrm{rtioMoleWetCo2}(\mathrm{mol\ mol}-1\ ) = \frac{\mathrm{fwMoleCo2}\ (\mu\mathrm{mol\ mol}-1\ )}{1000000} \tag{3.4}$$

fwMoleH2o (mmol mol-1 , L0 DP) is total wet mole fraction of water vapor in the air. It will be converted to rtioMoleWetH2o (mol mol-1 , L0p DP) below:

$$\mathrm{rtioMoleWetH2o(mol\ mol-1\ )}\ = \frac{\mathrm{fwMoleH2o\ (mmol\ mol-1\ )}}{1000} \tag{3.5}$$

Calculate CO_2 dry mole fraction $\mathrm{rtioMoleDryCo2\ (mol\ mol-1\ )}$ from wet mole fraction of CO_2 $\mathrm{rtioMoleWetCo2}$ (mol mol-1 , L0p DP) and wet mole fraction of water vapor $\mathrm{rtioMoleWetH2o}$ (mol mol-1 , L0p DP):

$$\mathrm{rtioMoleDryCo2}\ = \frac{\mathrm{rtioMoleWetCo2}}{(1-\mathrm{rtioMoleWetH2o})} \tag{3.6}$$

Calculate H_2O dry mole fraction $\mathrm{rtioMoleDryH2o(mol\ mol-1\ )}$ from wet mole fraction of H_2O $\mathrm{rtioMoleWetH2o}$ (mol mol-1 , L0p DP):

$$\mathrm{rtioMoleDryH2o}\ = \frac{\mathrm{rtioMoleWetH2o}}{(1-\mathrm{rtioMoleWetH2o})} \tag{3.7}$$

tempCell (°C) should be converted to temp (K):

$$\mathrm{temp\ (K)} = \mathrm{tempCell\ (°C)}+273.15 \tag{3.8}$$

presCell (kPa) should be converted to pres (Pa):

$$\mathrm{pres\ (Pa)} = \mathrm{presCell\ (kPa)} \times 1000 \tag{3.9}$$

3.3.3 QA/QC Procedure

Standard plausibility tests should be applied to all L0p DPs except for flags. An associated pass/fail flag will be generated for each test according to AD[02]. (Note: Gap, null and de-spiking plausibility tests will not be run.) Quality reports will be generated for temporally-averaged L1 DPs in a separate L1 ATBD document (to be written).

Table 3-3: Plausibility quality flags to be applied to all L0p DPs (except for L0p DPs that are quality flags).

Flag	Term modifier	Description
QF_{Cal}	qfCal	Quality flag for the Invalid Calibration test
QF_{Pers}	qfPers	Quality flag for the Persistence test
QF_{Rng}	qfRng	Quality flag for the Range test
QF_{Step}	qfStep	Quality flag for the Step test

When perform the Invalid Calibration test, CI should use the latest calibration coefficients for the test if no new calibration coefficients set is available, even after the valid date range is already expired.

As all flags will be applied to each individual L0p DPs they will follow a uniform naming convention, whereby the L0p DP term is augmented with the plausibility test flag term modifier. For example, the quality flag for the step test for Cell Temperature will be "qfStepTemp".

The following parameters will be provided by FIU for each L0p DP and maintained in the CI data store.

Table 3-4: Parameters required for plausibility tests.

Parameter	Description
Thsh_{Pers}	Threshold for the Persistence test
Time_{Pers}	Time parameter for the Persistence test
$\mathrm{Thsh}_{Rng,min}$	Minimum threshold for the Range test
$\mathrm{Thsh}_{Rng,max}$	Maximum threshold for the Range test
Thsh_{Step}	Threshold for the Step test

3.4 Uncertainty

NA

4 ANALYZER FOR ISOTOPIC CO_2

4.1 Data Product Description

This section describes the processes to convert L0 DPs from the isotopic CO_2 analyzer (Picarro G2131-i, *hereafter* referred to as CRD CO_2) under the DGD 0330600000 into 1 Hz L0p DPs. The CRD CO_2 is referred to as crdCo2 in reference to DPs.

4.1.1 Variables Reported

The crdCo2-related L0p reported variables as provided by the algorithms documented in this ATBD are displayed in **Error! Reference source not found.**.

Table 4-1: List of crdCo2-related L0p reported variables that are produced in this ATBD.

L0p DP	L0p fieldName	L0pDP Frequency (Hz)	Units	Input L0 DPs or L0p - fieldNames
Instrument status	sensStus	1	NA	instStat
Instrument status flag	qfSensStus	1	NA	sensStus*
Cavity pressure	pres	1	Pa	presCavi
Cavity temperature	temp	1	K	tempCavi

L0p DP	L0p fieldName	L0pDP Frequency (Hz)	Units	Input L0 DPs or L0p -fieldNames
Warm box temperature	tempWbox	1	K	tempWarmBox
Gas spectrum ID	idGas	1	NA	specID
CO2 wet mole fraction	rtioMoleWetCo2	1	mol mol^{-1}	fwMoleCO2
CO2 dry mole fraction	rtioMoleDryCo2	1	mol mol^{-1}	fdMoleCO2
12CO2 wet mole fraction	rtioMoleWet12CCo2	1	mol mol^{-1}	fwMole12CO2
12CO2 dry mole fraction	rtioMoleDry12CCo2	1	mol mol^{-1}	fdMole12CO2
13CO2 wet mole fraction	rtioMoleWet13CCo2	1	mol mol^{-1}	fwMole13CO2
13CO2 dry mole fraction	rtioMoleDry13CCo2	1	mol mol^{-1}	fdMole13CO2
$\delta^{13}C$	dlta13CCo2	1	‰	d13CO2
H2O wet mole fraction	rtioMoleWetH2o	1	mol mol^{-1}	percentFwMoleH2O
H2O dry mole fraction	rtioMoleDryH2o	1	mol mol^{-1}	rtioMoleWetH2o*

*L0p DP is used as an input to generate other L0p DPs.

4.1.2 Input Dependencies

Table 4-2 lists all crdCo2-related L0 DPs and specifies which L0 DPs will be used to produce L0p reported variables in this ATBD.

Table 4-2: List of crdCo2-related L0 DPs.

L0 DP	L0 DP fieldName	Sample Frequency	Units	Data Product Number	DPs that are used to produce L0p (Y/N)
Instrument status	instStat	~1 Hz	NA	NEON.DOM.SITE.DP0.00102.001.02306.700.000.000	Y
Cavity pressure	presCavi	~1 Hz	torr	NEON.DOM.SITE.DP0.00102.001.02307.700.000.000	Y
Cavity temperature	tempCavi	~1 Hz	C	NEON.DOM.SITE.DP0.00102.001.02308.700.000.000	Y
Temperature inside chassis	tempDas	~1 Hz	C	NEON.DOM.SITE.DP0.00102.001.02309.700.000.000	N
Etalon temperature	tempEtal	~1 Hz	C	NEON.DOM.SITE.DP0.00102.001.02310.700.000.000	N

L0 DP	L0 DP fieldName	Sample Frequency	Units	Data Product Number	DPs that are used to produce L0p (Y/N)
Warm box temperature	tempWarmBox	~1 Hz	C	NEON.DOM.SITE.DP0.00102.001.02311.700.000.000	Y
State of external rotary valve	posiMPV	~1 Hz	NA	NEON.DOM.SITE.DP0.00102.001.02312.700.000.000	N
Digitizer value of outlet proportional valve	valvOutl	~1 Hz	NA	NEON.DOM.SITE.DP0.00102.001.02313.700.000.000	N
State of external solenoid valves	valvSol	~1 Hz	NA	NEON.DOM.SITE.DP0.00102.001.02314.700.000.000	N
Gas spectrum ID	specID	~1 Hz	NA	NEON.DOM.SITE.DP0.00102.001.02315.700.000.000	Y
CO2 wet mole fraction	fwMoleCO2	~1 Hz	$\mu mol\ mol^{-1}$	NEON.DOM.SITE.DP0.00102.001.02316.700.000.000	Y
CO2 dry mole fraction	fdMoleCO2	~1 Hz	$\mu mol\ mol^{-1}$	NEON.DOM.SITE.DP0.00102.001.02191.700.000.000	Y
12CO2 wet mole fraction	fwMole12CO2	~1 Hz	$\mu mol\ mol^{-1}$	NEON.DOM.SITE.DP0.00102.001.02317.700.000.000	Y
12CO2 dry mole fraction	fdMole12CO2	~1 Hz	$\mu mol\ mol^{-1}$	NEON.DOM.SITE.DP0.00102.001.02318.700.000.000	Y
13CO2 wet mole fraction	fwMole13CO2	~1 Hz	$\mu mol\ mol^{-1}$	NEON.DOM.SITE.DP0.00102.001.02319.700.000.000	Y
13CO2 dry mole fraction	fdMole13CO2	~1 Hz	$\mu mol\ mol^{-1}$	NEON.DOM.SITE.DP0.00102.001.02320.700.000.000	Y
2 minutes box averaging of $\delta^{13}C$	2Mind13CO2	~1 Hz	‰	NEON.DOM.SITE.DP0.00102.001.02321.700.000.000	N
30 seconds box averaging of $\delta^{13}C$	30Secd13CO2	~1 Hz	‰	NEON.DOM.SITE.DP0.00102.001.02322.700.000.000	N
5 minutes box averaging of $\delta^{13}C$	5Mind13CO2	~1 Hz	‰	NEON.DOM.SITE.DP0.00102.001.02323.700.000.000	N
$\delta^{13}C$	d13CO2	~1 Hz	%	NEON.DOM.SITE.DP0.00102.001.02324.700.000.000	Y
H2O wet mole fraction in percent	percentFwMoleH2O	~1 Hz	%	NEON.DOM.SITE.DP0.00102.001.02325.700.000.000	Y
2 minutes box averaging of isotope CO2 ratio	2MinCO2IsoRatio	~1 Hz	dimensionless	NEON.DOM.SITE.DP0.00102.001.02326.700.000.000	N
30 seconds box averaging of isotope CO2 ratio	30SecCO2IsoRatio	~1 Hz	dimensionless	NEON.DOM.SITE.DP0.00102.001.02327.700.000.000	N

L0 DP	L0 DP fieldName	Sample Frequency	Units	Data Product Number	DPs that are used to produce L0p (Y/N)
5 minutes box averaging of isotope CO2 ratio	5MinCO2IsoRatio	~1 Hz	dimensionless	NEON.DOM.SITE.DP0.00102.001.02328.700.000.000	N
Isotope CO2 ratio	CO2IsoRatio	~1 Hz	dimensionless	NEON.DOM.SITE.DP0.00102.001.02329.700.000.000	N
CH4 wet mole fraction	fwMoleCH4	~1 Hz	$\mu mol\ mol^{-1}$	NEON.DOM.SITE.DP0.00102.001.02330.700.000.000	N
CH4 dry mole fraction	fdMoleCH4	~1 Hz	$\mu mol\ mol^{-1}$	NEON.DOM.SITE.DP0.00102.001.02331.700.000.000	N
CH4 high precision wet mole fraction	fwMoleHPCH4	~1 Hz	$\mu mol\ mol^{-1}$	NEON.DOM.SITE.DP0.00102.001.02332.700.000.000	N
CH4 high precision dry mole fraction	fdMoleHPCH4	~1 Hz	$\mu mol\ mol^{-1}$	NEON.DOM.SITE.DP0.00102.001.02333.700.000.000	N
Peak height of H2O line	peakHeigH2O	~1 Hz	partsPerBillionPerCentimeter	NEON.DOM.SITE.DP0.00102.001.02334.700.000.000	N
Maximum of the spline fit to the CH4 line	spliFitCH4	~1 Hz	partsPerBillionPerCentimeter	NEON.DOM.SITE.DP0.00102.001.02335.700.000.000	N
Peak height of 12C line	peakHeig12C	~1 Hz	partsPerBillionPerCentimeter	NEON.DOM.SITE.DP0.00102.001.02336.700.000.000	N
Peak height of 13C line	peakHeig13C	~1 Hz	partsPerBillionPerCentimeter	NEON.DOM.SITE.DP0.00102.001.02337.700.000.000	N

*: Only the L0 DPs in "Y" are selected to transform into L0p DPs reported in this ATBD.

4.1.3 Product Instances

All terrestrial sites across the NEON observatory have the CRD CO_2 analyzers; individual instances of all analyzer-related L0p data outputs are in **Error! Reference source not found.**.

4.1.4 Temporal Resolution and Extent

The temporal extent of the reported variables in **Error! Reference source not found.** is 1 Hz.

4.1.5 Spatial Resolution and Extent

The CRD CO_2 analyzer will be located within the tower hut infrastructure. However, the analyzer's measurements reflect the points in space where the sample inlets are located on the tower infrastructure, which are site-specific.

4.2 Scientific context

Measurements of isotopic CO_2 exchange between the biosphere and atmosphere provide a powerful tool to advance the understanding of carbon cycle processes on different temporal and spatial scales (Werner and Gessler, 2011). When stable CO_2 isotope measurements are used in conjunction with flux measurements (e.g., with eddy-covariance technique) further insight can be gained concerning partitioning of net ecosystem CO_2 fluxes into gross respiration and photosynthesis (Yakir and Wang, 1996; Bowling et al., 2001). Partitioning of net ecosystem CO_2 fluxes would increase understanding of how environmental factors affect ecosystem respiration and photosynthesis separately at relatively large spatial scales from ecosystem to region (Yakir and Wang, 1996; Griffis, 2013). In addition, comparing stable CO_2 isotopes among sites and domains can be used to determine the contribution of fossil fuel carbon in the free atmosphere. This will provide researchers with tracer information of how large changes in air masses interact with the surface environments at regional to continental scales (Randerson et al. 2002a, 2002b).

4.2.1 Theory of Measurement

The Picarro G2131-i is a laser-based analyzer that uses the cavity ring-down spectroscopy (CRDS) technique to measure the stable isotope of $\delta^{13}C$ in CO_2. The principle of CRDS is to determine the optical absorbance of a particular gas species of interest by measuring the rate of exponential decay of light intensity inside a stable optical resonator called the ring-down cavity (Busch and Busch, 1997; Balslev-Clausen, 2011; Wahl et al., 2006; Crosson, 2008). The main components in a typical CRDS system are a laser, a high-finesse optical cavity consisting of two or more high-reflectivity mirrors, and a photo detector (Figure 2). When the measurement is carried out, the light with characteristic wavelength from a laser source is injected into the cavity through one of the partially reflecting mirrors. The light intensity in the cavity starts to build up over time and once a preset intensity level is reached, the laser is shut-off. Then, the decay of the stored light transmitted out of the cavity through one of partially reflecting mirrors is monitored by the photo detector (Figure 2; Wahl et al., 2006).

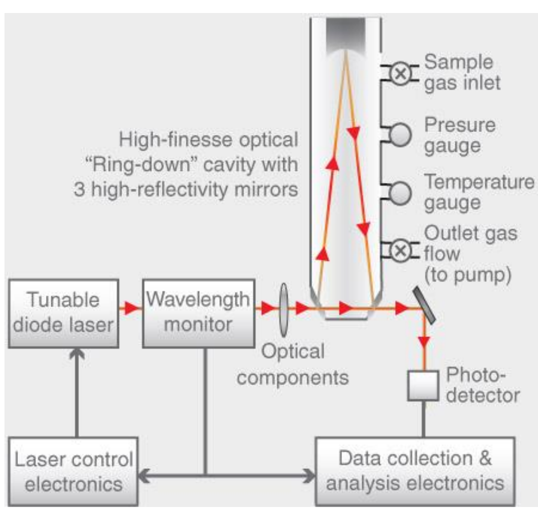

Figure 2. Schematic diagram of the components in the cavity ring-down spectroscopy analyzer. Source: http://www.picarro.com/

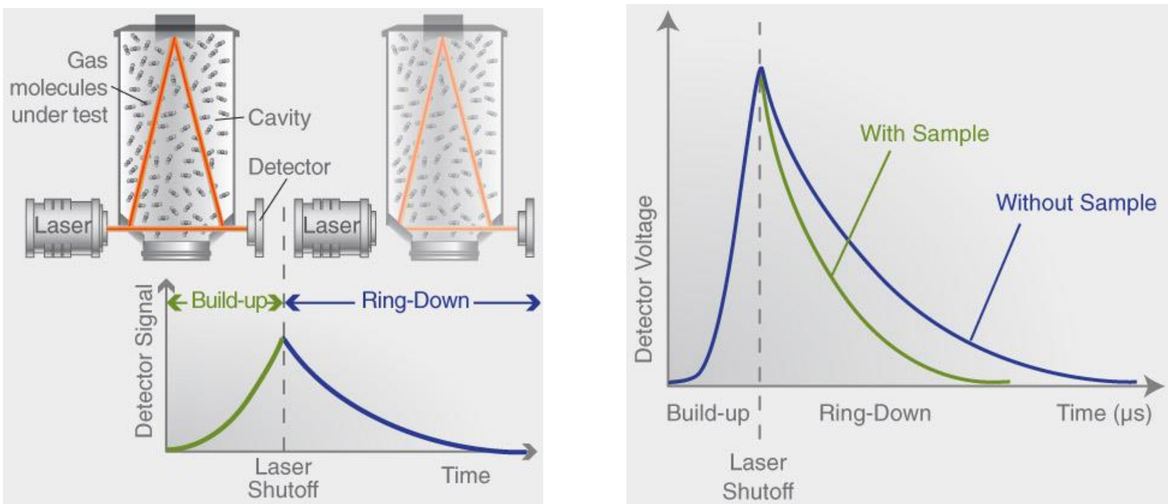

Figure 3. Left panel: a schematic of CRDS analyzer showing how a ring down measurement is carried out. Right panel: CRDS measure the decay of light intensity in the cavity with and without a sample having resonant absorbance. This demonstrates how optical loss (or absorption by gas) is rendered into a time measurement. Source: http://www.picarro.com/

4.2.2 Theory of Algorithm

Following Beer-Lambert law, the transmitted light, $I(t)$, from the cavity is given by:

$$I(t) = I_0 e^{-t/\tau} \tag{4.1}$$

where I_0 is the initial transmitted light intensity (i.e. at the time the laser is switched off), t is time, and τ is the ring-down time constant which describes how long it take for the intensity of light to reach $1/e$ of I_0. For an empty cavity, the transmitted light intensity decreases over time following an exponential decay characterized by a ring-down rate ($1/\tau$) that depends on the reflectivity of the mirrors, the separation between the mirrors, and the speed of light in the cavity (Wahl et al., 2006; Zare et al., 2009). If a gas species that absorbs the laser light is introduced into the cavity, the ring-down rate decreases compared with that for the empty cavity (Figure 2). This decay is proportional to the total optical losses inside the ring-down cavity including the round-trip scattering, mirror-transmission losses and the absorbance of a sample. Then, the mole fraction or isotopic ratio of the sample can be determined from the obtained absorption spectrum by calculating the difference between decay rates of the empty cavity and a cavity containing a sample (Wheeler et al., 1998; Korkiakoski, 2014).

For the Picarro G2131-i analyzer, the stable isotope of δ^{13}C is measured by measuring the absorption of two separate $^{12}CO_2$ and $^{13}CO_2$ spectral lines in the near-infrared region of the spectrum and the ratio of the peak heights of the lines is a measure of the ratio of the mole fractions of each of the two isotopologues (http://www.picarro.com/).

4.3 Algorithm Implementation

Data flow for L0p signal processing is outlined in the following order.

1. Select L0 data streams as indicated as "Y" in Table 4-2 in for further data processing.
2. Generate complete data with respect to 1 Hz frequency using a time regularization approach in accordance with AD[04], details are provided in section 4.3.2 for selected L0 data streams in step 1.
3. Identify timestamp corresponding to specID 105 and 11 and select all required data (Table 4-4) using these timestamps.
4. Generate complete data with respect to 1 Hz frequency using a time regularization approach in accordance with AD[04], details are provided in section 4.3.2 for all L0 DPs listed in Table 4-4.
5. Apply unit conversion to:
    a. cavity pressure (presCavi),
    b. cavity temperature (tempCavi),
    c. warm box temperature (tempWarmBox),
    d. wet and dry mole fraction of CO_2 (fwMoleCO2 and fdMoleCO2), 12CO_2, (fdMole12CO2, fwMole12CO2), 13CO_2 (fdMole13CO2, fwMole13CO2), and
    e. percentFwMoleH2O.

Details are provided in section 4.3.3

6. Determine and assign the instrumentation status flag (qfSensStus, i.e. '0' if there is no error and '1' if error is detected during the operation) to corresponding 1 Hz data, details are provided in section 4.3.4.
7. QA/QC Plausibility tests will be applied to the data stream in accordance with AD[02], details are provided in section 4.3.5.

4.3.1 Filter specific data stream by spectrum ID

The CRD CO_2 is capable of measuring multiple gas species, but measures only one gas species at a time and the analyzer will update only the most recent measured values. This will create duplicates of data in the data stream (see example in Table 4-3). The spectrum ID (specID) L0 DP, which indicates which gas species are being measured, will be used to filter only the raw measurement data for each L0 DPs in Table 4-4.

Table 4-3: Example of crdCo2 L0 data streams. Note that only L0 DPs of interest are shown in this table.

timeStamp	instStat	specID	fwMoleCO2	fdMoleCO2	fwMole12CO2	fdMole12CO2	fwMole13CO2	fdMole13	d13CO2	percentFwMoleH2O	fwMoleCH4	fdMoleCH4	fwMoleHPCH4	fdMoleHPCH4	CO2IsoRatio
2015-09-24T14:21:00.597Z	963	105	453.033997	465.119995	446.813995	458.738007	4.939	5.071	-11.62	1.539	0.011	2.044	2.082	2.047	2.081
2015-09-24T14:21:01.864Z	963	29	453.036987	465.122009	446.813995	458.738007	4.942	5.074	-11.077	1.539	0.011	2.047	2.084	2.047	2.081
2015-09-24T14:21:02.220Z	963	25	453.036987	465.122009	446.813995	458.738007	4.942	5.074	-11.077	1.539	0.011	2.047	2.084	2.048	2.082
2015-09-24T14:21:03.403Z	963	105	453.483002	465.579987	447.253998	459.190002	4.947	5.079	-11.077	1.539	0.011	2.047	2.084	2.048	2.082
2015-09-24T14:21:04.386Z	963	105	453.531006	465.630005	447.308014	459.244995	4.941	5.073	-12.42	1.539	0.011	2.047	2.084	2.048	2.082
2015-09-24T14:21:06.458Z	963	11	453.53299	465.588013	447.309998	459.20401	4.941	5.072	-12.483	1.534	0.011	2.047	2.084	2.048	2.082
2015-09-24T14:21:07.542Z	963	105	454.02301	466.091003	447.794006	459.700012	4.946	5.078	-12.483	1.534	0.011	2.047	2.084	2.048	2.082
2015-09-24T14:21:08.526Z	963	105	454.04599	466.11499	447.812988	459.720001	4.95	5.082	-11.687	1.534	0.011	2.047	2.084	2.048	2.082
2015-09-24T14:21:09.778Z	963	29	454.049011	466.118011	447.812988	459.720001	4.953	5.085	-11.133	1.534	0.011	2.043	2.08	2.048	2.082
2015-09-24T14:21:10.132Z	963	25	454.049011	466.118011	447.812988	459.720001	4.953	5.085	-11.133	1.534	0.011	2.043	2.08	2.047	2.081
2015-09-24T14:21:11.330Z	963	105	453.959991	466.026001	447.725006	459.630005	4.952	5.084	-11.133	1.534	0.011	2.043	2.08	2.047	2.081
2015-09-24T14:21:12.314Z	963	105	453.873993	465.937988	447.63501	459.537994	4.956	5.088	-10.133	1.534	0.011	2.043	2.08	2.047	2.081
2015-09-24T14:21:14.401Z	963	11	453.871002	465.938995	447.63501	459.541992	4.953	5.085	-10.756	1.534	0.011	2.043	2.08	2.047	2.081
2015-09-24T14:21:15.493Z	963	105	454.014008	466.085999	447.777008	459.687012	4.954	5.086	-10.756	1.534	0.011	2.043	2.08	2.047	2.081
2015-09-24T14:21:16.465Z	963	105	453.838989	465.906006	447.604004	459.509003	4.952	5.084	-10.734	1.534	0.011	2.043	2.08	2.047	2.081
2015-09-24T14:21:17.721Z	963	29	453.835999	465.903015	447.604004	459.509003	4.95	5.082	-11.284	1.534	0.011	2.05	2.087	2.047	2.081
2015-09-24T14:21:18.075Z	963	25	453.835999	465.903015	447.604004	459.509003	4.95	5.082	-11.284	1.534	0.011	2.05	2.087	2.047	2.081
2015-09-24T14:21:19.258Z	963	105	454.036011	466.108002	447.799988	459.710999	4.952	5.084	-11.284	1.534	0.011	2.05	2.087	2.047	2.081
2015-09-24T14:21:20.240Z	963	105	453.743011	465.808014	447.513	459.415985	4.948	5.08	-11.509	1.534	0.011	2.05	2.087	2.047	2.081
2015-09-24T14:21:22.334Z	963	11	453.742004	465.822998	447.511993	459.431	4.947	5.079	-11.593	1.536	0.011	2.05	2.087	2.047	2.081
2015-09-24T14:21:23.433Z	963	105	453.824005	465.907013	447.592987	459.514008	4.948	5.08	-11.593	1.536	0.011	2.05	2.087	2.047	2.081
2015-09-24T14:21:24.432Z	963	105	453.710999	465.790985	447.479004	459.397003	4.95	5.082	-10.984	1.536	0.011	2.05	2.087	2.047	2.081
2015-09-24T14:21:25.679Z	963	29	453.709991	465.789001	447.479004	459.397003	4.948	5.08	-11.288	1.536	0.011	2.034	2.071	2.047	2.081
2015-09-24T14:21:26.033Z	963	25	453.709991	465.789001	447.479004	459.397003	4.948	5.08	-11.288	1.536	0.011	2.034	2.071	2.048	2.082
2015-09-24T14:21:27.239Z	963	105	453.966003	466.052002	447.730988	459.656006	4.951	5.083	-11.288	1.536	0.011	2.034	2.071	2.048	2.082
2015-09-24T14:21:28.227Z	963	105	453.761993	465.842987	447.545013	459.464996	4.934	5.066	-14.404	1.536	0.011	2.034	2.071	2.048	2.082
2015-09-24T14:21:30.327Z	963	11	453.769989	465.878998	447.544006	459.490997	4.943	5.075	-12.524	1.54	0.011	2.034	2.071	2.048	2.082
2015-09-24T14:21:30.551Z	963	11	453.769989	465.878998	447.544006	459.490997	4.943	5.075	-12.524	1.54	0.011	2.034	2.071	2.048	2.082

Table 4-4: Spectrum ID and its corresponded L0 DPs.

Spectrum ID (specID)	L0 DPs
105	fwMoleCO2 fdMoleCO2 fwMole12CO2 fdMole12CO2 fwMole13CO2 fdMole13CO2 d13CO2
11	percentFwMoleH2O

4.3.2 Time regularization

CRD CO_2 measures data at ~1 Hz. To generate complete L0p data with respect to 1 Hz frequency, missing timestamps and the corresponding data values will be filled with NaN (not NA) following the procedures detailed in AD[04]. In this case we will use the default options in AD[04] with a windowing approach described by Eq. 3 in AD[04], and when multiple data values fall within a single window we will use the closest value determined by minimum absolute deviation, option 1 in AD[04].

4.3.3 Unit conversion

CRD CO_2 outputs in its standard units using its own internal propriety algorithm. However, some measurements need to be converted to NEON standard units as follow:

The unit of cavity pressure (presCavi) shall be converted to Pascal (Pa) by:

$$\text{pres in Pa} = 101325/760 * \text{presCavi in torr} \quad (4.2)$$

The units of cavity temperature (tempCavi) and warm box temperature (tempWarmBox) shall be converted to kelvin. The units of wet and dry mole fraction of CO_2 (fwMoleCO2 and fdMoleCO2), $12CO_2$, (fdMole12CO2, fwMole12CO2) and $13CO_2$ (fdMole13CO2, fwMole13CO2) are needed to convert to mole mole-1 by:

$$\mathrm{X} = 10^{-6} * \mathrm{Y} \quad (4.3)$$

where, X is rtioMoleWetCo2, rtioMoleDryCo2, rtioMoleWet12CCo2, rtioMoleDry12CCo2, rtioMoleWet13CCo2, or rtioMoleDry13CCo2 in mol mol^{-1} and Y is fwMoleCO2, fdMoleCO2, fwMole12CO2, fdMole12CO2, fwMole13CO2, or fdMole13CO2 in µmol mol^{-1}.

The total wet mole fraction in percent of water vapor (percentFwMoleH2O) is needed to convert to mol mol^{-1} by:

$$\text{rtioMoleWetH2o} = 10^{-2} * \text{percentFwMoleH2O} \quad (4.4)$$

and then dry mole fraction of water vapor can be calculated as:

$$\text{rtioMoleDryH2o} = \frac{\text{rtioMoleWetH2o}}{(1-\text{rtioMoleWetH2o})} \quad (4.5)$$

4.3.4 Sensor Flags

Instrumentation status flag will be generated as part of the L0p report variables to indicate that the analyzer was working properly and no error occurred during operation, which is defined as:

$$\text{qfSensStus} = \begin{cases} 0 \text{ if sensStus} = 963 \\ 1 \text{ if sensStus} \neq 963 \\ -1 \text{ if sensStus} = \text{NaNand continous sequence of NaNs} > 3\text{s duration} \\ \text{NaN if sensStus} = \text{NaN and continuous sequence of NaNs} \leq 3\text{s duration} \end{cases} \quad (4.6)$$

Additionally, to distinguish between NaNs that resulted from time regularization and NaNs that resulted from true missing values, the latter will be replaced by -1, see Eq. (4.6).

4.3.5 QA/QC Procedure

Standard plausibility tests should be applied to all L0p DPs except for qfSensStus, sensStus, and idGas. An associated pass/fail flag will be generated for each test according to AD[02]. Note: Gap, null, and de-spiking plausibility tests will not be run, due to the gap-filling described in section 4.3.1 Time Regularization. Quality reports will be generated for temporally-averaged L1 DPs at a later stage.

Table 4-5: Plausibility quality flags to be applied to all L0p DPs

Flag	Term modifier	Description
QF_{Cal}	qfCal	Quality flag for the Invalid Calibration test
QF_{Pers}	qfPers	Quality flag for the Persistence test
QF_{Rng}	qfRng	Quality flag for the Range test
QF_{Step}	qfStep	Quality flag for the Step test

When performing the Invalid Calibration test, CI should use the latest calibration coefficients for the test if no new calibration coefficients set is available, even after the valid date range is already expired.

As all flags will be applied to each individual L0p DPs they will follow a uniform naming convention, whereby the L0p DP term is augmented with the plausibility test flag term modifier. For example, the quality flag for the step test for $\delta^{13}C$ will be "qfStepDlta13CCo2".

The following parameters will be provided by FIU for each L0p DP and maintained in the CI data store.

Table 4-6: Parameters required for plausibility tests.

Parameter	Description
Thsh_{Pers}	Threshold for the Persistence test
Time_{Pers}	Time parameter for the Persistence test
$\mathrm{Thsh}_{Rng,min}$	Minimum threshold for the Range test
$\mathrm{Thsh}_{Rng,max}$	Maximum threshold for the Range test
Thsh_{Step}	Threshold for the Step test

4.4 Uncertainty

NA

5 ANALYZER FOR ISOTOPIC WATER

5.1 Data Product Description

This section describes the processes to convert L0 DPs from the isotopic H_2O analyzer (Picarro L2130-i, *hereafter* referred to as CRD H_2O) under the DGD 0328050000 into 1 Hz L0p DPs. The CRD H_2O is referred to as crdH2o in reference to DPs.

5.1.1 Variables Reported

The crdH2o-related L0p reported variables provided by the algorithms documented in this ATBD are displayed in Table 5-1: List of crdH2o-related L0p reported variables that produced in this ATBD.Table 5-1.

Table 5-1: List of crdH2o-related L0p reported variables that produced in this ATBD.

L0p DP	L0p fieldName	L0p DP Frequency	Units	Input L0 fieldNames
Instrument Status	sensStus	1 Hz	NA	instStat
Instrument status flag	qfSensStus	1 Hz	NA	sensStus
Cavity pressure	pres	1 Hz	Pa	presCavi
Cavity temperature	temp	1 Hz	K	tempCavi
Warm box temperature	tempWbox	1 Hz	K	tempWarmBox
ValveMask	valvCrdH2o	1 Hz	NA	valvMask
H2O wet mole fraction	rtioMoleWetH2o	1 Hz	mol mol-1	ppmvFwMoleH2O
H2O dry mole fraction	rtioMoleDryH2o	1 Hz	mol mol-1	rtioMoleWetH2o*
$\delta^{18}O$	dlta18OH2o	1 Hz	‰	d18OWater
$\delta^{2}H$	dlta2HH2o	1 Hz	‰	d2HWater
N2 flag	stusN2	1 Hz	NA	N2Flag
N2flag flag	qfStusN2	1 Hz	NA	stusN2
Low humidity flag	qfLowRtioMoleWetH2o	1 Hz	NA	rtioMoleWetH2o*

*: This is a L0p DP. It is used as an input to generate other L0p DP.

5.1.2 Input Dependencies

Table 5-2 lists all crdH2o-related L0 DPs and specifies which L0 DPs will be used to produce L0p reported variables in this ATBD.

Table 5-2: A full list of crdH2o L0 DPs.

L0 DP	L0 DP fieldName	Sample Frequency	Units	Data Product Number	DPs that are used to produce L0' (Y/N)*
Instrument status	instStat	~1 Hz	NA	NEON.DOM.SITE.DP0.00103.001.02306.700.000.000	Y
Cavity Pressure	presCavi	~1 Hz	torr	NEON.DOM.SITE.DP0.00103.001.02307.700.000.000	Y
Cavity Temperature	tempCavi	~1 Hz	°C	NEON.DOM.SITE.DP0.00103.001.02308.700.000.000	Y
Das Temperature	tempDas	~1 Hz	°C	NEON.DOM.SITE.DP0.00103.001.02309.700.000.000	N
Etalon Temperature	tempEtal	~1 Hz	°C	NEON.DOM.SITE.DP0.00103.001.02310.700.000.000	N
Warm Box Temperature	tempWarmBox	~1 Hz	°C	NEON.DOM.SITE.DP0.00103.001.02311.700.000.000	Y
MPV Position	posiMPV	~1 Hz	NA	NEON.DOM.SITE.DP0.00103.001.02312.700.000.000	N
Outlet Valve	valvOutl	~1 Hz	NA	NEON.DOM.SITE.DP0.00103.001.02313.700.000.000	N
Valve Mask	valvMask	~1 Hz	NA	NEON.DOM.SITE.DP0.00103.001.02338.700.000.000	Y
H2O wet concentration	ppmvFwMoleH2O	~1 Hz	$\mu mol\ mol^{-1}$	NEON.DOM.SITE.DP0.00103.001.02339.700.000.000	Y
$\delta^{18}O$	d18OWater	~1 Hz	‰	NEON.DOM.SITE.DP0.00103.001.02369.700.000.000	Y
$\delta^{2}H$	d2HWater	~1 Hz	‰	NEON.DOM.SITE.DP0.00103.001.02370.700.000.000	Y
CH4	fwMoleCH4	~1 Hz	$\mu mol\ mol^{-1}$	NEON.DOM.SITE.DP0.00103.001.02330.700.000.000	N
N2 flag	N2Flag	~1 Hz	NA	NEON.DOM.SITE.DP0.00103.001.02340.700.000.000	Y
Baseline shift	baseShift	~1 Hz	ppb/cm	NEON.DOM.SITE.DP0.00103.001.02341.700.000.000	N
Slope shift	slopShift	~1 Hz	ppb/cm	NEON.DOM.SITE.DP0.00103.001.02342.700.000.000	N
Residuals	resiRMS	~1 Hz	ppb/cm	NEON.DOM.SITE.DP0.00103.001.02343.700.000.000	N

*: Only the L0 DPs in "Y" are selected to transform into L0p DPs reported in this ATBD.

5.1.3 Product Instances

20 core sites plus Barrow relocatable site across the NEON observatory own the CRD H_2O analyzers. Individual instance of all analyzer-related L0p data outputs are in Table 5-1.

5.1.4 Temporal Resolution and Extent

The temporal extent of the reported variables in Table 5-1 is 1 Hz.

5.1.5 Spatial Resolution and Extent

The CRD H_2O analyzer will be located within the tower hut infrastructure. However, the analyzer's measurements reflect the points in space where the sample inlets are located on the tower infrastructure, which will be site specific.

5.2 Scientific context

To obtain detailed knowledge of the hydrological cycle, information on all three phases of water is required. Isotopic analysis of atmospheric trace gases provides a valuable tool for resolving their budgets because the physical, chemical, or biological processes involved fractionate isotopically in unique ways and leave characteristic isotopic signatures in the trace gas. In particular, water vapor isotopes provide information concerning the mechanisms of processes that occur in the water cycle, such as evaporation at the surface of the Earth and subsequent transport and phase changes in the atmosphere. Water-vapor isotope measurements can be used to reveal a possible relationship between water-vapor isotopes and ambient moisture, and to understand the processes such as evaporation and condensation in climatic simulations (Iannone et al., 2010). When the stable H_2O isotope measurements are used in conjunction with flux measurements (e.g., with eddy-covariance technique) further insight can be gained by partitioning the net ecosystem H_2O fluxes into evaporation and transpiration over an ecosystem (Yepez et al., 2003; Hu et al., 2014).

5.2.1 Theory of Measurement

The Picarro L2130-i is a laser-based analyzer that uses the cavity ring-down spectroscopy (CRDS) technique to measure the stable isotopes of $\delta^{18}O$ and $\delta^{2}H$ in H_2O. The underlying principle of CRDS can be found in section 4.2.1.

5.2.2 Theory of Algorithm

Details on theory of algorithm can be found in section 4.2.2. For Picarro L2130-i analyzer, the stable isotope of $\delta^{18}\mathrm{O}$ is measured by measuring the absorption of two separate spectral lines ($H_2{}^{18}O$ and $H_2{}^{16}O$) in the near-infrared region of the spectrum, and the ratio of the peak heights of the lines is measured by the ratio of the mole fractions of each of the two isotopologues. Similarly, the stable isotope of δD is measured by measuring the absorption of two separate spectral lines (${}^{2}H_2O$ and ${}^{1}H_2O$) in the near-infrared region of the spectrum, and the ratio of the peak heights of the lines is measured by the ratio of the mole fractions of each of the two isotopologues (http://www.picarro.com/).

5.3 Algorithm Implementation

Data flow for signal processing of L0p reported variables will be treated in the following order:

1. Select the following L0 data streams for further data processing: instStat, valvMask, ppmvFwMoleH2O, d18OWater, d2HWater, N2Flag . See Table 5-2.
2. Generate complete data with respect to 1 Hz frequency, using a time regularization approach in accordance with AD[04]. Details are provided in section 5.3.1.
3. Convert units according to Eq. () to () in section 5.3.2.
4. Determine and assign the Instrumentation status flag (qfSensStus) to corresponding 1 Hz data. Details are provided below. See section 5.3.3 a.
5. Determine and assign flag (qfStusN2) for carrier gas mode setting (N2Flag). See section 5.3.3 b.
6. Determine and assign the Low humidity flag (qfLowRtioMoleWetH2o) to corresponding 1 Hz data. Details are provided below. See section 5.3.3 c.
7. QA/QC Plausibility tests will be applied to the data stream in accordance with AD[02]. Details are provided below. See section 5.3.4 below.

5.3.1 Time regularization

CRD H_2O analyzer measures data at ~ 1 Hz. To generate a complete L0p dataset with respect to 1 Hz frequency, missing timestamps and the corresponding data values will be filled with NaN (not NA) following the procedures detailed in AD[04]. In this case we will use the default options in AD[04] with a windowing approach described by Eq. 3 in AD[04], and when multiple data values fall within a single window we will use the closest value determined by minimum absolute deviation, option 1 in AD[04].

5.3.2 Unit conversion

Measurements output from the CRD H_2O analysers are outputted in their standard units using their own internal propriety algorithm. However, some measurements such as ppmvFwMoleH2O are needed to convert to NEON standard units. The total wet mole fraction in ppmv of water vapor in the air shall be converted to wet mole fraction in mole mole^{-1} by:

$$\mathrm{rtioMoleWetH2o} = \mathrm{ppmvFwMoleH2O}/1000000 \tag{5.1}$$

and then dry mole fraction of water vapor will be calculated as:

$$\mathrm{rtioMoleDryH2o} = \frac{\mathrm{rtioMoleWetH2o}}{(1 - \mathrm{rtioMoleWetH2o}/1000)} \tag{5.2}$$

The unit of cavity pressure (presCavi) shall be converted to Pascal (Pa) by:

$$\mathrm{pres\ in\ Pa} = 101325/760 * \mathrm{presCavi\ in\ torr} \tag{5.3}$$

The unit of cavity temperature (tempCavi) shall be converted to Kelvin (K) by:

$$\mathrm{temp\ in\ K} = \mathrm{tempCavi\ in\ Celsius} + 273.15 \tag{5.4}$$

The unit of warm box temperature (tempWarmBox) shall be converted to Kelvin (K) by:

$$\text{tempWbox in K} = \text{tempWarmBox in Celsius} + 273.15 \tag{5.5}$$

5.3.3 Sensor Flags

a. **Instrumentation status flag** (qfSensStus) will be generated as part of the L0p report variables to indicate the status of the instrumentation during operation. 0 indicates there is no error and 1 indicates an error has been detected during the operation. In addition, the definition below also includes steps to distinguish the NaNs between data missing NaNs (NaN > 3s) or NaNs due to time regularization (NaN ≤ 3s). qfSensStus is defined as:

$$\text{qfSensStus} = \begin{cases} 0 \text{ if sensStus} = 963 \\ 1 \text{ if sensStus} \neq 963 \\ -1 \text{ if sensStus} = \text{NaN and continous sequence of NaNs} > 3\text{s duration} \\ \text{NaN if sensStus} = \text{NaN and continuous sequence of NaNs} \leq 3\text{s duration} \end{cases} \tag{5.6}$$

b. **Carrier gas setting status flag** (qfStusN2) will be generated as part of the L0p report variables to indicate if the carrier gas mode was set correctly in L2130-I and there is no error occurred during operation. For N2Flag, 0=air mode, 1=N2 mode. Because NEON will use zero air as carrier gas. Carrier gas setting N2Flag should be always 0 during normal operation. If N2Flag is 1, data should be flagged, indicating data will be not useful. Because we do time regularization first to generate StusN2, then StusN2 will be used to generate the quality flag qfStusN2 below. In other words, qfStusN2 = 0 (no error) when StusN2 = 0 (air mode), and qfStusN2 = 1 (has error) when StusN2 = 1 (N2 mode). Similarly, the definition below also includes steps to distinguish the NaNs between data missing NaNs (NaN > 3s) or NaNs due to time regularization (NaN ≤ 3s). Therefore, qfStusN2 is defined as:

$$\text{qfStusN2} = \begin{cases} 0 \text{ if StusN2} = 0 \\ 1 \text{ if StusN2} = 1 \\ -1 \text{ if StusN2} = \text{NaN and and continous sequence of NaNs} > 3\text{s duration} \\ \text{NaN if StusN2} = \text{NaN and continuous sequence of NaNs} \leq 3\text{s duration} \end{cases} \tag{5.7}$$

c. **Low humidity flag** (qfLowRtioMoleWetH2o) will be generated as part of the L0p report variables to indicate if the sensor is operated under low humidity. In the laboratory testing, we found the humidity dependence of the isotopic measurements became significantly pronounced for the humidity levels below 5000 ppmv (or 0.005 mol mol^{-1}). Here, 0 indicates the sensor operates under the humidity levels greater than 5000 ppmv and 1 indicates the sensor operates under the humidity levels below or equal to 5000 ppmv. In addition, the definition below also includes steps to distinguish the NaNs between data missing NaNs (NaN > 3s) or NaNs due to time regularization (NaN ≤ 3s). qfLowRtioMoleWetH2o is defined as:

$$\mathrm{qfLowRtioMoleWetH2o} = \begin{cases} 0 & \text{if rtioMoleWetH2o} > 0.005 \\ 1 & \text{if rtioMoleWetH2o} \leq 0.005 \\ -1 & \text{if rtioMoleWetH2o} = \text{NaN and continous sequence of NaNs} > \text{3s duration} \\ \text{NaN} & \text{if rtioMoleWetH2o} = \text{NaN and continuous sequence of NaNs} \leq \text{3s duration} \end{cases} \tag{5.8}$$

5.3.4 QA/QC Procedure

Standard plausibility tests should be applied to all L0p DPs, except for flags, instrument status (sensStus), valve mask (valvCrdH2o), and N2 Status (stusN2). An associated pass/fail flag will be generated for each test according to AD[02]. (Note. We will not be carrying out the "Gap test" and "Null test". We also will not run signal de-spike). Quality reports will be generated for temporally averaged L1 DPs at a later stage.

Table 5-3: Plausibility quality flags to be applied to all L0p DPs except for flags.

Flag	Term modifier	Description
QF_{Cal}	qfCal	Quality flag for the Invalid Calibration test
QF_{Pers}	qfPers	Quality flag for the Persistence test
QF_{Rng}	qfRng	Quality flag for the Range test
QF_{Step}	qfStep	Quality flag for the Step test

When perform the Invalid Calibration test, CI should use the latest calibration coefficients for the test if no new calibration coefficients set is available, even after the valid date range is already expired.

As all flags will be applied to each individual L0p DPs they will follow a uniform naming convention, whereby the L0p DP term is augmented with the plausibility test flag term modifier. For example, the quality flag for the step test for $\delta^{18}O$ will be "qfStepDlta18OH2o".

The following parameters will be provided by FIU for each L0p DP and maintained in the CI data store.

Table 5-4: Parameters required for plausibility tests.

Parameter	Description
Thsh_{Pers}	Threshold for the Persistence test
Time_{Pers}	Time parameter for the Persistence test
$\mathrm{Thsh}_{Rng,min}$	Minimum threshold for the Range test
$\mathrm{Thsh}_{Rng,max}$	Maximum threshold for the Range test
Thsh_{Step}	Threshold for the Step test

5.4 Uncertainty

NA

6 TEMPERATURE SENSOR IN THE HUT

6.1 Data Product Description

6.1.1 Variables Reported

The Comet T7610 sensor measuring the temperature, barometric pressure, relative humidity, and water mixing ratios in the hut is called envHut in reference to DPs. The envHut-related L0p variables provided by the algorithms documented in this ATBD are displayed in Table 6-1.

Table 6-1: List of envHut-related L0p reported variables that are produced in this ATBD.

L0p DP	L0p fieldName	L0p DP Frequency (Hz)	Units	Input L0 DPs or L0p fieldNames
Temperature in the instrument hut	temp	1	K	tempHut
Humidity in the instrument hut	rh	1	-	RHHut
Barometric pressure in the instrument hut	pres	1	Pa	baroPresHut

L0p DP	L0p fieldName	L0p DP Frequency (Hz)	Units	Input L0 DPs or L0p fieldNames
H2O wet mole fraction in the instrument hut	rtioMoleWetH2o	1	mol mol^{-1}	baroPresHut H2OMixRatioHut
Hut temperature flag	qfTemp	1	NA	temp*
Hut humidity flag	qfRh	1	NA	rtioMoleWetH2o*

*L0p DP is used as an input to generate other L0p DPs.

6.1.2 Input Dependencies

Table 6-2 details the envHut-related L0 DPs used to produce L0p reported variables in this ATBD.

Table 6-2: List of envHut-related L0 DPs that are transformed into L0p reported variables DPs in this ATBD.

L0 DP	L0 DP fieldName	Sample Frequency	Units	Data Product Number	DPs that are used to produce L0p (Y/N)
Temperature in the instrument hut	tempHut	1	C	NEON.DOM.SITE.DP0.00104.001.02344.700.000.000	Y
Humidity in the instrument hut	RHHut	1	%	NEON.DOM.SITE.DP0.00104.001.02345.700.000.000	Y
Barometric pressure in the instrument hut	baroPresHut	1	kPa	NEON.DOM.SITE.DP0.00104.001.02346.700.000.000	Y
H2O mixing ratio in the instrument hut	H2OMixRatioHut	1	g kg^{-1}	NEON.DOM.SITE.DP0.00104.001.02347.700.000.000	Y

*: Only the L0 DPs in "Y" are selected to transform into L0p DPs reported in this ATBD.

6.1.3 Product Instances

The Comet T7610 is located in the instrument hut within a radius of 50 cm from the LI840A. All terrestrial sites across the NEON observatory have the Comet T7610 sensors; individual instances of all L0p data outputs from this sensor are in Table 6-1.

6.1.4 Temporal Resolution and Extent

The temporal extent of the reported variables in Table 6-1 is 1 Hz.

6.1.5 Spatial Resolution and Extent

The Comet T7610 is located within the tower hut infrastructure. However, the measurements reflect the points in space where the sensor is located in the tower hut infrastructure. In the current design, the Comet T7610 is installed in the same rack as IRGA analyzer to represent hut environmental condition.

6.2 Scientific context

The Comet T7610 is used to monitor hut environmental condition, which includes ambient temperature, pressure, relative humidity and water mixing ratio. Because of the dependency of the IRGA analyzer to its ambient temperature variation, the temperature L0 DP output from this sensor will be used to create flags to indicate when the data from IRGA are delivered outside of the acceptable temperature ranges. . Furthermore, water mixing ratio output from this sensor will also be used to create flags to indicate when the data from CRD H_2O delivered outside of the acceptable humidity ranges. According to communication with manufacture, the high ambient humidity could interfere with the performance of CRD H_2O.

6.2.1 Theory of Measurement

The Comet T7610 is designed to measure temperature, relative humidity and atmospheric pressure in air without aggressive substances. The sensor also outputs computed quantities, including dew point temperature, absolute humidity, mixing ratio and specific enthalpy. In the current design, the mixing ratio was selected as the computed output and it will be used to generate the humidity flags for CRD H_2O.

6.2.2 Theory of Algorithm

NA

6.3 Algorithm Implementation

L0p signal processing consists of the following sequence:

1. Select L0 data streams as indicated as “Y” in Table 6-2 for further data processing.
2. Generate complete data with respect to 1 Hz frequency using the time regularization approach in accordance with AD[04], details are provided in section 6.3.1.
3. Apply unit conversion to tempHut, RHHUT, baroPresHut, and H2OMixRatioHut according to Eq. (6.1) to (6.4), respectively.
4. Determine and assign the temperature flag to its corresponding timestamp according to Eq. (6.5), details are provided below in section 6.3.3.
5. Determine and assign the humidity flag to its corresponding timestamp according to Eq. (6.6), details are provided below in section 6.3.3.
6. QA/QC Plausibility tests will be applied to the data stream in accordance with AD[02], details are provided below in section 6.3.4.

6.3.1 Time regularization

The Comet T7610 measures data at 1 Hz. To generate time regularized output, complete L0p data with respect to 1 Hz frequency by filling in missing timestamps and the corresponding data values with NaN (not NA) following the procedures detailed in AD[04]. In this case we will use the default options in AD[04] with a windowing approach described by Eq. 3 in AD[04], and when multiple data values fall within a single window we will use the closest value determined by minimum absolute deviation, option 1 in AD[04].

6.3.2 Unit conversion

The Comet T7610 sensor outputs data in digital form through Ethernet connections, therefore, no analog to digital (A/D) conversion is necessary. However, all measurements, including tempHut, RHHut, baroPresHut, and H2OMixRatioHut are needed to convert to the meaningful units as follow:

tempHut (NEON.DOM.SITE.DP0.00104.001.02344.700.000.000) in degree Celsius to Kelvin,

$$\text{temp in K} = \text{tempHut in degree °C} + 273.15 \tag{6.1}$$

RHHut (NEON.DOM.SITE.DP0.00104.001.02345.700.000.000) in percentage to fraction,

$$\text{rh in fraction} = \frac{\text{RHHut in percentage}}{100} \tag{6.2}$$

baroPresHut (NEON.DOM.SITE.DP0.00104.001.02346.700.000.000) in kPa to Pa,

$$\text{pres in Pa} = \text{baroPresHut in kPa} * 1000 \tag{6.3}$$

and H2OMixRatioHut (NEON.DOM.SITE.DP0.00104.001.02347.700.000.000) in g kg^{-1} to mol mol-1

$$\text{rtioMoleWetH2o} = \text{H2OMixRatioHut} * \frac{\text{MolmDry}}{\text{MolmH2o}} * \frac{\text{baroPresHut}}{101.325} * 10^{-3} \tag{6.4}$$

where MolmDry is molecular mass of dry air and equal to 28.97 (kg $kmol^{-1}$)

MolmH2o is molecular mass of water vapor and equal to 18.02 (kg $kmol^{-1}$)

baroPresHut is atmospheric pressure (kPa).

6.3.3 Sensor Flags

a. **Temperature flag** (qfTemp) – will be generated to indicate when data measured by IRGA sensor are delivered outside of the acceptable temperature ranges (at 10 degree Kelvin) The temperature flag at time t will be determined as follows:

$$1 \text{ if } N \geq 3420 \text{ and } |\text{maxTemp} - \text{minTemp}|_t > 10 \text{ K}$$

$$\mathrm{qfTemp}_t = \begin{cases} 0 \text{ if } N \geq 3420 \text{ and } |\mathrm{maxTemp} - \mathrm{minTemp}|_t \leq 10\ \mathrm{K} \\ -1\ otherwise. \end{cases} \quad (6.5)$$

where $\mathrm{maxTemp}$ is the maximum hut temperature in between $t - n\ and\ t$ (K)
$\mathrm{minTemp}$ is the minimum hut temperature in between $t - n\ and\ t$ (K)
n is seconds in hour and equal to 3600 (s)
N is the number of samples of $\mathrm{tempHut}$ in between $t - n\ and\ t$ that are used to determine $\mathrm{maxTemp}$ and $\mathrm{minTemp}$

b. **Humidity flag** (qfRh) – will be generated to indicate when data measured by CRD H2O sensor are delivered outside of the acceptable humidity ranges (greater than 0.03 mol mol^{-1}). The humidity flag will be determined as follows:

$$\mathrm{qfRh} = \begin{cases} 1 \text{ if } \mathrm{rtioMoleWetH2o} > 0.03 \\ 0 \text{ if } \mathrm{rtioMoleWetH2o} \leq 0.03 \\ -1\ otherwise. \end{cases} \quad (6.6)$$

where $\mathrm{rtioMoleWetH2o}$ is the wet mole fraction of water vapor (mol mol^{-1})

6.3.4 QA/QC Procedure

Standard plausibility tests should be applied to all L0p DPs, except for qfTemp and qfRh. An associated pass/fail flag will be generated for each test according to AD[02]. Note that we will not be carrying out the "gap test" or "null test". Quality reports will be generated for temporally averaged L1 DPs at a later stage. Because this sensor will never be sent back to CVAL for calibration once it is deployed at field, no valid calibration date will be provided to CI to generate calibration flag.

Plausibility quality flags to be applied to all L0p DPs, except for qfTemp and qfRh.

Flag	Term modifier	Description
QF_{Pers}	qfPers	Quality flag for the Persistence test
QF_{Rng}	qfRng	Quality flag for the Range test
QF_{Step}	qfStep	Quality flag for the Step test

As all flags will be applied to each individual L0p DPs they will follow a uniform naming convention, whereby the L0p DP term is augmented with the plausibility test flag term modifier. For example, the quality flag for the step test for $\delta^{13}C$ will be "qfStepDlta13CCo2".

Test following parameters will be provided by FIU for each L0p DP and maintained in the CI data store.

Parameters required for plausibility tests.

Parameter	Description
Thsh_{Pers}	Threshold for the Persistence test
Time_{Pers}	Time parameter for the Persistence test
$\mathrm{Thsh}_{Rng,min}$	Minimum threshold for the Range test
$\mathrm{Thsh}_{Rng,max}$	Maximum threshold for the Range test
Thsh_{Step}	Threshold for the Step test

6.4 Uncertainty

NA

7 GAS CYLINDER PRESSURE SENSOR

7.1 Data Product Description

This Chapter describes the processes to convert L0 DPs under delivery pressure sensor (DGD CA07140000) and cylinder pressure sensor (DGD CA07150000) into 1 Hz L0p DPs. The delivery pressure sensor is referred to as presValiRegOutStor in reference to DPs. The cylinder pressure sensor is referred to as presValiRegInStor in reference to DPs.

7.1.1 Variables Reported

The delivery pressure sensor (Omega PX319-100GI) and cylinder pressure sensor (Omega PX319-3KGI) related L0p reported variables provided by the algorithms documented in this ATBD are displayed in Table 7-1. Please note, although some L0p fieldnames for Delivery pressure sensor (DGD CA07140000) are identical to Cylinder pressure sensor (DGD CA07150000), they live in different data tables, thus this is not a problem of conflict. Because the L0p pressure output from each sensor will live in different tables of HDF5 file, it is ok to use generic term of "presDiff" for all delivery pressure and all cylinder pressure L0p outputs.

Table 7-1: List of presValiRegOutStor and presValiRegInStor related L0p reported variables that produced in this ATBD.

L0p DP	L0p fieldName	L0p DP Frequency	Units	Input L0 data products
presValiRegOutStor (DGD CA07140000)				
delivery pressure (ZERO)	presDiff	1 Hz	Pa	NEON.DOM.SITE.DP0.00110.001.02196.709.000.000
delivery pressure (ARCHIVE)	presDiff	1 Hz	Pa	NEON.DOM.SITE.DP0.00110.001.02196.710.000.000

L0p DP	L0p fieldName	L0p DP Frequency	Units	Input L0 data products
delivery pressure (ZERO for CRD H_2O)	presDiff	1 Hz	Pa	NEON.DOM.SITE.DP0.00110.001.02196.711.000.000
delivery pressure (LOW)	presDiff	1 Hz	Pa	NEON.DOM.SITE.DP0.00110.001.02196.712.000.000
delivery pressure (MEDIUM)	presDiff	1 Hz	Pa	NEON.DOM.SITE.DP0.00110.001.02196.713.000.000
delivery pressure (HIGH)	presDiff	1 Hz	Pa	NEON.DOM.SITE.DP0.00110.001.02196.714.000.000
delivery pressure flag (ZERO to CRD H_2O)	qfPresDiff	1 Hz	NA	presDiff from ZERO for CRD H_2O *
presValiRegInStor (DGD CA07150000)				
cylinder pressure (ZERO)	presDiff	1 Hz	Pa	NEON.DOM.SITE.DP0.00111.001.02196.709.000.000
cylinder pressure (ARCHIVE)	presDiff	1 Hz	Pa	NEON.DOM.SITE.DP0.00111.001.02196.710.000.000
cylinder pressure (ZERO to CRD H_2O)	presDiff	1 Hz	Pa	NEON.DOM.SITE.DP0.00111.001.02196.711.000.000
cylinder pressure (LOW)	presDiff	1 Hz	Pa	NEON.DOM.SITE.DP0.00111.001.02196.712.000.000
cylinder pressure (MEDIUM)	presDiff	1 Hz	Pa	NEON.DOM.SITE.DP0.00111.001.02196.713.000.000
cylinder pressure (HIGH)	presDiff	1 Hz	Pa	NEON.DOM.SITE.DP0.00111.001.02196.714.000.000
cylinder pressure flag (ZERO)	qfPresDiff	1 Hz	NA	presDiff from ZERO*
cylinder pressure flag (ARCHIVE)	qfPresDiff	1 Hz	NA	presDiff from ARCHIVE*
cylinder pressure flag (ZERO to CRD H_2O)	qfPresDiff	1 Hz	NA	presDiff from ZERO to CRD H_2O)*
cylinder pressure flag (LOW)	qfPresDiff	1 Hz	NA	presDiff from LOW*
cylinder pressure flag (MEDIUM)	qfPresDiff	1 Hz	NA	presDiff from MEDIUM*
cylinder pressure flag (HIGH)	qfPresDiff	1 Hz	NA	presDiff from HIGH*

*: This is a L0p DP. It is used as an input to generate other L0p DP.

7.1.2 Input Dependencies

Table 7-2 below lists all presValiRegOutStor and presValiRegInStor related L0 DPs and specifies which L0 DPs will be used to produce L0p reported variables in this ATBD.

Table 7-2: A full list of presValiRegOutStor and presValiRegInStor related L0 DPs.

L0 DP	L0 DP fieldName	Sample Frequency	Units	Data Product Number	DPs that are used to produce L0p (Y/N)*
presValiRegOutStor (DGD CA07140000)					
delivery pressure (ZERO)	presGage	1 Hz	kPa	NEON.DOM.SITE.DP0.00110.001.02196.709.000.000	Y
delivery pressure (ARCHIVE)	presGage	1 Hz	kPa	NEON.DOM.SITE.DP0.00110.001.02196.710.000.000	Y
delivery pressure (ZERO CRD H_2O)	presGage	1 Hz	kPa	NEON.DOM.SITE.DP0.00110.001.02196.711.000.000	Y
delivery pressure (LOW)	presGage	1 Hz	kPa	NEON.DOM.SITE.DP0.00110.001.02196.712.000.000	Y
delivery pressure (MEDIUM)	presGage	1 Hz	kPa	NEON.DOM.SITE.DP0.00110.001.02196.713.000.000	Y
delivery pressure (HIGH)	presGage	1 Hz	kPa	NEON.DOM.SITE.DP0.00110.001.02196.714.000.000	Y
presValiRegOutStor (DGD CA07150000)					
cylinder pressure (ZERO)	presGage	1 Hz	kPa	NEON.DOM.SITE.DP0.00111.001.02196.709.000.000	Y
cylinder pressure (ARCHIVE)	presGage	1 Hz	kPa	NEON.DOM.SITE.DP0.00111.001.02196.710.000.000	Y
cylinder pressure (ZERO CRD H_2O)	presGage	1 Hz	kPa	NEON.DOM.SITE.DP0.00111.001.02196.711.000.000	Y
cylinder pressure (LOW)	presGage	1 Hz	kPa	NEON.DOM.SITE.DP0.00111.001.02196.712.000.000	Y
cylinder pressure (MEDIUM)	presGage	1 Hz	kPa	NEON.DOM.SITE.DP0.00111.001.02196.713.000.000	Y
cylinder pressure (HIGH)	presGage	1 Hz	kPa	NEON.DOM.SITE.DP0.00111.001.02196.714.000.000	Y

*: Only the L0 DPs in "Y" are selected to transform into L0p DPs reported in this ATBD.

7.1.3 Product Instances

All TIS sites across the NEON observatory own 6 delivery pressure sensor (Omega PX319-100GI) and 6 cylinder pressure sensors (Omega PX319-3KGI) for Eddy Covariance Storage Exchange assembly. Each individual instance will generate one L0p data output listed in Table 7-1.

7.1.4 Temporal Resolution and Extent

The temporal extent of the reported variables in Table 7-1 is 1 Hz.

7.1.5 Spatial Resolution and Extent

The 6 delivery pressure sensor (Omega PX319-100GI) and 6 cylinder pressure sensors (Omega PX319-3KGI) will be located within the tower hut infrastructure. Each pair of the pressure sensors (1 Omega PX319-100GI and 1 Omega PX319-3KGI) is connected to a gas cylinder in the hut to monitor the gas cylinder pressure and the gas delivery pressure.

7.2 Scientific context

Multiple gas cylinders contain known CO_2 concentration will be used as reference gases to periodically validate the IRGA performance and CRD CO_2 performance. If the pressure of the gas inside the cylinders is too low (<400 PSIG), it is a potential that the gas deviates from the known concentration. The pressure sensors (Omega PX319-3KGI, DGD CA07150000) are used to monitor this cylinder pressure. If the delivery pressure from the gas tank is too high, the sensors and/or infrastructure components downstream of the gas path could be damaged. The pressure sensors (Omega PX319-100GI, DGD CA07140000) are used to monitor this delivery pressure.

7.2.1 Theory of Measurement

OMEGA's PX309 Series (including PX309, PX319, PX329, and PX359) high performance general purpose pressure transducers use two state-of-the-art silicon technologies. Pressure ranges below 100 psi use a high-accuracy silicon sensor protected by a fluid filled stainless steel diaphragm. Ranges 100 psi and above use high-accuracy silicon strain gages molecularly bonded to the stainless steel diaphragm. Both systems provide a rugged sensor with high accuracy and excellent long term stability (Source: http://www.omega.com/pptst/PX309.html).

7.2.2 Theory of Algorithm

NA

7.3 Algorithm Implementation

Data flow for signal processing of L0p DPs will be treated in the following order.

1. Select all 6 L0 pressGage data streams from delivery pressure sensor and all data streams from cylinder pressure sensor for further data processing. SeeTable 7-2.
2. Generate a complete data with respect to 1 Hz frequency using a time regularization approach in accordance with AD[04], details are provided in section 7.3.1.

3. Apply unit conversion to cylinder pressure and delivery pressure from kPa to Pa. See Eq. (7.1) and (7.2) below.
4. Determine and assign the gas delivery pressure flag and gas cylinder pressure flag to correspond 1 Hz data using Eq. (7.3) and (7.4) below.
5. QA/QC Plausibility tests will be applied to the data stream in accordance with AD[02], details are provided below. See section 7.3.4.

7.3.1 Time regularization

The gas cylinder pressure and the gas delivery pressure sensors measure data at 1 Hz. To generate a complete L0p dataset with respect to 1 Hz frequency, missing timestamps and the corresponding data values will be filled with NaN (not NA) following the procedures detailed in AD[04]. In this case we will use the default options in AD[04], and when multiple data values fall within a single window we will use the closest value determined by minimum absolute deviation, option 1 in AD[04].

7.3.2 Unit conversion

Convert L0 DPs of cylinder pressure (NEON.DOM.SITE.DP0.00111.001.02196.HOR.VER.000) and delivery pressure (NEON.DOM.SITE.DP0.00110.001.02196.HOR.VER.000) from kPa to Pa. The fieldName for both cylinder pressure and delivery pressure L0 DPs is presGage.

Cylinder pressure:

$$\mathrm{presDiff\ in\ Pa} = \mathrm{presGage\ in\ kPa} * 1000 \tag{7.1}$$

Delivery pressure:

$$\mathrm{presDiff\ in\ Pa} = \mathrm{presGage\ in\ kPa} * 1000 \tag{7.2}$$

7.3.3 Sensor Flags

a. **Delivery pressure flag for zero air gas cylinder delivery pressure used for CRD H_2O** (qfPresDiff from ZERO for CRD H_2O) will be generated as part of the L0p report variables to indicate if the delivery pressure of zero air is out of range 2.5±0.5 psig (17237±3447 Pa) during CRD H_2O field validation/annual calibration. It is only applied to this L0 data stream NEON.DOM.SITE.DP0.00110.001.02196.711.000.000. After time regularization, the L0p data will be presDiff (from ZERO for CRD H_2O), Therefore, qfPresDiff is defined as:

$$\mathrm{qfPresDiff} = \begin{cases} 1 \text{ if presDiff} > 20684 \text{ Pa or presDiff} < 13790 \text{ Pa} \\ 0 \text{ if } 13790 \text{ Pa} < \text{presDiff} < 20684 \text{ Pa} \end{cases} \tag{7.3}$$

$-1\ otherwise.$

b. **Cylinder pressure flag** (qfPresDiff) will be generated as part of the L0p report variables to indicate if the gas cylinder press is lower than 400 psig (2757903 Pa). This will apply to all data streams from DGD CA07150000. It is defined as:

$$\text{qfPresDiff} = \begin{cases} 1 \text{ if presDiff} < 2757903 \text{ Pa} \\ 0 \text{ if presDiff } \geq 2757903 \text{ Pa} \\ \text{-1 otherwise} \end{cases} \tag{7.4}$$

7.3.4 QA/QC Procedure:

Standard plausibility tests should be applied to all L0p DPs except for flags. An associated pass/fail flag will be generated for each test according to AD[02]. (Note. We will not be carrying out the "gap test" and "null test"). Quality reports will be generated for temporally averaged L1 DPs at a later stage. Because this sensor will never be sent back to CVAL for calibration once it is deployed at field, thus no valid calibration date will be provided to CI to generate calibration flag.

Table 7-3: Plausibility quality flags to be applied to all L0p DPs except for flags

Flag	Term modifier	Description
QF_{Pers}	qfPers	Quality flag for the Persistence test
QF_{Rng}	qfRng	Quality flag for the Range test
QF_{Step}	qfStep	Quality flag for the Step test

As all flags will be applied to each individual L0p DPs they will follow a uniform naming convention, whereby the L0p DP term is augmented with the plausibility test flag term modifier. For example, the quality flag for the step test for the cylinder pressure from a pressure gauge on a low CO2 concentration cylinder will be "qfStepPresDiff".

Test following parameters will be provided by FIU for each L0p DP and maintained in the CI data store.

Table 7-4: Parameters required for plausibility tests.

Parameter	Description
Thsh_{Pers}	Threshold for the Persistence test
Time_{Pers}	Time parameter for the Persistence test
$\text{Thsh}_{Rng,min}$	Minimum threshold for the Range test
$\text{Thsh}_{Rng,max}$	Maximum threshold for the Range test
Thsh_{Step}	Threshold for the Step test

7.4 Uncertainty

NA

8 ABSOLUTE PRESSURE TRANSDUCER

8.1 Data Product Description

This Chapter describes the processes to convert L0 DPs under absolute pressure transducer (DGD CA08830000) at ECSE inlets into 1 Hz L0p DPs. The absolute pressure transducer at inlet is referred to as presInlt in reference to DPs.

8.1.1 Variables Reported

The Omega PX319-030AI absolute pressure transducer is used to monitor the inlet pressure at each tower measurement level. The presInlt-related L0p reported variables provided by the algorithms documented in this ATBD are displayed in Table 8-1. Because the L0p pressure output from each sensor will live in different tables of HDF5 file, it is ok to use generic term of "presDiff" for all inlet pressure L0p outputs.

Table 8-1: List of The presInlt-related L0p reported variables that produced in this ATBD.

L0p DP	L0p fieldName	L0p DP Frequency	Units	Input L0 data products
Inlet pressure (ML1)	presDiff	1 Hz	Pa	NEON.DOM.SITE.DP0.00109.001.02196.000.010.000
Inlet pressure (ML2)	presDiff	1 Hz	Pa	NEON.DOM.SITE.DP0.00109.001.02196.000.020.000
Inlet pressure (ML3)	presDiff	1 Hz	Pa	NEON.DOM.SITE.DP0.00109.001.02196.000.030.000
Inlet pressure (ML4)	presDiff	1 Hz	Pa	NEON.DOM.SITE.DP0.00109.001.02196.000.040.000
Inlet pressure (ML5)	presDiff	1 Hz	Pa	NEON.DOM.SITE.DP0.00109.001.02196.000.050.000
Inlet pressure (ML6)	presDiff	1 Hz	Pa	NEON.DOM.SITE.DP0.00109.001.02196.000.060.000
Inlet pressure (ML7)	presDiff	1 Hz	Pa	NEON.DOM.SITE.DP0.00109.001.02196.000.070.000
Inlet pressure (ML8)	presDiff	1 Hz	Pa	NEON.DOM.SITE.DP0.00109.001.02196.000.080.000
Inlet pressure flag (ML1)	qfPresDiff	1 Hz	NA	presDiff from ML1*
Inlet pressure flag (ML2)	qfPresDiff	1 Hz	NA	presDiff from ML2*

L0p DP	L0p fieldName	L0p DP Frequency	Units	Input L0 data products
Inlet pressure flag (ML3)	qfPresDiff	1 Hz	NA	presDiff from ML3*
Inlet pressure flag (ML4)	qfPresDiff	1 Hz	NA	presDiff from ML4*
Inlet pressure flag (ML5)	qfPresDiff	1 Hz	NA	presDiff from ML5*
Inlet pressure flag (ML6)	qfPresDiff	1 Hz	NA	presDiff from ML6*
Inlet pressure flag (ML7)	qfPresDiff	1 Hz	NA	presDiff from ML7*
Inlet pressure flag (ML8)	qfPresDiff	1 Hz	NA	presDiff from ML8*

*: These are L0p DPs. They are used as inputs to generate other L0p DPs.

8.1.2 Input Dependencies

Table 8-2 below list all the presInlt-related L0 DPs and specifies which L0 DPs will be used to produce L0p reported variables in this ATBD.

Table 8-2: A full list of presInlt-related L0 DPs.

L0 DP	L0 DP fieldName	Sample Frequency	Units	Data Product Number	DPs that are used to produce L0p (Y/N)*
Inlet pressure (ML1)	presGage	1 Hz	kPa	NEON.DOM.SITE.DP0.00109.001.02196.000.010.000	Y
Inlet pressure (ML2)	presGage	1 Hz	kPa	NEON.DOM.SITE.DP0.00109.001.02196.000.020.000	Y
Inlet pressure (ML3)	presGage	1 Hz	kPa	NEON.DOM.SITE.DP0.00109.001.02196.000.030.000	Y
Inlet pressure (ML4)	presGage	1 Hz	kPa	NEON.DOM.SITE.DP0.00109.001.02196.000.040.000	Y
Inlet pressure (ML5)	presGage	1 Hz	kPa	NEON.DOM.SITE.DP0.00109.001.02196.000.050.000	Y
Inlet pressure (ML6)	presGage	1 Hz	kPa	NEON.DOM.SITE.DP0.00109.001.02196.000.060.000	Y
Inlet pressure (ML7)	presGage	1 Hz	kPa	NEON.DOM.SITE.DP0.00109.001.02196.000.070.000	Y
Inlet pressure (ML8)	presGage	1 Hz	kPa	NEON.DOM.SITE.DP0.00109.001.02196.000.080.000	Y

*: Only the L0 DPs in “Y” are selected to transform into L0p DPs reported in this ATBD.

8.1.3 Product Instances

All TIS sites across the NEON observatory own up to 8 Omega PX319-030AI inlet pressure sensors (depending on the number of measurement levels at a specific site) for Eddy Covariance Storage Exchange (ECSE) assembly. Each individual instance will generate one L0 data product in Table 8-2, which represents the inlet pressure at each measurement level (ML). Measurement level varies from 1 to 8 at each site. Each individual instance will generate one L0p data output listed in Table 8-1.

8.1.4 Temporal Resolution and Extent

The temporal extent of the reported variables in Table 8-1 is 1 Hz.

8.1.5 Spatial Resolution and Extent

The Omega PX319-030AI inlet pressure sensor will be located behind a critical orifice of the ECSE sample inlet at each measurement level on tower structure to monitor the pressure in the sample line.

8.2 Scientific context

The air samples from each measurement level are pulled through the sample line continuously by a pump dedicated to that line. The flow rate of the air should be high enough to maintain the pressure in the sample line at 40%-50% of the ambient pressure to prevent condensation in the sample line. Absolute pressure transducer (DGD CA08830000) on each sample line is used to monitor the air pressure inside that sample line.

8.2.1 Theory of Measurement

OMEGA's PX309 Series (including PX309, PX319, PX329, and PX359) high performance general purpose pressure transducers use two state-of-the-art silicon technologies. Pressure ranges below 100 psi use a high-accuracy silicon sensor protected by a fluid filled stainless steel diaphragm. Ranges 100 psi and above use high-accuracy silicon strain gages molecularly bonded to the stainless steel diaphragm. Both systems provide a rugged sensor with high accuracy and excellent long term stability (Source: http://www.omega.com/pptst/PX309.html).

8.2.2 Theory of Algorithm

NA

8.3 Algorithm Implementation

Data flow for signal processing of L0p DPs will be treated in the following order.

1. Select all L0 pressGage data streams from inlet pressure sensors (Table 8-2) for further data processing.
2. Generate a complete data with respect to 1 Hz frequency using a time regularization approach in accordance with AD[04], details are provided in section 8.3.1.
3. Apply unit conversion to inlet pressure from kPa to Pa. See Eq. (8.1) below.
4. Determine and assign the inlet pressure flag to correspond 1 Hz data using Eq. (8.2).
5. QA/QC Plausibility tests will be applied to the data stream in accordance with AD[02], details are provided below in 8.3.4.

8.3.1 Time regularization

The inlet pressure sensor measures data at ~ 1 Hz. To generate a complete L0p dataset with respect to 1 Hz frequency, missing timestamps and the corresponding data values will be filled with NaN (not NA) following the procedures detailed in AD[04]. In this case we will use the default options in AD[04], and when multiple data values fall within a single window we will use the closest value determined by minimum absolute deviation, option 1 in AD[04].

8.3.2 Unit conversion

Convert all inlet pressure (NEON.DOM.SITE.DP0.00109.001.02196.000.VER.000) data streams from kilopascal to pascal. The fieldName for inlet pressure is presGage

$$\text{presDiff in Pa} = \text{presGage in kpa} * 1000 \tag{8.1}$$

8.3.3 Sensor Flags

a. **Inlet pressure flag** (qfPresDiff) will be generated as part of the L0p report variables for inlet pressure data streams at all measurement levels to indicate if the inlet pressure is >45% +/- 5% of ambient pressure. Ambient pressure for each site will be provided by FIU and maintained in the CI data store.

$$\text{qfPresDiff} = \begin{cases} 1 & \text{if presDiff} > 50\% \times \text{ambient pressure or presDiff} < 40\% \times \text{ambient pressure} \\ 0 & \text{if } 40\% \times \text{ambient pressure} \le \text{presDiff} \le 50\% \times \text{ambient pressure} \end{cases} \tag{8.2}$$

Table 8-3: Ambient pressure at each NEON sites used for ATBD data processing.

Domain	Site	Site code	Site Type	Latitude	Longitude	Elevation (m)	Barometric pressure (Pa)
1	Harvard Forest	HARV	core	42.54	-72.17	348	97210
1	Bartlett Experimental Forest	BART	relocatable	44.06	-71.29	273	98080
2	Blandy	BLAN	relocatable	39.06	-78.07	182	99160
2	Smithsonian CRC (SCBI)	SCBI	core	38.89	-78.14	355	97130
2	Smithsonian ERC	SERC	relocatable	38.89	-76.56	10	101210
3	Ordway	OSBS	core	29.69	-81.99	48	100750
3	Jones	JERC	relocatable	31.19	-84.47	47	100770
3	Disney	DSNY	relocatable	28.13	-81.44	20	101090
4	Guanica	GUAN	core	17.97	-66.87	126	99820

4	Lajas	LAJA	relocatable	18.02	-67.08	16	101130
5	Steigerwaldt	STEI	relocatable	45.51	-89.58	477	95720
5	Tree Haven	TREE	relocatable	45.49	-89.59	461	95910
5	UNDERC	UNDE	core	46.23	-89.54	520	95230
6	Konza - Core	KONZ	core	39.10	-96.56	415	96440
6	Konza - Relocatable	KONA	relocatable	39.11	-96.61	323	97500
6	U Kansas Bio Station	UKFS	relocatable	39.04	-95.19	321	97530
7	Oak Ridge	ORNL	core	35.96	-84.28	342	97290
7	Great Smokey Mtns	GRSM	relocatable	35.69	-83.50	661	93630
7	Mountain Lake	MLBS	relocatable	37.38	-80.52	1170	88030
8	Talladega	TALL	core	32.95	-87.39	164	99370
8	Dead Lake	DELA	relocatable	32.54	-87.80	32	100940
8	Lenoir Landing	LENO	relocatable	31.85	-88.16	12	101180
9	Dakota-Coteau	DCFS	relocatable	47.16	-99.11	575	94600
9	Northern Great Plains	NOGP	relocatable	46.77	-100.92	589	94440
9	Woodworth	WOOD	core	47.13	-99.24	590	94430
10	CPER	CPER	core	40.82	-104.75	1653	82970
10	Sterling	STER	relocatable	40.46	-103.03	1365	85960
10	RMNP Castnet	RMNP	relocatable	40.28	-105.55	2742	72430
11	LBJ/Caddo	CLBJ	core	33.40	-97.57	272	98100
11	Klemme	OAES	relocatable	35.41	-99.06	520	95230
12	Yellowstone	YELL	core	44.95	-110.54	2129	78220
13	Niwot	NIWO	core	40.05	-105.58	3478	65930
13	Moab	MOAB	relocatable	38.25	-109.39	1800	81480
14	Santa Rita	SRER	core	31.91	-110.84	999	89880
14	Jornada	JORN	relocatable	32.59	-106.84	1321	86420
15	Onaqui	ONAQ	core	40.18	-112.45	1654	82960
16	Wind River	WREF	core	45.82	-121.95	368	96980
16	Abby Road	ABBY	relocatable	45.76	-122.33	367	96990
17	Soaproot	SOAP	relocatable	37.03	-119.26	1210	87600
17	Teakettle	TEAK	relocatable	37.01	-119.01	2149	78030
17	San Joaquin	SJER	core	37.11	-119.73	397	96650
18	Toolik	TOOL	relocatable	68.66	-149.37	827	91770
18	Barrow	BARR	relocatable	71.28	-156.62	7	101240
19	Caribou-Poker	BONA	core	65.15	-147.50	239	98480
19	Delta Junction	DEJU	relocatable	63.88	-145.75	504	95410
19	Healy	HEAL	relocatable	63.88	-149.21	171	99290
20	Puumakaala	PUUM	core	19.55	-155.32	1684	91480

8.3.4 QA/QC Procedure

Standard plausibility tests should be applied to all L0p DPs except for flags. An associated pass/fail flag will be generated for each test according to AD[02]. (Note. We will not be carrying out the "gap test" and "null test"). Quality reports will be generated for temporally averaged L1 DPs at a later stage. Because this sensor will never be sent back to CVAL for calibration once it is deployed at field, thus no valid calibration date will be provided to CI to generate calibration flag.

Table 8-4: Plausibility quality flags to be applied to all L0p DPs except for flags

Flag	Term modifier	Description
QF_{Pers}	qfPers	Quality flag for the Persistence test
QF_{Rng}	qfRng	Quality flag for the Range test
QF_{Step}	qfStep	Quality flag for the Step test

As all flags will be applied to each individual L0p DPs they will follow a uniform naming convention, whereby the L0p DP term is augmented with the plausibility test flag term modifier. For example, the quality flag for the step test for inlet pressure at ML1 will be "qfStepPresDiff".

Test following parameters will be provided by FIU for each L0p DP and maintained in the CI data store.

Table 8-5: Parameters required for plausibility tests.

Parameter	Description
Thsh_{Pers}	Threshold for the Persistence test
Time_{Pers}	Time parameter for the Persistence test
$\mathrm{Thsh}_{Rng,min}$	Minimum threshold for the Range test
$\mathrm{Thsh}_{Rng,max}$	Maximum threshold for the Range test
Thsh_{Step}	Threshold for the Step test

8.4 Uncertainty

NA

9 MASS FLOW METER IN SAMPLE LINES

9.1 Data Product Description

This Chapter describes the processes to convert L0 DPs under mass flow meter (DGD 0341530000) into 1 Hz L0p DPs. The mass flow meter is referred to as mfm in reference to DPs.

9.1.1 Variables Reported

The mfm-related L0p reported variables provided by the algorithms documented in this ATBD are displayed in the accompanying file Table 9-1. Because the L0p outputs from each sensor will live in different tables of HDF5 file, it is ok to use generic term of "frt00", "frt", "presAtm", "temp" for mass flow meter L0p outputs.

Table 9-1: List of mfm-related L0p reported variables that produced in this ATBD.

L0p DP	L0p fieldName	Sample Frequency	Units	Input L0 DPs or L0p DP fieldNames
Mass flow rate (ML1)	frt00	1	$m^3\ s^{-1}$	NEON.DOM.SITE.DP0.00108.001.01951.700.010.000
Volumetric flow rate (ML1)	frt	1	$m^3\ s^{-1}$	NEON.DOM.SITE.DP0.00108.001.01950.700.010.000
Pressure (ML1)	presAtm	1	Pa	NEON.DOM.SITE.DP0.00108.001.01948.700.010.000
Gas temperature (ML1)	temp	1	K	NEON.DOM.SITE.DP0.00108.001.01949.700.010.000
Mass flow rate (ML2)	frt00	1	$m^3\ s^{-1}$	NEON.DOM.SITE.DP0.00108.001.01951.700.020.000
Volumetric flow rate (ML2)	frt	1	$m^3\ s^{-1}$	NEON.DOM.SITE.DP0.00108.001.01950.700.020.000
Pressure (ML2)	presAtm	1	Pa	NEON.DOM.SITE.DP0.00108.001.01948.700.020.000
Gas temperature (ML2)	temp	1	K	NEON.DOM.SITE.DP0.00108.001.01949.700.020.000
Mass flow rate (ML3)	frt00	1	$m^3\ s^{-1}$	NEON.DOM.SITE.DP0.00108.001.01951.700.030.000
Volumetric flow rate (ML3)	frt	1	$m^3\ s^{-1}$	NEON.DOM.SITE.DP0.00108.001.01950.700.030.000
Pres (ML3)ure	presAtm	1	Pa	NEON.DOM.SITE.DP0.00108.001.01948.700.030.000
Gas temperature (ML3)	temp	1	K	NEON.DOM.SITE.DP0.00108.001.01949.700.030.000

Mass flow rate (ML4)	frt00	1	$m^3\ s^{-1}$	NEON.DOM.SITE.DP0.00108.001.01951.700.040.000
Volumetric flow rate (ML4)	frt	1	$m^3\ s^{-1}$	NEON.DOM.SITE.DP0.00108.001.01950.700.040.000
Pressure (ML4)	presAtm	1	Pa	NEON.DOM.SITE.DP0.00108.001.01948.700.040.000
Gas temperature (ML4)	temp	1	K	NEON.DOM.SITE.DP0.00108.001.01949.700.040.000
Mass flow rate (ML5)	frt00	1	$m^3\ s^{-1}$	NEON.DOM.SITE.DP0.00108.001.01951.700.050.000
Volumetric flow rate (ML5)	frt	1	$m^3\ s^{-1}$	NEON.DOM.SITE.DP0.00108.001.01950.700.050.000
Pressure (ML5)	presAtm	1	Pa	NEON.DOM.SITE.DP0.00108.001.01948.700.050.000
Gas temperature (ML5)	temp	1	K	NEON.DOM.SITE.DP0.00108.001.01949.700.050.000
Mass flow rate (ML6)	frt00	1	$m^3\ s^{-1}$	NEON.DOM.SITE.DP0.00108.001.01951.700.060.000
Volumetric flow ra (ML6)te	frt	1	$m^3\ s^{-1}$	NEON.DOM.SITE.DP0.00108.001.01950.700.060.000
Pressure (ML6)	presAtm	1	Pa	NEON.DOM.SITE.DP0.00108.001.01948.700.060.000
Gas temperature (ML6)	temp	1	K	NEON.DOM.SITE.DP0.00108.001.01949.700.060.000
Mass flow rate (ML7)	frt00	1	$m^3\ s^{-1}$	NEON.DOM.SITE.DP0.00108.001.01951.700.070.000
Volumetric flow rate (ML7)	frt	1	$m^3\ s^{-1}$	NEON.DOM.SITE.DP0.00108.001.01950.700.070.000
Pressure (ML7)	presAtm	1	Pa	NEON.DOM.SITE.DP0.00108.001.01948.700.070.000
Gas temperature (ML7)	temp	1	K	NEON.DOM.SITE.DP0.00108.001.01949.700.070.000
Mass flow rate (ML8)	frt00	1	$m^3\ s^{-1}$	NEON.DOM.SITE.DP0.00108.001.01951.700.080.000
Volumetric flow rate (ML8)	frt	1	$m^3\ s^{-1}$	NEON.DOM.SITE.DP0.00108.001.01950.700.080.000
Pressure (ML8)	presAtm	1	Pa	NEON.DOM.SITE.DP0.00108.001.01948.700.080.000

Gas temperature (ML8)	temp	1	K	NEON.DOM.SITE.DP0.00108.001.01949.700.080.000

9.1.2 Input Dependencies

Table 9-2 details the mfm-related L0 DPs used to produce L0p reported variables in this ATBD.

Table 9-2: A full list of mfm-related L0 DPs.

L0 DP	L0 DP fieldName	Sample Frequency	Units	L0 Data Product Number	DPs that are used to produce L0p (Y/N)
			ML1		
Mass flow rate	frt0	1	LPM	NEON.DOM.SITE.DP0.00108.001.01951.700.010.000	Y
Volumetric flow rate	frt	1	LPM	NEON.DOM.SITE.DP0.00108.001.01950.700.010.000	Y
Pressure	presAtm	1	kPa	NEON.DOM.SITE.DP0.00108.001.01948.700.010.000	Y
Gas temperature	temp	1	°C	NEON.DOM.SITE.DP0.00108.001.01949.700.010.000	Y
			ML2		
Mass flow rate	frt0	1	LPM	NEON.DOM.SITE.DP0.00108.001.01951.700.020.000	Y
Volumetric flow rate	frt	1	LPM	NEON.DOM.SITE.DP0.00108.001.01950.700.020.000	Y
Pressure	presAtm	1	kPa	NEON.DOM.SITE.DP0.00108.001.01948.700.020.000	Y
Gas temperature	temp	1	°C	NEON.DOM.SITE.DP0.00108.001.01949.700.020.000	Y
			ML3		
Mass flow rate	frt0	1	LPM	NEON.DOM.SITE.DP0.00108.001.01951.700.030.000	Y
Volumetric flow rate	frt	1	LPM	NEON.DOM.SITE.DP0.00108.001.01950.700.030.000	Y
Pressure	presAtm	1	kPa	NEON.DOM.SITE.DP0.00108.001.01948.700.030.000	Y

L0 DP	L0 DP fieldName	Sample Frequency	Units	L0 Data Product Number	DPs that are used to produce L0p (Y/N)
Gas temperature	temp	1	°C	NEON.DOM.SITE.DP0.00108.001.01949.700.030.000	Y
	ML4				
Mass flow rate	frt0	1	LPM	NEON.DOM.SITE.DP0.00108.001.01951.700.040.000	Y
Volumetric flow rate	frt	1	LPM	NEON.DOM.SITE.DP0.00108.001.01950.700.040.000	Y
Pressure	presAtm	1	kPa	NEON.DOM.SITE.DP0.00108.001.01948.700.040.000	Y
Gas temperature	temp	1	°C	NEON.DOM.SITE.DP0.00108.001.01949.700.040.000	Y
	ML5				
Mass flow rate	frt0	1	LPM	NEON.DOM.SITE.DP0.00108.001.01951.700.050.000	Y
Volumetric flow rate	frt	1	LPM	NEON.DOM.SITE.DP0.00108.001.01950.700.050.000	Y
Pressure	presAtm	1	kPa	NEON.DOM.SITE.DP0.00108.001.01948.700.050.000	Y
Gas temperature	temp	1	°C	NEON.DOM.SITE.DP0.00108.001.01949.700.050.000	Y
	ML6				
Mass flow rate	frt0	1	LPM	NEON.DOM.SITE.DP0.00108.001.01951.700.060.000	Y
Volumetric flow rate	frt	1	LPM	NEON.DOM.SITE.DP0.00108.001.01950.700.060.000	Y
Pressure	presAtm	1	kPa	NEON.DOM.SITE.DP0.00108.001.01948.700.060.000	Y
Gas temperature	temp	1	°C	NEON.DOM.SITE.DP0.00108.001.01949.700.060.000	Y
	ML7				
Mass flow rate	frt0	1	LPM	NEON.DOM.SITE.DP0.00108.001.01951.700.070.000	Y

L0 DP	L0 DP fieldName	Sample Frequency	Units	L0 Data Product Number	DPs that are used to produce L0p (Y/N)
Volumetric flow rate	frt	1	LPM	NEON.DOM.SITE.DP0.00108.001.01950.700.070.000	Y
Pressure	presAtm	1	kPa	NEON.DOM.SITE.DP0.00108.001.01948.700.070.000	Y
Gas temperature	temp	1	°C	NEON.DOM.SITE.DP0.00108.001.01949.700.070.000	Y
	ML8				
Mass flow rate	frt0	1	LPM	NEON.DOM.SITE.DP0.00108.001.01951.700.080.000	Y
Volumetric flow rate	frt	1	LPM	NEON.DOM.SITE.DP0.00108.001.01950.700.080.000	Y
Pressure	presAtm	1	kPa	NEON.DOM.SITE.DP0.00108.001.01948.700.080.000	Y
Gas temperature	temp	1	°C	NEON.DOM.SITE.DP0.00108.001.01949.700.080.000	Y

9.1.3 Product Instances

All sites across the NEON observatory own 4 to 8 Alicat Scientific MW-20 SLPM-NEON mass flow meters (depending on the number of measurement levels at a specific site) for Eddy Covariance Storage Exchange assembly. Each individual instance will generate one L0p data output listed in Table 9-1.

9.1.4 Temporal Resolution and Extent

The temporal extent of the reported variables in Table 9-1 is 1 Hz.

9.1.5 Spatial Resolution and Extent

The Alicat Scientific MW-20 SLPM-NEON mass flow meters will be located within the tower hut infrastructure. Each flow meter will be located upstream of a sample line pump to monitor the flow rate of the air that pass through the sample line of that measurement level.

9.2 Scientific context

The air samples from each measurement level are pulled through the sample line continuously by a pump dedicated to that line. The flow rate of the air should be high enough to maintain the pressure in the sample line at 40%-50% of the ambient pressure to prevent condensation in the sample line.

Decrease in flow rate could be a result from clogging or ice buildup at the inlet, or malfunction of a pump, etc. The mass flow meter (DGD 0341530000) on each sample line is used to monitor the air flow rate of that sample line.

9.2.1 Theory of Measurement

All M-Series Gas Flow Meters (and MC Series Gas Flow Controllers) are based on the accurate measurement of volumetric flow. The volumetric flow rate is determined by creating a pressure drop across a unique internal restriction, known as a Laminar Flow Element (LFE), and measuring differential pressure across it. The restriction is designed so that the gas molecules are forced to move in parallel paths along the entire length of the passage; hence laminar (streamline) flow is established for the entire range of operation of the device. Unlike other flow measuring devices, in laminar flow meters the relationship between pressure drop and flow is linear (source: http://www.alicat.com/documents/manuals/Gas_Flow_Meter_Manual.pdf).

9.2.2 Theory of Algorithm

NA

9.3 Algorithm Implementation

Data flow for signal processing of L0p DPs will be treated in the following order.

1. Select L0 DPs from Table 9-2 for further data processing.
2. Generate a complete data with respect to 1 Hz frequency using a time regularization approach in accordance with AD[04], details are provided in section 9.3.1.
3. Apply unit conversion to frt0, frt, temp and pressAtm according to Eq. (9.1) to (9.4), respectively.
4. QA/QC Plausibility tests will be applied to the data stream in accordance with AD[02], details are provided below. See section 9.3.4

9.3.1 Time regularization

Mass flow meter measures data at ~ 1 Hz. To generate a complete L0p dataset with respect to 1 Hz frequency, missing timestamps and the corresponding data values will be filled with NaN (not NA) following the procedures detailed in AD[04]. In this case we will use the default options in AD[04] with a windowing approach described by Eq. 3 in AD[04], and when multiple data values fall within a single window we will use the closest value determined by minimum absolute deviation, option 1 in AD[04].

9.3.2 Unit conversion

The mass flow meter sensor outputs data in digital form through Ethernet connections, therefore, no analog to digital (A/D) conversion is necessary. However, some measurements included frt0, frt, temp and presAtm, are needed to convert from LPM to m^3 s^{-1}, from LPM to m^3 s^{-1}, from to °C to K, and from kPa to Pa, respectively.

Convert frt0 (L0 DP) in LPM to frt00 (L0p DP) in m^3 s^{-1}:

$$\text{frt00 in } m^3\, s^{-1} = \text{ frt in LPM} * 0.000017 \tag{9.1}$$

Convert frt (L0 DP) in LPM to frt (L0p DP) in m^3 s^{-1}:

$$\text{frt in } m^3\, s^{-1} = \text{ frt in LPM} * 0.000017 \tag{9.2}$$

Convert temp in degree °C to temp in K,

$$\text{temp in K} = \text{ temp in °C } + 273.15 \tag{9.3}$$

presAtm in kPa to presAtm in Pa,

$$\text{presAtm in Pa } = \text{ presAtm in kPa } * 1000 \tag{9.4}$$

9.3.3 QA/QC Procedure

Standard plausibility tests should be applied to all L0p DPs except for flags. An associated pass/fail flag will be generated for each test according to AD[02]. (Note. We will not be carrying out the “gap test” and “null test”). Quality reports will be generated for temporally averaged L1 DPs at a later stage. Because this sensor will never be sent back to CVAL for calibration once it is deployed at field, thus no valid calibration date will be provided to CI to generate calibration flag.

Table 9-3: Plausibility quality flags to be applied to all L0p DPs except for flags

Flag	Term modifier	Description
QF_{Pers}	qfPers	Quality flag for the Persistence test
QF_{Rng}	qfRng	Quality flag for the Range test
QF_{Step}	qfStep	Quality flag for the Step test

As all flags will be applied to each individual L0p DPs they will follow a uniform naming convention, whereby the L0p DP term is augmented with the plausibility test flag term modifier. For example, the quality flag for the step test for the temperature from mass flow meter for ML01 will be “qfStepTemp”.

Test following parameters will be provided by FIU for each L0p DP and maintained in the CI data store.

Table 9-4: Parameters required for plausibility tests.

Parameter	Description
Thsh_{Pers}	Threshold for the Persistence test

Time_{Pers}	Time parameter for the Persistence test
$\mathrm{Thsh}_{Rng,min}$	Minimum threshold for the Range test
$\mathrm{Thsh}_{Rng,max}$	Maximum threshold for the Range test
Thsh_{Step}	Threshold for the Step test

9.4 Uncertainty

NA

10 MASS FLOW CONTROLLER

10.1 Data Product Description

10.1.1 Variables Reported

The mass flow controller for field validation gas: Alicat Scientific MC-5 SLPM-NEON and mass flow controller for IRGA: Alicat Scientific MCRW-5 SLPM-DS-NEON related L0p reported variables provided by the algorithms documented in this ATBD are displayed in Table 10-1. The mass flow controller for field validation gas is referred to as mfcValiStor in reference to DPs. The mass flow controller for IRGA is referred to as mfcSampStor in reference to DPs.

Table 10-1: List of mfcValiStor and mfcSampStor related L0p reported variables that are produced in this ATBD.

L0p DP	L0p fieldName	L0p DP Frequency (Hz)	Units	Input L0 DP or L0p fieldNames
mfcValiStor (DGD 0341500000)				
Flow rate set point	frtSet00	1	$m^3\ s^{-1}$	NEON.DOM.SITE.DP0.00107.001.01952.700.000.000
Flow rate at NIST standard condition	frt00	1	$m^3\ s^{-1}$	NEON.DOM.SITE.DP0.00107.001.01951.700.000.000
Flow rate at site	frt	1	$m^3\ s^{-1}$	NEON.DOM.SITE.DP0.00107.001.01950.700.000.000
Atmospheric pressure	presAtm	1	Pa	NEON.DOM.SITE.DP0.00107.001.01948.700.000.000
Temperature	temp	1	K	NEON.DOM.SITE.DP0.00107.001.01949.700.000.000
Validation flow rate flag	qfFrt00	1	NA	frtSet00* frt00*
mfcSampStor (DGD 0341570000)				

L0p DP	L0p fieldName	L0p DP Frequency (Hz)	Units	Input L0 DP or L0p fieldNames
Flow rate set point	frtSet00	1	$m^3 s^{-1}$	NEON.DOM.SITE.DP0.00106.001.01952.700.000.000
Flow rate at NIST standard condition	frt00	1	$m^3 s^{-1}$	NEON.DOM.SITE.DP0.00106.001.01951.700.000.000
Flow rate at site	frt	1	$m^3 s^{-1}$	NEON.DOM.SITE.DP0.00106.001.01950.700.000.000
Atmospheric pressure	presAtm	1	Pa	NEON.DOM.SITE.DP0.00106.001.01948.700.000.000
Temperature	temp	1	K	NEON.DOM.SITE.DP0.00106.001.01949.700.000.000
IRGA sample flow rate flag	qfFrt00	1	NA	frt00*

*L0p DP is used as an input to generate other L0p DPs

10.1.2 Input Dependencies

Table 10-2 details the mfcValiStor and mfcSampStor related L0 DPs and specifies which L0 DPs will be used to produce L0p reported variables in this ATBD.

Table 10-2: List of mfcValiStor and mfcSampStor related L0 DPs.

L0 DP	L0 DP fieldName	Sample Frequency	Units	Data Product Number	DPs that are used to produce L0p (Y/N)
mfcValiStor (DGD 0341500000)					
Flow rate set point	frtSet0	1	LPM	NEON.DOM.SITE.DP0.00107.001.01952.700.000.000	Y
Flow rate at NIST standard condition	frt0	1	LPM	NEON.DOM.SITE.DP0.00107.001.01951.700.000.000	Y
Flow rate at site	frt	1	LPM	NEON.DOM.SITE.DP0.00107.001.01950.700.000.000	Y
Atmospheric pressure	presAtm	1	kPa	NEON.DOM.SITE.DP0.00107.001.01948.700.000.000	Y
Temperature	temp	1	C	NEON.DOM.SITE.DP0.00107.001.01949.700.000.000	Y
mfcSampStor (DGD 0341570000)					
Flow rate set point	frtSet0	1	LPM	NEON.DOM.SITE.DP0.00106.001.01952.700.000.000	Y

L0 DP	L0 DP fieldName	Sample Frequency	Units	Data Product Number	DPs that are used to produce L0p (Y/N)
Flow rate at NIST standard condition	frt0	1	LPM	NEON.DOM.SITE.DP0.00106.001.01951.700.000.000	Y
Flow rate at site	frt	1	LPM	NEON.DOM.SITE.DP0.00106.001.01950.700.000.000	Y
Atmospheric pressure	presAtm	1	kPa	NEON.DOM.SITE.DP0.00106.001.01948.700.000.000	Y
Temperature	temp	1	C	NEON.DOM.SITE.DP0.00106.001.01949.700.000.000	Y

10.1.3 Product Instances

Mass flow controller for field validation gases (DGD 0341500000) and mass flow controller for IRGA (DGD 0341570000) are located in the instrument hut. All terrestrial sites across the NEON observatory have both MFCs. How the individual instances of all valves relate to L0p data outputs is summarized in Table 10-1.

10.1.4 Temporal Resolution and Extent

The temporal extent of the reported variables in Table 10-1 is 1 Hz.

10.1.5 Spatial Resolution and Extent

Both mass flow controller for field validation gases and IRGA are located in the tower hut infrastructure. However, the measurements reflect the points in space where the mass flow controllers are located in the hut infrastructure. Mass flow controller for field validation gases is located between the validation gas manifold and the T splitter to the CRD CO_2 sample manifold and the IRGA sample manifold and mass flow controller for IRGA is located between IRGA and its external pump.

10.2 Scientific context

During the measurements, the IRGA sample cell must be continually flushed which requires an external air pump that supplies a flow rate of 1 LPM ± 0.2 LPM at NIST standard consitions. The MFC (DGD 0341570000) is used to maintain and monitor to make sure that a constant flow of sample goes through and does not damage the LI840A sample cell. During the field validation of IRGA and CRD CO_2, the consumption of validation gases shall be minimized and no sign of leakage is apparent. For this purpose the flow rates of validation gases shall be monitored continuously using the mass flow controller (DGD 0341500000).

10.2.1 Theory of Measurement

The Alicat Scientific gas flow controllers are based on the accurate measurement of volumetric flow. The volumetric flow rate is determined by creating a pressure drop across a unique internal restriction, called a Laminar Flow Element (LFE), and measuring differential pressure across the LFE (RD [07]). The LFE forces the gas molecules to move in parallel paths along entire length of the passage; hence laminar flow is established for the entire range of operation of the device (RD [07]). Given a known temperature and pressure the mass flow rate can be determine from volumetric flow rate.

10.2.2 Theory of Algorithm

NA

10.3 Algorithm Implementation

L0p signal processing consists of the following sequence:

1. Select L0 data streams as indicated as "Y" in Table 10-2 for further data processing.
2. Generate complete data with respect to 1 Hz frequency using a time regularization approach in accordance with AD[04]. Details are provided in section 10.3.1.
3. Apply unit conversion to L0 DPs. Details are provided below in section 10.3.2.
4. Determine and assign the validation flow rate flag, and IRGA sample flow rate flag to corresponding timestamps. Details are provided below in section 10.3.3.
5. QA/QC Plausibility tests will be applied to the data stream in accordance with AD[02]. Details are provided below in section 10.3.4.

10.3.1 Time regularization

The Alicat Scientific mass flow controllers measure data at 1 Hz. To generate complete L0p data with respect to 1 Hz frequency, missing timestamps and the corresponding data values will be filled with NaN (not NA) following the procedures detailed in AD[04]. In this case we will use the default options in AD[04] with a windowing approach described by Eq. 3 in AD[04], and when multiple data values fall within a single window we will use the closest value determined by minimum absolute deviation, option 1 in AD[04].

10.3.2 Unit conversion

L0 data product measurements from both mass flow controllers should be converted to L0p as follows: flow rate set point (frtSet0), flow rate at NIST standard condition (frt0), and flow rate at site (frt) in LPM shall be converted to m3 s-1

$$\text{flow rate in m}^3\,\text{s}^{-1} = \text{flow rate in LPM} * 1.666667 * 10^{-5}, \tag{10.1}$$

$$\text{presAtm in Pa} = \text{presAtm in kPa} * 1000\,, \tag{10.2}$$

and

$$\text{temp in K} = \text{temp in degree °C} + 273.15 \tag{10.3}$$

10.3.3 Sensor Flags

Flags will be generated for the sensor tests including the validation flow rate flag and IRGA sample flow rate flag, which are defined below. These flags will be generated as part of the L0p processing to indicate when the flow rate is outside the requirement range.

a. **Validation flow rate flag** (qfFrt00) – will be generated to indicate the flow rate of the validation gas mass flow controller (DGD 0341500000) while performing IRGA and CRD CO_2 validation is outside the requirement range. The validation flow rate flag will be determined as follows:

$$\text{qfFrt00} = \begin{cases} 1 & \text{if frtSet00} = (0.5 * 1.666667 * 10^{-5}) \text{ and frt00} > (0.5 * 1.666667 * 10^{-5}) \text{ or} \\ & \text{if frtSet00} = (1.3 * 1.666667 * 10^{-5}) \text{and frt00} < (1.2 * 1.666667 * 10^{-5}) \text{ or frt00} > (1.35 * 1.666667 * 10^{-5}) \text{ or} \\ & \text{if } 0 < \text{frtSet00} < (1.3 * 1.666667 * 10^{-5}) \\ 0 & \text{if frtSet00} = (0.5 * 1.666667 * 10^{-5}) \text{ and frt00} \le (0.5 * 1.666667 * 10^{-5}) \text{ or} \\ & \text{if frtSet00} = (1.3 * 1.666667 * 10^{-5}) \text{ and } (1.2 * 1.666667 * 10^{-5}) \le \text{frt00} \le (1.35 * 1.666667 * 10^{-5}) \\ -1 & \textit{otherwise}. \end{cases} \tag{10.4}$$

where frtSet00 is the flow rate set point from mfcVali
frt00 is the flow rate at NIST standard condition from mfcVali

b. **LI840A sample flow rate flag** (qfFrt00) – will be generated to indicate the flow rate of mass flow controller (DGD 0341570000) during IRGA performed both sampling and validation is outside the requirement range. The IRGA sample flow rate flag will be determined as follows:

$$1 \text{ if frt00} < (0.8 * 1.666667 * 10^{-5}) \text{ or frt00 } > (1.2 * 1.666667 * 10^{-5})$$

$$qfFrt00 = \begin{cases} 0 \text{ if } (0.8 * 1.666667 * 10^{-5}) \leq \text{frt00} \leq (1.2 * 1.666667 * 10^{-5}) \\ -1 \; otherwise. \end{cases} \qquad (10.5)$$

where frt00 is the flow rate at NIST standard condition from irgaMfcSamp

10.3.4 QA/QC Procedure

Standard plausibility tests should be applied to all L0p DPs except for frtSet00 and qfFrt00. No persistence test for frt00 is required since it is very stable. But range test and step test for frt00 should be performed. An associated pass/fail flag will be generated for each test according to AD[02]. Note that we will not be carrying out the "gap test" or "null test". Quality reports will be generated for temporally averaged L1 DPs at a later stage. Because this sensor will never be sent back to CVAL for calibration, once it is deployed at field, no valid calibration date will be provided to CI to generate calibration flag.

Table 10-3: Plausibility quality flags to be applied to all L0p DPs

Flag	Term modifier	Description
QF_{Pers}	qfPers	Quality flag for the Persistence test
QF_{Rng}	qfRng	Quality flag for the Range test
QF_{Step}	qfStep	Quality flag for the Step test

As all flags will be applied to each individual L0p DPs they will follow a uniform naming convention, whereby the L0p DP term is augmented with the plausibility test flag term modifier. For example, the quality flag for the step test for $\delta^{13}C$ will be "qfStepDlta13CCo2".

Test following parameters will be provided by FIU for each L0p DP and maintained in the CI data store.

Table 10-4: Parameters required for plausibility tests.

Parameter	Description
Thsh_{Pers}	Threshold for the Persistence test
Time_{Pers}	Time parameter for the Persistence test
$\text{Thsh}_{Rng,min}$	Minimum threshold for the Range test
$\text{Thsh}_{Rng,max}$	Maximum threshold for the Range test
Thsh_{Step}	Threshold for the Step test

10.4 Uncertainty

NA

11 SAMPLE LINE PUMPS

11.1 Data Product Description

This Chapter describes the processes to convert L0 DPs under pumps (DGD CD07150000) into 1 Hz L0p DPs. The pump is referred to as pumpStor in reference to DPs.

11.1.1 Variables Reported

The pumpStor L0p reported variable provided by the algorithms documented in this ATBD are displayed in the Table 11-1. Because the L0p outputs from each sensor will live in different tables of HDF5 file, it is ok to use generic term of "pumpVolt" for pump voltage L0p outputs.

Table 11-1: List of pumpStor-related L0p reported variables that produced in this ATBD.

L0p DP	L0p fieldName	L0p DP Frequency	Units	Input L0 DPs or L0p DPs
Pump voltage (ML1)	pumpVolt	1 Hz	volt	NEON.DOM.SITE.DP0.00112.001.02351.700.010.000
Pump Voltage (ML2)	pumpVolt	1 Hz	volt	NEON.DOM.SITE.DP0.00112.001.02351.700.020.000
Pump Voltage (ML3)	pumpVolt	1 Hz	volt	NEON.DOM.SITE.DP0.00112.001.02351.700.030.000
Pump Voltage (ML4)	pumpVolt	1 Hz	volt	NEON.DOM.SITE.DP0.00112.001.02351.700.040.000
Pump Voltage (ML5)	pumpVolt	1 Hz	volt	NEON.DOM.SITE.DP0.00112.001.02351.700.050.000
Pump Voltage (ML6)	pumpVolt	1 Hz	volt	NEON.DOM.SITE.DP0.00112.001.02351.700.060.000
Pump Voltage (ML7)	pumpVolt	1 Hz	volt	NEON.DOM.SITE.DP0.00112.001.02351.700.070.000
Pump Voltage (ML8)	pumpVolt	1 Hz	volt	NEON.DOM.SITE.DP0.00112.001.02351.700.080.000
Pump Voltage (IRGA)	pumpVolt	1 Hz	volt	NEON.DOM.SITE.DP0.00112.001.02351.700.000.000

11.1.2 Input Dependencies

Table 11-2 details the pump related L0 DPs used to produce L0p reported variables in this ATBD.

Table 11-2: List of pumpStor-related L0 DPs that are transformed into L0p reported variables in this ATBD.

L0 DP	L0 DP fieldName	Sample Frequency *	Units	Data Product Number	DPs that are used to produce L0p (Y/N)
Pump voltage (ML1)	pumpVoltage	varies	volt	NEON.DOM.SITE.DP0.00112.001.02351.700.010.000	Y

L0 DP	L0 DP fieldName	Sample Frequency *	Units	Data Product Number	DPs that are used to produce L0p (Y/N)
Pump Voltage (ML2)	pumpVoltage	varies	volt	NEON.DOM.SITE.DP0.00112.001.02351.700.020.000	Y
Pump Voltage (ML3)	pumpVoltage	varies	volt	NEON.DOM.SITE.DP0.00112.001.02351.700.030.000	Y
Pump Voltage (ML4)	pumpVoltage	varies	volt	NEON.DOM.SITE.DP0.00112.001.02351.700.040.000	Y
Pump Voltage (ML5)	pumpVoltage	varies	volt	NEON.DOM.SITE.DP0.00112.001.02351.700.050.000	Y
Pump Voltage (ML6)	pumpVoltage	varies	volt	NEON.DOM.SITE.DP0.00112.001.02351.700.060.000	Y
Pump Voltage (ML7)	pumpVoltage	varies	volt	NEON.DOM.SITE.DP0.00112.001.02351.700.070.000	Y
Pump Voltage (ML8)	pumpVoltage	varies	volt	NEON.DOM.SITE.DP0.00112.001.02351.700.080.000	Y
Pump Voltage (IRGA)	pumpVoltage	varies	volt	NEON.DOM.SITE.DP0.00112.001.02351.700.000.000	Y

Note: *pump voltage L0 data is available whenever pump speed is adjusted to meet the inlet pressure setting. The time interval when pump voltage is available varies from 1 second to >20 s.

11.1.3 Product Instances

All sites across the NEON observatory own 4 to 8 Gast 2032-101-G644 Pumps for sample lines (depending on the number of measurement levels at a specific site) and 1 Gast 2032-101-G644 Pump for LI840A IRGA in the Eddy Covariance Storage Exchange assembly. Each individual instance will generate one L0p data output listed in Table 11-1.

11.1.4 Temporal Resolution and Extent

The temporal extent of the reported variables in Table 11-2 varies from 1 second to > 20 s.

11.1.5 Spatial Resolution and Extent

The Gast 2032-101-G644 Pumps will be located within the tower hut infrastructure. Each sample line pump will be located downstream of all sensors in a sample line to pull the air through the sample line of that measurement level. The IRGA pump locates down stream of LI840A sensor to pull the air samples through IRGA cell for measurements.

11.2 Scientific context

The air samples from each measurement level are pulled through the sample line continuously by a pump dedicated to that line. The flow rate of the air should be high enough to maintain the pressure in the sample line at 40%-50% of the ambient pressure to prevent condensation in the sample line. The Gast pump (DGD CD07150000) dedicated to each sample line is use to pull sufficient air through the sample line to generate the required sample line pressure.

The Gast pump (DGD CD07150000) dedicated to IRGA is used to pull 1 SLPM air flow through the IRGA cell for sampling measurements.

11.2.1 Theory of Measurement

A rotary vane pump is a positive-displacement pump that consists of vanes mounted to a rotor that rotates inside of a cavity. The faster the vanes rotate, the higher volume of air flow will be pulled. How fast the vanes inside a pump will rotate during profile measurements is determined by how much power is supplied to the pump, which is eventually controlled by the pressure gradient between the ambient pressure and sample line pressure. The higher the power supplier is, the faster the vanes will spin. This power supply (in volts) to each pump is monitored to determine the status of the pump.

11.2.2 Theory of Algorithm

NA

11.3 Algorithm Implementation

Data flow for signal processing of L0p DPs will be treated in the following order.

1. Select all L0 pumpVoltage data streams from Table 11-2 for further data processing.
2. Generate a complete data with respect to 1 Hz frequency using a time regularization approach in accordance with AD[04], details are provided in section 11.3.1.
3. QA/QC Plausibility tests will be applied to the data stream in accordance with AD[02], details are provided below in 11.3.3.

11.3.1 Time regularization

The time interval when pump voltage is available varies from 1 second to > 20 s. To generate a complete L0p dataset with respect to 1 Hz frequency, missing timestamps and the corresponding data values will be filled with previous value. When multiple data values fall within a single window we will use the closest value determined by minimum absolute deviation, option 1 in AD[04].

11.3.2 QA/QC Procedure

Standard plausibility tests should be applied to all L0p DPs except for flags. An associated pass/fail flag will be generated for each test according to AD[02]. (Note. We will not be carrying out the “gap test” and “null test”). Quality reports will be generated for temporally averaged L1 DPs at a later stage.

Because this sensor will never be sent back to CVAL for calibration once it is deployed at field, thus no valid calibration date will be provided to CI to generate calibration flag.

Table 11-3: Plausibility quality flags to be applied to all L0p DPs except for flags

Flag	Term modifier	Description
QF_{Pers}	qfPers	Quality flag for the Persistence test
QF_{Rng}	qfRng	Quality flag for the Range test
QF_{Step}	qfStep	Quality flag for the Step test

As all flags will be applied to each individual L0p DPs they will follow a uniform naming convention, whereby the L0p DP term is augmented with the plausibility test flag term modifier. For example, the quality flag for the step test for pump voltage at ML01 will be "qfStepPumpVolt".

Test following parameters will be provided by FIU for each L0p DP and maintained in the CI data store.

Table 11-4: Parameters required for plausibility tests.

Parameter	Description
Thsh_{Pers}	Threshold for the Persistence test
Time_{Pers}	Time parameter for the Persistence test
$\mathrm{Thsh}_{Rng,min}$	Minimum threshold for the Range test
$\mathrm{Thsh}_{Rng,max}$	Maximum threshold for the Range test
Thsh_{Step}	Threshold for the Step test

11.4 Uncertainty

NA

12 HEATER

12.1 Data Product Description

This Chapter describes the processes to generate 1 Hz heating flags (L0p DPs) using L0 DPs from HMP155 Related Humidity Sensor at the tower top and in the soil array. The DGD number for the HMP155 relative humidity sensor is CA04430000.The temperature and dewpoint measurements from these two sensors are used to trigger heater on/off. The HMP155 data is referred to as rhSens in reference to L0p DPs. The heater flag (qfHeat) generated using HMP155 data will be placed under qfqm/irgaStor, qfqm/crdCo2, and qfqm/crdH2o folders of L0p HDF5 file. See section 19 for more details.

12.1.1 Variables Reported

The heater related L0p reported variable provided by the algorithms documented in this ATBD are displayed in Table 12-1. Since heater will be turn on at the same time for all measurement levels once the environmental conditions are reached, the heater flag will apply to all measurement levels.

Table 12-1: List of heatInlt related L0p reported variables that produced in this ATBD.

L0p DP	L0p fieldName	L0p DP Frequency	Units	Input L0 fieldNames
Heater flag	qfHeat	1 Hz	NA	sensorTemp, dewPoint from HMP155 AT tower top: NEON.DOM.SITE.DP0.00098.001.01309.000.VER.000 NEON.DOM.SITE.DP0.00098.001.01358.000.VER.000 SensorTemp, dewPoint from HMP155 at soil array: NEON.DOM.SITE.DP0.00098.001.01309.003.000.000 NEON.DOM.SITE.DP0.00098.001.01358.003.000.000
Relative humidity	rh	1 Hz	-	NEON.D10.CPER.DP0.00098.001.01357.000.VER*.000
Temperature	temp	1 Hz	K	NEON.D10.CPER.DP0.00098.001.01309.000.VER*.000
Dew point/frost point temperature	tempDew	1 Hz	K	NEON.D10.CPER.DP0.00098.001.01358.000.VER*.000
Sensor error flag	qfSens	1 Hz	NA	NEON.D10.CPER.DP0.00098.001.01359.000.VER*.000
Relative humidity	rh	1 Hz	-	NEON.D10.CPER.DP0.00098.001.01357.003.000.000
Temperature	temp	1 Hz	K	NEON.D10.CPER.DP0.00098.001.01309.003.000.000
Dew point/frost point temperature	tempDew	1 Hz	K	NEON.D10.CPER.DP0.00098.001.01358.003.000.000
Sensor error flag	qfSens	1 Hz	NA	NEON.D10.CPER.DP0.00098.001.01359.003.000.000

*: Vertical measurement level (VER) where the HMP155 locates at tower top varies from site to site.

Please be aware that the unit for relative humidity L0p data (rh) is fraction, using "-" to represent it.

12.1.2 Input Dependencies

Table 12-2 details the relative humidity HMP 155 sensors related L0 DPs used to produce L0p reported variables in this ATBD.

Table 12-2: List of relative humidity HMP 155 related L0 DPs that are transformed into L0p reported variables in this ATBD.

L0 DP	L0 DP fieldName	Sample Frequency*	Units	Data Product Number	DPs that are used to produce L0p (Y/N)
Relative humidity sensor at the tower top (DGD CA04430000)					
Relative humidity	RH	1	%	NEON.D10.CPER.DP0.00098.001.01357.000.VER*.000	Y
Temperature	sensorTemp	1	°C	NEON.D10.CPER.DP0.00098.001.01309.000.VER*.000	Y
Dew point/frost point temperature	dewPoint	1	°C	NEON.D10.CPER.DP0.00098.001.01358.000.VER*.000	Y
Sensor error flag	RHStatus	1	NA	NEON.D10.CPER.DP0.00098.001.01359.000.VER*.000	Y
Relative humidity sensor at the soil array (DGD CA04430000)					
Relative humidity	RH	1	%	NEON.D10.CPER.DP0.00098.001.01357.000.VER*.000	Y
Temperature	sensorTemp	1	°C	NEON.D10.CPER.DP0.00098.001.01309.000.VER*.000	Y
Dew point/frost point temperature	DewPoint	1	°C	NEON.D10.CPER.DP0.00098.001.01358.000.VER*.000	Y
Sensor error flag	RHStatus	1	NA	NEON.D10.CPER.DP0.00098.001.01359.000.VER*.000	Y

*: Vertical measurement level (VER) where the HMP155 locates at tower top varies from site to site.

12.1.3 Product Instances

All sites across the NEON observatory own 4 to 8 heaters (depending on the number of measurement levels at a specific site) for Eddy Covariance Storage Exchange assembly. They will be turned on/off at the same time at a site. Therefore, only one L0p data output of heater flag listed in Table 12-1, which will apply to all measurement levels.

12.1.4 Temporal Resolution and Extent

The temporal extent of the reported variables in Table 12-1 is 1 Hz.

12.1.5 Spatial Resolution and Extent

The heater will be wrapped outside each Eddy Covariance Storage Exchange inlet at heated sites only. The list of the heated site can be found below in Table 12-3:

Table 12-3: List of NEON heated sites.

Domain	Site	Site Code
1	Harvard Forest	HARV
1	Bartlett Experimental Forest	BART
2	SCBI	SCBI
2	Blandy Experimental Farm	BLAN
2	Smithsonian Environmental Research Center	SERC
5	UNDERC	UNDE
5	Steigerwald Land Services	STEI
5	Tree Haven	TREE
6	Konza Prairie Biological Station	KONZ
6	Konza Prairie Biological Station (Agricultural Lowland)	KONA
6	The University of Kansas Field Station	UKFS
7	Oak Ridge	ORNL
7	Great Smoky Mountains National Park, Twin Creeks	GRSM
7	Mountain Lake Biological Station (SW Virginia)	MLBS
9	Woodworth	WOOD
9	Dakota Coteau Field School	DCFS
9	Northern Great Plains Research Laboratory	NOGP
10	Central Plains Experimental Range	CPER
10	North Sterling, CO	STER
10	RMNP, CASTNET	RMNP
11	Caddo/LBJ	CLBJ
11	Klemme Range Research Station	OAES
12	Yellowstone Northern Range (Frog Rock)	YELL
13	Niwot Ridge/Mountain Research Station	NIWO
13	Moab, Canyonlands Ecological Research Site	MOAB
15	Onaqui-Ault	ONAQ
16	Wind River Experimental Forest	WREF
16	Abby road	ABBY
17	San Joaquin	SJER
17	Soaproot Saddle	SOAP
17	Lower Teakettle	TEAK
18	Toolik Lake	TOOL
18	Barrow	BARR
19	Caribou Creek (CPCRW)	BONA
19	Eight Mile Lake, Healy Alaska, Alpine Tundra, Thermokarsting	HEAL
19	Delta Junction, Non-permafrost	DEJU

12.2 Scientific context

To avoid ice or rime ice clogging the inlet and critical flow orifice, heating should be applied to the screened inlet and critical flow orifice at each tower measurement levels. Heating should be low (maximum 50 W and not exceed heating of 70 Celsius at any time) to avoid the stable isotopic fractionation.

12.2.1 Theory of Measurement

Heater control is based on the ambient air and the conditions when rime ice could happen (when the air temperature equals or is lower than the dew point temperature, and the air temperature reads close to or below water freezing point (0 °C). So, if air temperature is within 2 °C above the dew point temperature, and air temperature is ≤0°C, then turn on the heater. After the heater is switched on, heating should be maintained at 10 Celsius +/- 5 Celsius above dewpoint temperature. When air temperature is 5 °C higher than dew point temperature, then turn the heater off.

The dewpoint temperature and air temperature outputted by HMP155 sensors assembly at the tower top and at ground level at the soil array, which typically bound the worst freezing conditions, will be used for above heater command and control. The logic is to monitor the conditions at the tower top and at ground level, and if one of them approaches the frost conditions, then turn on the screened inlet heaters on all profile levels at the same time. When air temperature is 5 °C higher than dew point temperature at both tower top and at ground level, turn off the screened inlet heaters on all profile levels at the same time. To minimize the uncertainty among sampling levels, heating applied to intake tube inlet at all measurement levels at that site shall be triggered on and/or off at the same time (+/- 5 s).

Because the heater used in the profile system does not have a chip, it is not a data generating device (DGD), and therefore the heater on/off status cannot be streamed back to CI as a L0 data product. The heating flag generated in the post data process in this document. See details below.

12.2.2 Theory of Algorithm

NA

12.3 Algorithm Implementation

Data flow for signal processing of L0p DPs will be treated in the following order.

1. Select four L0 data streams from HMP155 sensor at the tower top and in the soil array. See Table 12-2.

2. Generate a complete data with respect to 1 Hz frequency using a time regularization approach in accordance with AD[04], details are provided in section 12.3.1.
3. Determine and assign the heater on/off flag to correspond 1 Hz data using Eq. (12.1). This should be done based on the raw L0 data products before unit conversion.
4. Perform the unit conversion to generate L0p data according to Eq. (12.2) and (12.3)
5. No need to perform QA/QC Plausibility tests on HMP155 data streams. This is to mimic the filed command and control on heater using raw HMP155 data.
6. No need to perform plausibility test on heater flags.

12.3.1 Time regularization

The HMP155 sensor measures data at ~ 1 Hz. To generate a complete L0p dataset with respect to 1 Hz frequency, missing timestamps and the corresponding data values will be filled with NaN (not NA) following the procedures detailed in AD[04]. In this case we will use the default options in AD[04] with a windowing approach described by Eq. 3 in AD[04], and when multiple data values fall within a single window we will use the closest value determined by minimum absolute deviation, option 1 in AD[04].

12.3.2 Sensor Flags

a. **Heater Flag** (qfHeat) will be generated to indicate if the heater is turned on/off at a site. There will be only one control for heater on inlets at all measurement levels. In other word, heaters at all measurement levels will be turn on or turn off at the same time. Therefore, there will be only one heater flag in this document, which will be apply to all measurement level in a later QAQC process (not part of the discussion in this document). The heater flag at time *t* will be determined as follows:

$$\text{qfHeat (t)} = \begin{cases} 1 & \text{If } (T_{air\_top} < T_{dew\_top} + 2\ °\text{C and } T_{air\_top} \leq 0\ °\text{C}); \\ & \text{or if } (T_{air\_sp3} < T_{dew\_sp3} + 2\ °\text{C and } T_{air\_sp3} \leq 0\ °\text{C}); \\ & \text{or if } (T_{air\_top} < T_{dew\_top} + 5\ °\text{C and } qfHeat\ (t\text{-}1) = 1); \\ & \text{or } T_{air\_sp3} < T_{dew\_sp3} + 5\ °\text{C and } qfHeat\ (t\text{-}1) = 1); \\ 0 & \text{If } T_{air\_top} \geq T_{d\_top} + 5\ °\text{C and } T_{air\_sp3} \geq T_{dew\_sp3} + 5\ °\text{C}; \\ & \text{or if } (T_{dew\_top} + 5\ °\text{C} \leq T_{air\_top} \leq T_{dew\_top} + 2\ °\text{C and } qfHeat\ (t\text{-}1) = 0); \\ & \text{or if } (T_{dew\_sp3} + 5\ °\text{C} \leq T_{air\_sp3} \leq T_{dew\_sp3} + 2\ °\text{C and } qfHeat\ (t\text{-}1) = 0); \\ -1 & otherwise \end{cases} \quad (12.1)$$

where T_{dew_top} is HMP155 dew point temperature at tower-top at time t, unit is °C;
T_{dew_sp3} is HMP155 dew point temperature at soil plot 3 at time t, unit is °C;
T_{air_top} is HMP155 air temperatures at tower top at time t, unit is °C;
T_{air_b} is HMP155 air temperature at soil array at time t, unit is °C;
t is current time, unit is s.

12.3.3 Unit conversion

sensorTemp (°C) L0 DP should be converted to temp (K) L0p DP:

$$\text{temp (K)} = \text{sensorTemp (°C)} + 273.15 \qquad (12.2)$$

dewPoint (°C) L0 DP should be converted to temp (K) L0p DP:

$$\text{tempDew (K)} = \text{dewPoint (°C)} + 273.15 \qquad (12.3)$$

12.3.4 QA/QC Procedure

No standard plausibility test is required for this sensor.

12.4 Uncertainty

NA

13 MEASUREMENT TYPE SEPARATION

13.1 Data Product Description

Here we define measurement type as a sampling mode (samp) or a validation mode (vali). This chapter describes the processes to distinguish the measurement type of the data measured by LI-COR LI-840A (*hereafter* referred to as IRGA), isotopic CO_2 analyzer (Picarro G2131-i, *hereafter* referred to as CRD CO_2), and isotopic H_2O analyzer (Picarro L2130-i, hereafter referred to CRD H_2O) based on the status of auxiliary gas valves under the DGD CD06640002. The auxiliary gas valves referred to as valvAux in reference to DPs.

13.1.1 Variables Reported

The valvAux -related L0p reported variables provided by the algorithms documented in this ATBD are displayed in Table 13-1.

Table 13-1: List of valvAux-related L0p reported variables that produced in this ATBD.

L0p DP	L0p fieldName	L0p DP Frequency (Hz)	Units	Input L0 DPs or L0p DP fieldNames
Status of CRD H_2O wavelength monitor (WLM) purge valve	valv01	1	NA	valvCmd1
Status of CRD CO_2 validation gas valve	valv02	1	NA	valvCmd2
Status of IRGA vent valve	valv03	1	NA	valvCmd3
Status of IRGA validation gas valve	valv04	1	NA	valvCmd4
CRD H_2O measurement type	measTypeCrdH2o	1	NA	valv01*
CRD CO_2 measurement type	measTypeCrdCo2	1	NA	valv02*
IRGA vent valve flag	qfValvIrga	1	NA	valv03*
IRGA measurement type	measTypeIrga	1	NA	valv04*

*L0p DP is used as an input to generate other L0p DPs.

13.1.2 Input Dependencies

Table 13-2 details the valvAux-related L0 DPs and specifies which L0 DPs will be used to indicate the measurement type of the data measured by IRGA LI-840A, Picarro G2131-i, and L2130-i.

Table 13-2: List of valvAux-related L0 DPs.

L0 DP	L0 DP fieldName	Sample Frequency	Units	Data Product Number	DPs that are used to produce L0p (Y/N)
*Status of CRD H_2O WLM purge valve	valvCmd1	0.2	NA	NEON.DOM.SITE.DP0.00114.001.02360.HOR.VER.000	Y
Status of CRD CO_2 validation gas valve	valvCmd2	0.2	NA	NEON.DOM.SITE.DP0.00114.001.02361.HOR.VER.000	Y
Status of IRGA vent valve	valvCmd3	0.2	NA	NEON.DOM.SITE.DP0.00114.001.02362.HOR.VER.000	Y
Status of IRGA validation gas valve	valvCmd4	0.2	NA	NEON.DOM.SITE.DP0.00114.001.02364.HOR.VER.000	Y

*Note that there are no L0 DPs for those sites that do not own Picarro H2O analyzer.

13.1.3 Product Instances

The IRGA validation gas valve, the CRD CO_2 validation gas valve, and the CRD H_2O WLM purge valve are located in the instrument hut. All terrestrial sites across the NEON observatory have IRGA validation gas valve and the CRD CO_2 validation gas valve, and 21 sites (20 NEON core sites and 1 relocatable site at D18 Barrow) have the CRD H_2O WLM purge valve. How the individual instances of all valves relate to L0p data outputs is summarized in Table 13-1.

13.1.4 Temporal Resolution and Extent

The temporal resolution of the reported variables in Table 13-1 is 1 Hz.

13.1.5 Spatial Resolution and Extent

All four valves defined in Table 13-2 are located in the tower hut infrastructure. However, the measurements reflect the points in the flow path where the valves are located within the tower hut infrastructure. IRGA validation gas valve will be located between the T splitter to the CRD CO_2 sample manifold and the IRGA sample manifold and the T splitter to IRGA vent valve and the IRGA sample manifold. CRD CO_2 validation gas valve will be located between the T splitter to the CRD CO_2 sample manifold and the IRGA sample manifold and the CRD CO_2 sample manifold. CRD H_2O WLM purge valve will be located between the CRD H_2O analyzer and zero gas cylinder.

13.2 Scientific context

13.2.1 Theory of Measurement

Irrespective of whether L0 DPs were collected from the IRGA, CRD CO_2, or CRD H_2O the data must be preprocessed to relate the measurement for specific time to its respective measurement type. In this section, we will describe how to distinguish the measurement type for all 3 analyzers. However, the measurement type of IRGA needs a further step to differentiate between validation and calibration mode, details can be found in section 16.

During the sampling mode, the sample valves will be opened at scheduled times to draw atmospheric samples. During the validation/calibration mode the sample valves will be closed and the validation gas select valve, IRGA validation gas valve, the CRD CO_2 validation gas valve, and the CRD H_2O WLM purge valve will be opened. However, the topmost measurement level sample valve of IRGA will remain opened during validation/calibration to maintain stable pressure in the IRGA cell.

13.2.2 Theory of Algorithm

NA

13.3 Algorithm Implementation

L0p signal processing consists of the following sequence:

1. Select L0 data streams as indicated as "Y" in Table 13-2 for further data processing.
2. Generate L0p DPs from L0 DPs by converting to 1 Hz frequency using a time regularization approach in accordance with AD[04], details are provided in section 13.3.1.
3. Replace the NaN in L0p DPs according to Eq. (13.1).
4. Determine the measurement type for IRGA according to Eq. (13.2).
5. Determine the measurement type for CRD CO_2 according to Eq. (13.3).
6. For those sites that have the CRD H_2O analyzer, determine the measurement type for CRD H_2O according to Eq. (13.4).
7. Determine the IRGA vent flag according to Eq. (13.5).
8. When perform above data processing, it is suggested to include data one hour before and after the target processing time period to help identify validation across boundaries (days).

13.3.1 Time regularization

The IRGA validation gas valve, the CRD CO_2 validation gas valve, and the CRD H_2O WLM purge valve output L0 data at 0.2 Hz or every 5 seconds. To generate L0p DPs from L0 DPs by converting to 1 Hz frequency, missing timestamps and the corresponding data values are inserted following the procedures detailed in AD[04]. Here we use the default options in AD[04] with a windowing approach described by

Eq. 3 in AD[04]. In case multiple data values fall within a single window the last value used (option 3 in AD[04]).

13.3.2 Replacing NaN values

After time regularization, the missing L0p values will be filled with NaN. To be able to continue data processing, the L0p which equal to NaN are replaced by the following:

$$\mathrm{L0p} = \begin{cases} \text{previous L0p value if continuous sequence of NaNs} \leq 6\text{s duration} \\ -1 \text{ if continous sequence of NaNs} > 6\text{s duration} \end{cases} \quad (13.1)$$

where L0p is valvIdx and Idx is 01, 02,03, and 04.

13.3.3 IRGA measurement type

The measurement type specific for IRGA measurements can be determined as:

$$\mathrm{measTypeIrga} = \begin{cases} \text{samp if valv04} = 0 \\ \text{vali if valv04} = 1 \\ -1 \text{ if valv04} = -1 \end{cases} \quad (13.2)$$

13.3.4 CRD CO_2 measurement type

The measurement type specific for CRD CO_2 measurements can be determined as:

$$\mathrm{measTypeCrdCo2} = \begin{cases} \text{samp if valv02} = 0 \\ \text{vali if valv02} = 1 \\ -1 \text{ if valv02} = -1 \end{cases} \quad (13.3)$$

13.3.5 CRD H_2O measurement type

The measurement type specific for CRD H_2O measurements can be determined as:

$$\text{measTypeCrdH2o} = \begin{vmatrix} \text{samp if valv01} = 0 \\ \text{vali if valv01} = 1 \\ -1 \text{ if valv01} = -1 \end{vmatrix} \quad (13.4)$$

13.3.6 Sensor Flags

During the normal operation the IRGA vent valve is closed (equal to '0'). The IRGA vent flag (qfValvIrga) will be generated as part of the L0p variables to indicate that the system is working properly:

$$\text{qfValvIrga} = \begin{vmatrix} 0 \text{ if valv03} = 0 \\ 1 \text{ if valv03} = 1 \\ -1 \text{ if valv03} = -1 \end{vmatrix} \quad (13.5)$$

13.3.7 QA/QC Procedure

NA

13.4 Uncertainty

NA

14 MEASUREMENT LOCATION SEPARATION

14.1 Data Product Description

This section describes the processes to distinguish the measurement location of the data measured by LI-COR LI-840A (*hereafter* referred to as IRGA), isotopic CO_2 analyzer (Picarro G2131-i, *hereafter* referred to as CRD CO_2), and isotopic H_2O analyzer (Picarro L2130-I, hereafter referred to CRD H_2O) based on the state of solenoids in the sample manifolds under the DGD: CD06640001. The sample manifolds of IRGA, CRD CO_2, and CRD H_2O referred to as irgaValvLvl, crdCo2ValvLvl, and crdH2oValvLvl in reference to DPs, respectively.

14.1.1 Variables Reported

The sample manifold-related L0p reported variables provided by the algorithms documented in this ATBD are displayed in Table 14-1.

Table 14-1: List of sample manifold-related L0p reported variables that produced in this ATBD.

L0p DP	**L0p fieldName**	**L0p DP Frequency (Hz)**	**Units**	**Input L0 DPs or L0p DP fieldNames**
		irgaValvLvl (DGD CD06640001)		
Status of sample valve of ML01	valv01	1	NA	NEON.DOM.SITE.DP0.00113.001.02360.701.000.000
Status of sample valve of ML02	valv02	1	NA	NEON.DOM.SITE.DP0.00113.001.02361.701.000.000
Status of sample valve of ML03	valv03	1	NA	NEON.DOM.SITE.DP0.00113.001.02362.701.000.000
Status of sample valve of ML04	valv04	1	NA	NEON.DOM.SITE.DP0.00113.001.02364.701.000.000
Status of sample valve of ML05	valv05	1	NA	NEON.DOM.SITE.DP0.00113.001.02365.701.000.000
Status of sample valve of ML06	valv06	1	NA	NEON.DOM.SITE.DP0.00113.001.02366.701.000.000
Status of sample valve of ML07	valv07	1	NA	NEON.DOM.SITE.DP0.00113.001.02367.701.000.000
Status of sample valve of ML08	valv08	1	NA	NEON.DOM.SITE.DP0.00113.001.02368.701.000.000
IRGA measurement location	lvlIrga	1	NA	valv01* valv02* valv03* valv04* valv05* valv06* valv07* valv08*
		crdCo2ValvLvl (DGD CD06640001)		

L0p DP	L0p fieldName	L0p DP Frequency (Hz)	Units	Input L0 DPs or L0p DP fieldNames
Status of sample valve of ML01	valv01	1	NA	NEON.DOM.SITE.DP0.00113.001.02360.702.000.000
Status of sample valve of ML02	valv02	1	NA	NEON.DOM.SITE.DP0.00113.001.02361.702.000.000
Status of sample valve of ML03	valv03	1	NA	NEON.DOM.SITE.DP0.00113.001.02362.702.000.000
Status of sample valve of ML04	valv04	1	NA	NEON.DOM.SITE.DP0.00113.001.02364.702.000.000
Status of sample valve of ML05	valv05	1	NA	NEON.DOM.SITE.DP0.00113.001.02365.702.000.000
Status of sample valve of ML06	valv06	1	NA	NEON.DOM.SITE.DP0.00113.001.02366.702.000.000
Status of sample valve of ML07	valv07	1	NA	NEON.DOM.SITE.DP0.00113.001.02367.702.000.000
Status of sample valve of ML08	valv08	1	NA	NEON.DOM.SITE.DP0.00113.001.02368.702.000.000
CRD CO_2 measurement location	lvlCrdCo2	1	NA	valv01* valv02* valv03* valv04* valv05* valv06* valv07* valv08*
crdH2oValvLvl (DGD CD06640001)				
Status of sample valve of ML01	valv01	1	NA	NEON.DOM.SITE.DP0.00113.001.02360.704.000.000
Status of sample valve of ML02	valv02	1	NA	NEON.DOM.SITE.DP0.00113.001.02361.704.000.000

L0p DP	L0p fieldName	L0p DP Frequency (Hz)	Units	Input L0 DPs or L0p DP fieldNames
Status of sample valve of ML03	valv03	1	NA	NEON.DOM.SITE.DP0.00113.001.02362.704.000.000
Status of sample valve of ML04	valv04	1	NA	NEON.DOM.SITE.DP0.00113.001.02364.704.000.000
Status of sample valve of ML05	valv05	1	NA	NEON.DOM.SITE.DP0.00113.001.02365.704.000.000
Status of sample valve of ML06	valv06	1	NA	NEON.DOM.SITE.DP0.00113.001.02366.704.000.000
Status of sample valve of ML07	valv07	1	NA	NEON.DOM.SITE.DP0.00113.001.02367.704.000.000
Status of sample valve of ML08	valv08	1	NA	NEON.DOM.SITE.DP0.00113.001.02368.704.000.000
CRD H_2O measurement location	lvlCrdH2o	1	NA	valv01* valv02* valv03* valv04* valv05* valv06* valv07* valv08*

*L0p DP is used as an input to generate other L0p DPs.

14.1.2 Input Dependencies

Table 14-2 details sample manifold-related L0 DPs used to produce L0p reported variables in this ATBD.

Table 14-2: List of sample manifold-related L0 DPs that are transformed into L0p in this ATBD.

L0 DP	L0 DP fieldName	Sample Frequency	Units	Data Product Number	DPs that are used to produce L0p (Y/N)
irgaValvLvl (DGD CD06640001)					

L0 DP	L0 DP fieldName	Sample Frequency	Units	Data Product Number	DPs that are used to produce L0p (Y/N)
Status of sample valve of ML01	valvCmd1	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02360.701.000.000	Y
Status of sample valve of ML02	valvCmd2	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02361.701.000.000	Y
Status of sample valve of ML03	valvCmd3	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02362.701.000.000	Y
Status of sample valve of ML04	valvCmd4	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02364.701.000.000	Y
Status of sample valve of ML05	valvCmd5	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02365.701.000.000	Y
Status of sample valve of ML06	valvCmd6	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02366.701.000.000	Y
Status of sample valve of ML07	valvCmd7	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02367.701.000.000	Y
Status of sample valve of ML08	valvCmd8	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02368.701.000.000	Y
crdCo2ValvLvl (DGD CD06640001)					
Status of sample valve of ML01	valvCmd1	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02360.702.000.000	Y
Status of sample valve of ML02	valvCmd2	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02361.702.000.000	Y
Status of sample valve of ML03	valvCmd3	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02362.702.000.000	Y
Status of sample valve of ML04	valvCmd4	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02364.702.000.000	Y

L0 DP	L0 DP fieldName	Sample Frequency	Units	Data Product Number	DPs that are used to produce L0p (Y/N)
Status of sample valve of ML05	valvCmd5	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02365.702.000.000	Y
Status of sample valve of ML06	valvCmd6	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02366.702.000.000	Y
Status of sample valve of ML07	valvCmd7	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02367.702.000.000	Y
Status of sample valve of ML08	valvCmd8	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02368.702.000.000	Y
crdH2oValvLvl (DGD CD06640001)					
*Status of sample valve of ML01	valvCmd1	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02360.704.000.000	Y
*Status of sample valve of ML02	valvCmd2	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02361.704.000.000	Y
*Status of sample valve of ML03	valvCmd3	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02362.704.000.000	Y
*Status of sample valve of ML04	valvCmd4	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02364.704.000.000	Y
*Status of sample valve of ML05	valvCmd5	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02365.704.000.000	Y
*Status of sample valve of ML06	valvCmd6	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02366.704.000.000	Y
*Status of sample valve of ML07	valvCmd7	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02367.704.000.000	Y
*Status of sample valve of ML08	valvCmd8	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02368.704.000.000	Y

*Note: These status L0 DPs exist only for those sites that have the Picarro H_2O analyzer installed.

14.1.3 Product Instances

The sample manifolds are located in the instrument hut. All terrestrial sites across the NEON observatory have both IRGA and CRD CO_2 sample manifolds and only 21 sites (20 NEON core sites and 1 relocatable site at D18 Barrow) own the CRD H_2O sample manifolds. Individual instance of all sample manifold-related L0p data outputs are in Table 14-1.

14.1.4 Temporal Resolution and Extent

The temporal extent of the reported variables in Table 14-1 is 1 Hz.

14.1.5 Spatial Resolution and Extent

The sample manifolds will be located within the tower hut infrastructure. However, the measurements reflect the points in space where the sample inlets are located on the tower infrastructure, which is site specific.

14.2 Scientific context

14.2.1 Theory of Measurement

The EC Profile Assembly will be accompanied by a number of sample manifolds. These manifolds and their associated solenoid valves control the air sample delivered to each sensor. Each sample manifold consists of 9 inlet ports and one outlet port. The first 8 inlet ports will be connected to the sample solenoid valves, and one additional inlet port will be used for validation gases. The outlet port will be used to deliver air from the selected measurement level or validation gas to the analyzer. The status of the solenoid valves indicate the type of air sample measured for a specific time.

During sampling mode, the sample solenoid valves are opened at the scheduled time to receive atmospheric samples. During the validation/calibration mode all sample valves of CRD CO_2 and CRD H_2O sample manifolds are closed. However, the topmost measurement level sample valve of IRGA sample manifolds will remain opened during validation/calibration to maintain stable pressure in IRGA's cell.

The location controller dictates which valve in the sampling manifold is opened, which allows gas from only one measurement level (ML) to enter into the manifold at a time. The sequence of the sample solenoid valves always start from the highest to lowest measurement level (ML01), where the highest measurement level is site specific and can vary from 4 to 8.

14.2.2 Theory of Algorithm

NA

14.3 Algorithm Implementation

L0p signal processing consists of the following sequence:

1. Select L0 data streams indicated with "Y" in Table 14-2 for further data processing.
2. Generate L0p DPs from L0 DPs by converting to 1 Hz frequency using a time regularization approach in accordance with AD[04], details are provided in section 14.3.1.
3. Replace the NaN in L0p DPs according to Eq. (14.1).
4. Determine the measurement location for IRGA according to Eq. (14.2).
5. Determine the measurement location for CRD CO_2 according to Eq. (14.3).
6. For those sites that have a CRD H_2O analyzer, determine the measurement location for CRD H_2O according to Eq. (14.4).

14.3.1 Time regularization

The L0 DPs of IRGA, CRD CO_2, and CRD H_2O sample manifolds were recorded at 0.2 Hz or every 5 seconds. To generate L0p DPs from L0 DPs by converting to 1 Hz frequency, missing timestamps and the corresponding data values are inserted following the procedures detailed in AD[04]. Here we use the default options in AD[04] with a windowing approach described by Eq. 3 in AD[04] In case, multiple data values fall within a single window the last value used (option 3 in AD[04]).

14.3.2 Replacing NaN values

After time regularization, the missing L0p values will be filled with NaN. To be able to continue data processing, the L0p which equal to NaN are replaced by the following:

$$\mathrm{L0p} = \left| \begin{array}{l} \text{previous L0p value if continuous sequence of NaN} \\ \qquad\qquad \leq \text{6s duration} \\ \\ -1 \text{ if continuous sequence of NaN} > \text{6s duration} \end{array} \right. \tag{14.1}$$

where L0p is valvIdx in IRGA, CRD CO_2, and CRD H_2O sample manifolds

Idx is index for the location and equal to 01, 02, 03,…. n

n is the site-specific highest measurement level and can be vary from 04 to 08.

14.3.3 IRGA measurement location

The measurement location specific for IRGA measurements can be determined as:

$$\text{lvlIrga} = \left| \begin{array}{l} \text{lvlIdx if only one of valvIdx} = 1 \\ \text{vali if all valvIdx} = 0 \\ \text{negl if more than one valvIdx} = 1 \\ -1 \text{ if any valvIdx} = -1 \end{array} \right. \tag{14.2}$$

where: valvIdx is the solenoid valve in the IRGA sample manifold

Idx is index for the location and equal to 01, 02, 03,…. n

n is the site-specific highest measurement level and can be vary from 04 to 08.

14.3.4 CRD CO_2 measurement location

The measurement location specific for CRD CO_2 measurements can be determined as:

$$\text{lvlCrdCo2} = \left| \begin{array}{l} \text{lvlIdx if only one of valvIdx} = 1 \\ \text{vali if all valvIdx} = 0 \\ \text{negl if more than one valvIdx} = 1 \\ -1 \text{ any valvIdx} = -1 \end{array} \right. \tag{14.3}$$

where: valvIdx is the solenoid valve in the CRD CO_2 sample manifold

Idx is index for the location and equal to 01, 02, 03,…. n

n is the site-specific highest measurement level and can be vary from 04 to 08.

14.3.5 CRD H_2O measurement location

The measurement location specific for CRD H_2O measurements can be determined as:

$$\left| \text{lvlIdx if only one of valvIdx} = 1 \right.$$

$$\mathrm{lvlCrdH2o} = \begin{cases} \mathrm{vali\ if\ all\ valvIdx} = 0 \\ \mathrm{negl\ if\ more\ than\ one\ valvIdx} = 1 \\ -1\ \mathrm{any\ valvIdx} = -1 \end{cases} \quad (14.4)$$

where: $\mathrm{valvIdx}$ is the solenoid valve in the CRD H_2O sample manifold

Idx is index for the location and equal to 01, 02, 03,…. n

n is the site-specific highest measurement level and can be vary from 04 to 08.

14.3.6 QA/QC Procedure

NA

14.4 Uncertainty

NA

15 VALIDATION TYPE SEPARATION

15.1 Data Product Description

This section describes the processes to distinguish the validation/calibration type of the data measured by LI-COR LI-840A (*hereafter* referred to as IRGA), isotopic CO_2 analyzer (Picarro G2131-i, *hereafter* referred to as CRD CO_2), and isotopic H_2O analyzer (Picarro L2130-i, hereafter referred to CRD H_2O) based on the status of solenoids in validation manifold under the DGD: CD06640001 and the status of vaporizer 3-way valve under the DGD: CA10210000. The validation manifold and the vaporizer 3-way valve referred to as valvValiStor and crdH2oValvVali, respectively.

15.1.1 Variables Reported

The valvValiStor and crdH2oValvVali L0p reported variables provided by the algorithms documented in this ATBD are displayed in Table 15-1.

Table 15-1: List of valvValiStor and crdH2oValvVali L0p reported variables that produced in this ATBD.

L0p DP	L0p fieldName	L0p DP Frequency (Hz)	Units	Input L0 DPs or L0p DP fieldNames
valvValiStor (DGD CD06640001)				

L0p DP	L0p fieldName	L0p DP Frequency (Hz)	Units	Input L0 DPs or L0p DP fieldNames
Status of validation valve for low CO_2	valv02	1	NA	NEON.DOM.SITE.DP0.00113.001.02361.703.000.000
Status of validation valve for intermediate CO_2	valv03	1	NA	NEON.DOM.SITE.DP0.00113.001.02362.703.000.000
Status of validation valve for high CO_2	valv04	1	NA	NEON.DOM.SITE.DP0.00113.001.02364.703.000.000
Status of validation valve for archive CO_2	valv05	1	NA	NEON.DOM.SITE.DP0.00113.001.02365.703.000.000
Status validation valve for zero air	valv06	1	NA	NEON.DOM.SITE.DP0.00113.001.02366.703.000.000
Status validation valve for CRD H_2O shutdown	valv07	1	NA	NEON.DOM.SITE.DP0.00113.001.02367.703.000.000
Status of validation valve for CRD H_2O validation	valv08	1	NA	NEON.DOM.SITE.DP0.00113.001.02368.703.000.000
Validation gas type	typeGas	1	NA	valv02* valv03* valv04* valv05* valv06*
Validation gas type for crdH2o	typeGasCrdH2o			valv07* valv08*
crdH2oValvVali (DGD CA10210000)				
Status of vaporizer 3-way Valve	valv	1	NA	NEON.DOM.SITE.DP0.00115.001.02352.700.000.000
Validation injection number	injNum	1	NA	valv*
Validation H2O type	typeH2o	1	NA	valInj*

*L0p DP is used as an input to generate other L0p DPs.

15.1.2 Input Dependencies

Table 15-2 details valvValiStor and crdH2oValvVali L0 DPs and specifies which L0 DPs will be used to produce L0p reported variables in this ATBD.

Table 15-2: List of valvValiStor and crdH2oValvVali L0 DPs.

L0 DP	L0 DP fieldName	Sample Frequency	Units	Data Product Number	DPs that are used to produce L0p (Y/N)
valvValiStor (DGD CD06640001)					
Status of validation valve for low CO_2	valvCmd2	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02361.703.000.000	Y
Status of validation valve for intermediate CO_2	valvCmd3	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02362.703.000.000	Y
Status of validation valve for high CO_2	valvCmd4	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02364.703.000.000	Y
Status of validation valve for archive CO_2	valvCmd5	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02365.703.000.000	Y
Status validation valve for zero air	valvCmd6	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02366.703.000.000	Y
*Status validation valve for CRD H_2O shutdown	valvCmd7	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02367.703.000.000	Y
*Status of validation valve for CRD H_2O validation	valvCmd8	0.2	NA	NEON.DOM.SITE.DP0.00113.001.02368.703.000.000	Y
crdH2oValvVali (DGD CA10210000)					
*Status of vaporizer 3-way valve	valvStat1	varies, only occur when status changes	NA	NEON.DOM.SITE.DP0.00115.001.02352.700.000.000	Y

*Note that these status L0 DPs are only defined for those sites that have a CRD H_2O installed.

15.1.3 Product Instances

The validation manifold and vaporizer 3-way valve are located in the instrument hut. All sites across the NEON observatory have the validation manifolds and 21 sites (20 NEON core sites and 1 relocatable site at D18 Barrow) have the vaporizer 3-way valve. The relationships between the individual instances of validation manifold and 3-way valve to L0p data outputs are summarized in Table 15-1.

15.1.4 Temporal Resolution and Extent

The temporal resolution of the reported variables in Table 15-1 is 1 Hz.

15.1.5 Spatial Resolution and Extent

Both the validation manifold and the vaporizer 3-way valve are located within the tower hut infrastructure. However, the measurements reflect the points in flow path where they are located in the tower hut infrastructure. The validation manifold and its associated valves are located between the validation gas cylinders and the mass flow controller for field validation gases, while the vaporizer 3-way valve are located between CRD H_2O sample manifold and T split between gas valve for CRD H_2O shutdown and gas valve for CRD H_2O validation.

15.2 Scientific context

The validation gas manifold and its associated valves control the validation gas standards delivered to the IRGA and CRD CO_2 for field validation. The routine validation will be performed every 23 hours. However, to minimize the interference between both analyzers, the routine validation of these two analyzers is scheduled to not occur at the same time. The validation gas sequence for the IRGA routine validation shall be as follows; zero air and then the three validation gases from lowest to highest concentration. The sequence of validation gas for the CRD CO_2 routine validation is similar to IRGA but without zero air. In addition to the routine validation, both analyzers are scheduled to validate against the archive CO_2 on a monthly basis.

To minimize the IRGA drift, the field calibration is scheduled to repeat every 6 days. However, the IRGA analyzer drifts after the IRGA's sample cell experiences large pressure fluctuation (≥ 1.2 kPa). Therefore IRGA field calibration also occurs after the analyzer resumes measurements after interruptions (e.g., power failure, periodical instrument shut down for maintenance, etc.) and large pressure perturbations. The gas sequence for the IRGA field calibration includes only zero air and high CO_2 concentration gas.

15.2.1 Theory of Measurement

The validation gas manifold consists of 6 inlet ports and one outlet port. The first inlet port is idle. The second to sixth ports are equipped with validation gas select valves to intake validation gases. Moreover, there are two additional L0 DPs for the gas valve for CRD H_2O shutdown and gas valve for CRD H_2O validation also bundled into this validation gas manifold (DGD CD06640001). The gas valve for CRD H_2O validation will be opened to allow the zero air to flow to the vaporizer and CRD H_2O analyzer during field validation. While the gas valve for CRD H_2O shutdown will be only opened before the CRD H_2O is shut down to allow the zero air to flush out water.

During the routine field validation of the CRD H_2O, the analyzer will cease to measure the atmospheric vapor from the tower profiles and measure water standards by using the zero air as a carrier gas. The vaporizer 3-way valve is controlled to switch between the air sample and validation sample. Water standards are injected through the vaporizer (A0211 Liquid Sample High Precision Vaporizer: NEON P/N: 0300280001) using the autosampler (A0325 Auto Sampler: NEON P/N 0328050001) and a syringe. Field validation is performed for 3 standards (NEON Tertiary Low, Mid, and High standard) and each standard is injected 6 times. The procedure typically takes around 9 minutes per injection.

When the instrument is set up at field initially or after the water tray is changed periodically, field tech need inject some liquid water to vaporizer to train the instrument before proper operation. The raw data in the training period appear like the ones in validation period. The water used for training is typically local distilled water. All injections during training period should have similar $\delta^{18}O$ and δ^2H values. However, three different water reference standards are used for validation. The $\delta^{18}O$ and δ^2H values during validation period will vary greatly. The absolute difference between the max and min δ^2H values at the training period should be < 160 permil, while the absolute difference between the max and min δ^2H values at the validation period should be >200 permil. There will be a ~2 min or more break between training period and validation period. CI codes should be capable of distinguish these two types activities.

15.2.2 Theory of Algorithm

NA

15.3 Algorithm Implementation

L0p signal processing consists of the following sequence:

7. Select L0 data streams as indicated as "Y" in Table 15-2 for further data processing.
8. Generate L0p DPs from L0 DPs by converting to 1 Hz frequency using a time regularization approach in accordance with AD[04], details are provided in section 15.3.1.
9. Replace the NaN in L0p DPs, details are provided in section 15.3.2.
10. Determine validation/calibration gas type (typeGas) according to Eq. (15.2).
11. Determine validation gas type for crdH2o (typeGasCrdH2o) according to Eq. (15.3).
12. Replace gas type by "training" during the training period when the absolute difference between the max and min δ^2H values (NEON.DOM.SITE.DP0.00103.001.02370.700.000.000) at the training period/validation period is < 160 permil.
13. For sites that have a CRD H_2O, determine validation injection number according to Eq. (15.4) and then the validation H_2O type can be determined according to Eq. **(**15.5).
14. The training and validation activities could span two days, either the day before the target processing day and the target day, or the target day and the day after target day. It is suggested

select 12 hours before target day, plus target day, plus 12 hours after target day for above data processing steps.

15.3.1 Time regularization

The L0 DPs of the validation gas manifold were recorded at 0.2 Hz or every 5 seconds, while the vaporizer 3-way valve L0 DPs L0 is only available when the valve state changes (open or close). To generate L0p DPs from L0 DPs by converting to 1 Hz frequency, missing timestamps and the corresponding data values are inserted following the procedures detailed in AD[04]. Here we use the default options in AD[04] with a windowing approach described by Eq. 3 in AD[04] In case multiple data values fall within a single window, the vaporizer 3-way valve should use the first one and last one in the window, while other valves will use the last value in the window (option 3 in AD[04]).

15.3.2 Replacing NaN values

After time regularization, the missing L0p values of the validation gas manifold will be filled with NaN. To be able to continue data processing, the L0p which equal to NaN are replaced by the following:

$$\mathrm{L0p} = \begin{cases} \text{previous L0p value if continuous sequence of NaN} \\ \qquad \le 6\text{s duration} \\ -1 \text{ if continuous sequence of NaN} > 6\text{s duration} \end{cases} \tag{15.1}$$

where L0p is valvIdx in the validation manifold

Idx is index for the valve location and equal to 02, 03, 04,…. 08

As mentioned above that the vaporizer 3-way valve L0 DPs is only available when the valve state changes (open or close), therefore, it is impossible to distinguish between NaN's that resulted from time regularization and NaN's that resulted from true missing values. In this case, all of NaN in vaporizer 3-way valve L0p will be filled with previous value.

15.3.3 Validation/calibration gas type

The validation/calibration type can be determined as:

$$\begin{cases} \text{co2Low if only valv02} = 1 \\ \text{co2Med if only valv03} = 1 \end{cases}$$

$$\text{typeGas} = \begin{cases} \text{co2High if only valv04} = 1 \\ \text{co2Arch if only valv05} = 1 \\ \text{co2Zero if only valv06} = 1 \\ \text{samp if all valvIdx} = 0 \\ \text{negl if more than one valvIdx} = 1 \\ -1 \text{ any valvIdx} = -1 \end{cases} \qquad (15.2)$$

where: valvIdx is the solenoid valve in the validation manifold

Idx is index for the valve and equal to 02, 03, 04, 05, and 06

15.3.4 Validation gas type for crdH2o

The validation gas type for crdH2o can be determined as:

$$\text{typeGasCrdH2o} = \begin{cases} \text{h2oZeroOff if only valv07} = 1 \\ \text{h2oZeroVali if only valv08} = 1 \\ \text{samp if valv07} = 0 \text{ and valv08} = 0 \\ \text{negl if valv07} = 1 \text{ and valv08} = 1 \\ -1 \text{ valv07} = -1 \text{ and/or valv08} = -1 \end{cases} \qquad (15.3)$$

where: valv07 and valv08 are the solenoid valve number 7 and 8 in the validation manifold

15.3.5 Validation injection number

During the sampling mode of CRD H_2O, the vaporizer 3-way valve will be closed (valvStat1 = '0') and it will be opened (valvStat1 = '1') during the field validation mode. As mentioned in section 15.2.1 that each field validation cycle will be performed using 3 standards and each standard will be injected for 6 times, therefore, the validation injection number will be run from 01 to 18. Note that each injection will last for

~9 minutes. Once it done, the vaporizer 3-way valve always switches back to '0' for less than 5 seconds before starting a new injection. The validation injection number can be determined as:

$$\text{injNum} = \begin{cases} i \ \text{ for injStart}_i \leq \text{time} \leq \text{injEnd}_i \text{ if valv} = 1 \\ 00 \text{ if valv } = 0 \\ -1 \text{ if valv } = -1 \end{cases} \tag{15.4}$$

where: i is 01, 02, 03, …, 18

time is corresponding timestamps

injStart_i is the time when injection i begins and can be determined as the initial timestamp that $\text{valv } = 1$

injEnd_i is the time when injection i ends and can be determined as the initial timestamp that $\text{valv } = 0$.

15.3.6 Validation H_2O type

The validation H_2O type can be determined as:

$$\text{typeH2o} = \begin{cases} \text{h2oHigh if injNum } = \text{ 01 to 06} \\ \text{h2oMed if injNum } = \text{ 07 to 12} \\ \text{h2oLow if injNum } = \text{ 13 to 18} \\ \text{samp if injNum} = 00 > 6\text{s} \\ \text{vali if injNum} = 00 \leq 6\text{s} \\ \text{negl if injNum} = -1 \end{cases} \tag{15.5}$$

15.3.7 QA/QC Procedure

NA

15.4 Uncertainty

NA

16 IRGA MEASUREMENT TYPE SEPARATION

16.1 Data Product Description

This chapter describes the processes to distinguish between validation and calibration mode of the data measured by IRGA.

16.1.1 Variables Reported

The IRGA measurement type-related L0p reported variables provided by the algorithms documented in this ATBD are displayed in Table 16-1.

Table 16-1: List of measurement type-related L0p reported variables that produced in this ATBD.

L0p DP	L0p fieldName	L0p DP Frequency (Hz)	Units	Input L0 DPs or L0p DP fieldNames
IRGA measurement type	measTypeIrga	1	NA	measTypeIrga typeGas

16.1.2 Input Dependencies

Table 16-2 details input L0p DPs used to produce L0p reported variables in this ATBD.

Table 16-2: List of input L0p DPs that are transformed into reported L0p in this ATBD.

L0p DP	L0p DP fieldName	Sample Frequency	Units	DPs that are used to produce L0p (Y/N)
IRGA Measurement Type (Chapter 13)				
IRGA measurement type	measTypeIrga	1	NA	Y
Validation/Calibration Gas Type (Chapter 15)				
Validation gas type	typeGas	1	NA	Y

16.1.3 Product Instances

All sites across the NEON observatory own a sensor production the L0p reported variables defined in Table 16-1.

16.1.4 Temporal Resolution and Extent

The temporal extent of the reported variables in Table 16-1 is 1 Hz.

16.1.5 Spatial Resolution and Extent

Spatial resolution and extent of L0p reported variables defined in Table 16-1 can be found in section 13.1.5 and 15.1.5.

16.2 Scientific context

16.2.1 Theory of Measurement

Section 13 details how to distinguish the measurement type for all 3 analyzers into a sampling mode and validation mode. However, the measurement type of IRGA needs a further step to differentiate between validation and calibration mode. As mentioned in section 15, the field calibration of IRGA occurs every 6 days and every time after the analyzer resumes from the interruptions to minimize the IRGA drift. The gas sequence for the IRGA field calibration is different from the routine field validation since it uses only zero air and high CO_2 concentration. In this section we describe how to differentiate that calibration period.

16.2.2 Theory of Algorithm

NA

16.3 Algorithm Implementation

Determine the measurement type for IRGA according to Eq. (**16.1**).

16.3.1 IRGA measurement type

We need to determine whether the IRGA is in a calibration or validation time period by analyzing the typeGas values. The switch in sequential values from co2Zero to co2High only occurs during the calibration period and can be used to identify this process. The measTypeIrga is set to a value of cal for the time period from the first typeGas co2zero value in the continuous time series of typeGas co2Zero values prior to the co2Zero – co2High switch, to the last typeGas co2High values in the continuous time series of typeGas co2High values after the co2Zero-co2High switch. See Eq. (**16.1**) and example table below.

The measurement type specific for IRGA measurements can be determined as:

$$\text{measTypeIrga} = \begin{cases} \text{samp if measTypeIrga} = \text{samp} \\ \text{cal if measTypeIrga} = \text{vali} \\ \quad \text{\& order of valGas is co2Zero, followed by co2High} \\ \text{vali, otherwise} \end{cases} \tag{16.1}$$

Table 16-3:Example of input and output for IRGA measurement type.

Input measTypeIrga	Input typeGas	Output measTypeIrga
samp	samp	samp
⋮	⋮	⋮
samp	samp	samp
vali	co2Zero	cal
vali	co2Zero	cal
vali	co2Zero	cal
vali	co2Zero	cal
vali	co2Zero	cal
vali	co2High	cal
vali	co2High	cal
vali	co2High	cal
vali	co2High	cal
vali	co2High	cal
samp	samp	samp
⋮	⋮	⋮
samp	samp	samp
vali	co2Zero	vali
vali	co2Zero	vali
vali	co2Zero	vali
vali	co2Zero	vali
vali	co2Low	vali
vali	co2Low	vali
vali	co2Low	vali
vali	co2Low	vali
vali	co2Low	vali

vali	co2Med	vali
vali	co2Med	vali
vali	co2Med	vali
vali	co2Med	vali
vali	co2Med	vali
vali	co2High	vali
vali	co2High	vali
vali	co2High	vali
vali	co2High	vali
vali	co2High	vali
samp	samp	samp
⋮	⋮	⋮
samp	samp	samp
vali	co2Zero	cal
vali	co2Zero	cal
vali	co2Zero	cal
vali	co2Zero	cal
vali	co2Zero	cal
vali	co2High	cal
vali	co2High	cal
vali	co2High	cal
vali	co2High	cal
vali	co2High	cal
vali	co2Zero	vali
vali	co2Zero	vali
vali	co2Zero	vali
vali	co2Zero	vali
vali	co2Low	vali
vali	co2Low	vali
vali	co2Low	vali
vali	co2Low	vali
vali	co2Low	vali
vali	co2Med	vali
vali	co2Med	vali
vali	co2Med	vali
vali	co2Med	vali
vali	co2Med	vali
vali	co2High	vali
vali	co2High	vali
vali	co2High	vali
vali	co2High	vali
vali	co2High	vali

samp	samp	samp
⋮	⋮	⋮
samp	samp	samp

16.3.2 QA/QC Procedure

NA

16.4 Uncertainty

NA

17 GAS CYLINDER CONCENTRATIONS

17.1 Data Product Description

This section describes the processes to convert L0 DPs under DGD 0353710000 into 1 Hz L0p DPs. The gas cylinder concentrations referred to as gasRefe in reference to DPs.

Four CO_2 gas standards (low, med, high, archive) will be used to perform field validation/calibration on IRGA and CRD CO_2. There are two cylinders of zero air. One will be used as a carrier gas during CRD H_2O validation and used to dry CRD H_2O cavity prior to shut down. Another one is used for IRGA field calibration and validation, and used to dry CRD CO_2 cavity prior to shut down. The concentration of each CO_2 cylinder will be certified by NEON CVAL. The concentrations of the four CO_2 gas standards will be provided by CVAL and will be ingested by CI as L0p data. But the zero air cylinders will be purchased locally with no certification info for L0p data products.

17.1.1 Variables Reported

The gasRefe-related L0p reported variables provided by the algorithms documented in this ATBD are displayed in Table 17-1. Because the L0p outputs for each cylinder will live in different tables of HDF5 file, it is ok to use generic term of “rtioMoleDryCo2Refe”, “dlta13CCo2Refe”, “rtioMoleDry12CCo2Refe”, “rtioMoleDry13CCo2Refe” for CO_2 gas cylinder L0p outputs.

Table 17-1: List of gasRefe-related L0p reported variables that produced in this ATBD.

L0p DP	L0p fieldName	L0p DP Frequency	Units	Input L0 DPs
CO2 Gas Standard Archive				
Dry mole fraction of CO2 (Archive)	rtioMoleDryCo2Refe	1 Hz	mol mol-1	NEON.DOM.SITE.DP0.00118.001.02191.710.000.000

L0p DP	L0p fieldName	L0p DP Frequency	Units	Input L0 DPs
ratio of 13C:12C in CO2 (Archive)	dlta13CCo2Refe	1 Hz	‰	NEON.DOM.SITE.DP0.00118.001.02324.710.000.000
Dry molar fraction of 12CO2 (Archive)	rtioMoleDry12CCo2Refe	1 Hz	mol mol-1	NEON.DOM.SITE.DP0.00118.001.02318.710.000.000
Dry molar fraction of 13CO2 (Archive)	rtioMoleDry13CCo2Refe	1 Hz	mol mol-1	NEON.DOM.SITE.DP0.00118.001.02320.710.000.000
CO2 Gas Standard Low				
Dry mole fraction of CO2 (Low)	rtioMoleDryCo2Refe	1 Hz	mol mol-1	NEON.DOM.SITE.DP0.00118.001.02191.712.000.000
ratio of 13C:12C in CO2 (Low)	dlta13CCo2Refe	1 Hz	‰	NEON.DOM.SITE.DP0.00118.001.02324.712.000.000
Dry molar fraction of 12CO2 (Low)	rtioMoleDry12CCo2Refe	1 Hz	mol mol-1	NEON.DOM.SITE.DP0.00118.001.02318.712.000.000
Dry molar fraction of 13CO2 (Low)	rtioMoleDry13CCo2Refe	1 Hz	mol mol-1	NEON.DOM.SITE.DP0.00118.001.02320.712.000.000
CO2 Gas Standard Medium				
Dry mole fraction of CO2 (Medium)	rtioMoleDryCo2Refe	1 Hz	mol mol-1	NEON.DOM.SITE.DP0.00118.001.02191.713.000.000
ratio of 13C:12C in CO2 (Medium)	delta13CCo2Refe	1 Hz	‰	NEON.DOM.SITE.DP0.00118.001.02324.713.000.000
Dry molar fraction of 12CO2 (Medium)	rtioMoleDry12CCo2Refe	1 Hz	mol mol-1	NEON.DOM.SITE.DP0.00118.001.02318.713.000.000
Dry molar fraction of 13CO2 (Medium)	rtioMoleDry13CCo2Refe	1 Hz	mol mol-1	NEON.DOM.SITE.DP0.00118.001.02320.713.000.000
CO2 Gas Standard High				
Dry mole fraction of CO2 (High)	rtioMoleDryCo2Refe	1 Hz	mol mol-1	NEON.DOM.SITE.DP0.00118.001.02191.714.000.000
ratio of 13C:12C in CO2 (High)	delta13CCo2Refe	1 Hz	‰	NEON.DOM.SITE.DP0.00118.001.02324.714.000.000
Dry molar fraction of 12CO2 (High)	rtioMoleDry12CCo2Refe	1 Hz	mol mol-1	NEON.DOM.SITE.DP0.00118.001.02318.714.000.000
Dry molar fraction of 13CO2 (High)	rtioMoleDry13CCo2Refe	1 Hz	mol mol-1	NEON.DOM.SITE.DP0.00118.001.02320.714.000.000

*: These are L0p DPs. They are used as inputs to generate other L0p DPs.

17.1.2 Input Dependencies

Table 17-2 details gasRefe-related L0 DPs used to produce L0p reported variables in this ATBD.

Table 17-2: List of gasRefe-related L0 DPs that are transformed into L0p reported variables in this ATBD.

L0 DP	L0 DP fieldName	Sample Frequency *	Units	Data Product Number	CVAL coefficients	DPs that are used to produce L0p (Y/N)
	CO2 Gas Standard Archive					
Dry mole fraction of CO2 (Archive)	fdMoleCO2	NA	umol mol-1	NEON.DOM.SITE.DP0.00118.001.02191.710.000.000	CVALC0	Y
ratio of 13C:12C in CO2 (Archive)	d13CO2	NA	‰	NEON.DOM.SITE.DP0.00118.001.02324.710.000.000	CVALD0	Y
Dry molar fraction of 12CO2 (Archive)	fdMole12CO2	NA	umol mol-1	NEON.DOM.SITE.DP0.00118.001.02318.710.000.000	CVALA0	Y
Dry molar fraction of 13CO2 (Archive)	fdMole13CO2	NA	umol mol-1	NEON.DOM.SITE.DP0.00118.001.02320.710.000.000	CVALB0	Y
	CO2 Gas Standard Low					
Dry mole fraction of CO2 (Low)	fdMoleCO2	NA	umol mol-1	NEON.DOM.SITE.DP0.00118.001.02191.712.000.000	CVALC0	Y
ratio of 13C:12C in CO2 (Low)	d13CO2	NA	‰	NEON.DOM.SITE.DP0.00118.001.02324.712.000.000	CVALD0	Y
Dry molar fraction of 12CO2 (Low)	fdMole12CO2	NA	umol mol-1	NEON.DOM.SITE.DP0.00118.001.02318.712.000.000	CVALA0	Y
Dry molar fraction of 13CO2 (Low)	fdMole13CO2	NA	umol mol-1	NEON.DOM.SITE.DP0.00118.001.02320.712.000.000	CVALB0	Y
	CO2 Gas Standard Medium					
Dry mole fraction of CO2 (Medium)	fdMoleCO2	NA	umol mol-1	NEON.DOM.SITE.DP0.00118.001.02191.713.000.000	CVALC0	Y
ratio of 13C:12C in CO2 (Medium)	d13CO2	NA	‰	NEON.DOM.SITE.DP0.00118.001.02324.713.000.000	CVALD0	Y
Dry molar fraction of 12CO2 (Medium)	fdMole12CO2	NA	umol mol-1	NEON.DOM.SITE.DP0.00118.001.02318.713.000.000	CVALA0	Y
Dry molar fraction of 13CO2 (Medium)	fdMole13CO2	NA	umol mol-1	NEON.DOM.SITE.DP0.00118.001.02320.713.000.000	CVALB0	Y
	CO2 Gas Standard High					
Dry mole fraction of CO2 (High)	fdMoleCO2	NA	umol mol-1	NEON.DOM.SITE.DP0.00118.001.02191.714.000.000	CVALC0	Y
ratio of 13C:12C in CO2 (High)	d13CO2	NA	‰	NEON.DOM.SITE.DP0.00118.001.02324.714.000.000	CVALD0	Y
Dry molar fraction of 12CO2 (High)	fdMole12CO2	NA	umol mol-1	NEON.DOM.SITE.DP0.00118.001.02318.714.000.000	CVALA0	Y
Dry molar fraction of 13CO2 (High)	fdMole13CO2	NA	umol mol-1	NEON.DOM.SITE.DP0.00118.001.02320.714.000.000	CVALB0	Y

*: L0 DP sample frequency is not applicable here. These L0 DPs are just dummy data. See section 17.3.1 for more info.

17.1.3 Product Instances

Each of the 47 sites across the NEON observatory will have 4 CO_2 gas standard cylinders for ECSE sensor field validation/calibration. Individual instance of all gas cylinder related L0p data outputs are in Table 17-1. Each instance will generate 4 L0p data products.

17.1.4 Temporal Resolution and Extent

The temporal extent of the reported L0p variables in Table 17-1 is 1 Hz.

17.1.5 Spatial Resolution and Extent

The gas cylinders will be located within the gas room of the instrument hut side by side.

17.2 Scientific context

NA

17.2.1 Theory of Measurement

NA

17.2.2 Theory of Algorithm

NA

17.3 Algorithm Implementation

Data flow for signal processing of L0p DPs will be treated in the following order.

1. Select L0 DPs and CVAL coefficients in Table 17-2 from database, and parse the coefficients to the associated L0 DPs for further data processing. When extract the calibration coefficients, CI should use the latest calibration coefficients if no new calibration coefficients set is available, even after the valid date range is already expired.
2. Convert L0 DPs to generate 1 Hz L0p DPs using a time regularization approach in accordance with AD[04], details are provided in section 17.3.1.
3. Perform unit conversion. Details are provided in section 17.3.2
4. Perform calibration test, but no other QA/QC Plausibility tests are needed. When perform the Invalid Calibration test, CI should use the latest calibration coefficients for the test if no new calibration coefficients set is available, even after the valid date range is already expired.

17.3.1 Time regularization

L0 in Table 17-2 are just dummy data. CO_2 concentrations and associated uncertainties for each gas cylinder will be provided by CVAL as coefficients in database. CI will be responsible to process these concentration coefficient values (see Table 17-2) into 1 Hz L0p DPs. The uncertainty values should be processed as attributes of hdf5 file as shown in golden hdf5 file example provided by science team. The specific ingest and conversion method wills be detailed by CI.

17.3.2 Unit conversion

The calibration coefficients from CVAL have different units than the required L0p units. We need to convert some of them to eddy covariance standard units. See below:

$$\mathrm{rtioMoleDryCo2Refe(mol\ mol-1\ )} = \frac{\mathrm{fdMoleCo2\ (\mu mol\ mol-1\ )}}{1000000} \tag{17.1}$$

$$\mathrm{rtioMoleDry12CCo2Refe(mol\ mol-1\ )} = \frac{\mathrm{fdMole12Co2\ (\mu mol\ mol-1\ )}}{1000000} \tag{17.2}$$

$$\mathrm{rtioMoleDry13CCo2Refe(mol\ mol-1\ )} = \frac{\mathrm{fdMole13Co2\ (\mu mol\ mol-1\ )}}{1000000} \tag{17.3}$$

17.3.3 QA/QC Procedure

It is no need to perform standard plausibility tests on all data streams, except for calibration test, which indicates the CVAL certification date for the gas cylinders has been expired.

Table 17-3: Plausibility quality flags to be applied to all L0p DPs (except for L0p DPs that are quality flags)

Flag	Term modifier	Description
QF_{Cal}	qfCal	Quality flag for the Invalid Calibration test

17.4 Uncertainty

The uncertainties provided by CVAL along with the CVAL coefficients in Table 17-2 can be mapped to the following metadata terms in the HDF5 file attributes:

Table 17-4: Mapping between CVAL uncertainty terms and HDF5 metadata terms.

HDF5 metadata terms	CVAL uncertainties
sd	U_CVALA2
dfUcrtRaw	U_CVALD1
ucrtRaw	U_CVALA1
ucrtAve	U_CVALA3
dfUcrtAve	U_CVALD3
dfSd	U_CVALD2

18 REFERENCE WATER STANDARDS

18.1 Data Product Description

This section describes the processes to convert L0 DPs under DGD 0361660000 into 1 Hz L0p DPs. The reference water standards referred to as h2oRefe in reference to DPs.

Asset 0361660000 is a tray that holds 12-vial of liquid reference water standards (include equal number of low, medium and high standard) for routine field validation of CRD H_2O, which can provide supplies for 4 weeks.

18.1.1 Variables Reported

The isotopic values of $\delta^{18}O$ and δ^2H for each type of reference water standard (low, medium, or high) will be certified by CVAL and provided to CI on xml files. CI will ingest these values as L0 DPs (Table 18-2) and then further convert them to L0p DPs (Table 18-1).

The h2oRefe-related L0p reported variables provided by the algorithms documented in this ATBD are displayed in Table 18-1. Because the L0p outputs for all water standards will live in a same data table of HDF5 file, it is not ok to use generic term of "dlta2HH2oLow", "dlta18OH2oLow" for water standard L0p outputs. The indication of "Low", "Med", and "High" should stay in the L0p fieldnames for water standards.

Table 18-1: List of h2oRefe-related L0p reported variables that produced in this ATBD.

L0p DP	L0p fieldName	L0p DP Frequency	Units	Input L0 DPs
δ^2H in water standard Low	dlta2HH2oRefeLow	1 Hz	‰	NEON.DOM.SITE.DP0.00120.001.02850.700.000.000
$\delta^{18}O$ in water standard Low	dlta18OH2oRefeLow	1 Hz	‰	NEON.DOM.SITE.DP0.00120.001.02851.700.000.000
δ^2H in water standard Med	dlta2HH2oRefeMed	1 Hz	‰	NEON.DOM.SITE.DP0.00120.001.02852.700.000.000
$\delta^{18}O$ in water standard Med	dlta18OH2oRefeMed	1 Hz	‰	NEON.DOM.SITE.DP0.00120.001.02853.700.000.000

L0p DP	L0p fieldName	L0p DP Frequency	Units	Input L0 DPs
δ^2H in water standard High	dlta2HH2oRefeHigh	1 Hz	‰	NEON.DOM.SITE.DP0.00120.001.02854.700.000.000
$\delta^{18}O$ in water standard High	dlta18OH2oRefeHigh	1 Hz	‰	NEON.DOM.SITE.DP0.00120.001.02855.700.000.000

*: These are L0p DPs. They are used as inputs to generate other L0p DPs.

18.1.2 Input Dependencies

Table 18-2 details h2oRefe-related L0 DPs used to produce L0p reported variables in this ATBD.

Table 18-2: List of h2oRefe-related L0 DPs that are transformed into L0p reported variables in this ATBD.

L0 DP	L0 DP fieldName	Sample Frequency*	Units	Data Product Number	CVAL coefficients	DPs that are used to produce L0p (Y/N)
δ^2H in water standard Low	d2HWaterLow	NA	‰	NEON.DOM.SITE.DP0.00120.001.02850.700.000.000	CVALA1	Y
$\delta^{18}O$ in water standard Low	d18OWaterLow	NA	‰	NEON.DOM.SITE.DP0.00120.001.02851.700.000.000	CVALB1	Y
δ^2H in water standard Med	d2HWaterMed	NA	‰	NEON.DOM.SITE.DP0.00120.001.02852.700.000.000	CVALA2	Y
$\delta^{18}O$ in water standard Med	d18OWaterMed	NA	‰	NEON.DOM.SITE.DP0.00120.001.02853.700.000.000	CVALB2	Y
δ^2H in water standard High	d2HWaterHigh	NA	‰	NEON.DOM.SITE.DP0.00120.001.02854.700.000.000	CVALA3	Y
$\delta^{18}O$ in water standard High	d18OWaterHigh	NA	‰	NEON.DOM.SITE.DP0.00120.001.02855.700.000.000	CVALB3	Y

*: L0 DP sample frequency is not applicable here. These L0 DPs are just dummy data. See section 18.3.1 for more info.

18.1.3 Product Instances

Each of the 20 TIS core sites across the NEON observatory plus one relocatable site (D18 Barrow) will have a 12-vial tray for CRD H_2O field validation. Individual instance of all 12-vial tray related L0p data outputs are in Table 18-1. Each instance will generate 6 L0p data products.

18.1.4 Temporal Resolution and Extent

The temporal extent of the reported L0p variables in Table 18-1 is 1 Hz.

18.1.5 Spatial Resolution and Extent

The 12-vial tray for reference water standards will be located within the instrument room of the instrument hut on CRD instrument rack.

18.2 Scientific context

NA

18.2.1 Theory of Measurement

NA

18.2.2 Theory of Algorithm

NA

18.3 Algorithm Implementation

Data flow for signal processing of L0p DPs will be treated in the following order.

1. Select L0 DPs and CVAL coefficients in Table 18-2 from database, and parse the coefficients to the associated L0 DPs for further data processing. When extract the calibration coefficients, CI should use the latest calibration coefficients if no new calibration coefficients set is available, even after the valid date range is already expired.
2. Convert L0 DPs to generate 1 Hz L0p DPs using a time regularization approach in accordance with AD[04], details are provided in section 18.3.1.
3. Perform calibration test, but no other QA/QC Plausibility tests are needed. When perform the Invalid Calibration test, CI should use the latest calibration coefficients for the test if no new calibration coefficients set is available, even after the valid date range is already expired.

18.3.1 Time regularization

L0 in Table 18-2 are just dummy data. The isotopic values of $\delta^{18}O$ and $\delta^{2}H$ and associated uncertainties for each type of reference water standard (low, medium or high) will be provided by CVAL as coefficients in database. CI will be responsible to process these concentration coefficient values (see Table 18-2) into 1 Hz L0p DPs. The uncertainty values should be processed as attributes of hdf5 file as shown in golden hdf5 file example provided by science team. The specific conversion method will be detailed by CI.

18.3.2 QA/QC Procedure

It is no need to perform standard plausibility tests on all data streams, except for calibration test, which indicates the CVAL certification date for the water standards has been expired.

Table 18-3: Plausibility quality flags to be applied to all L0p DPs (except for L0p DPs that are quality flags)

Flag	Term modifier	Description
QF_{Cal}	qfCal	Quality flag for the Invalid Calibration test

18.4 Uncertainty

The uncertainties provided by CVAL along with the CVAL coefficients in Table 18-2 can be mapped to the following metadata terms in the HDF5 file attributes:

Table 18-4: Mapping between CVAL uncertainty terms and HDF5 metadata terms.

HDF5 metadata terms	CVAL uncertainties
sd	U_CVALA2
dfUcrtRaw	U_CVALD1
ucrtRaw	U_CVALA1
ucrtAve	U_CVALA3
dfUcrtAve	U_CVALD3
dfSd	U_CVALD2

19 HDF5 FILES GENERATION

This section describes the processes to organize L0p data which are going to use to generate the HDF5 files.

19.1 Data Product Description

19.1.1 Variables Reported

L0p preprocessed data are provided in the HDF5 files format.

19.1.2 Input Dependencies

L0p DPs used to produce L0p reported variables in this ATBD can be found in Table 3-1 to Table 18-1.

19.1.3 Product Instances

All sites across the NEON observatory own the HDF5 files. The files will be generated with a file name describing the subsystem, 4-letter site code, and the date (ex. ECSE_SERC_20160621.h5).

19.1.4 Temporal Resolution and Extent

The HDF5 files are generated for each 24 hour period. The temporal extent of the L0p preprocessed data in the HDF5 files is 1 Hz.

19.1.5 Spatial Resolution and Extent

NA

19.2 Scientific context

19.2.1 Theory of Measurement

NA

19.2.2 Theory of Algorithm

Hierarchical Data Format (HDF), currently distributed as HDF5, provides a file format with high compressibility, fast efficient reading and writing capabilities, directory-style files, and metadata attachment. The HDF5 file formats allow us to package various data sets into a single file with built-in structure for managing both data and metadata. The current NEON processing design utilizing the Eddy4r package within a Docker framework utilizes HDF5 files for input/output operations. The NEON HDF5 file structure was developed following the data product naming convention provided in AD[08], where portions of the naming convention as described below were selected to develop the hierarchical structure of the HDF5 file (Figure 4):

NEON.DOM.SITE.DPL.PRNUM.REV.TERMS.HOR.VER.TMI

WHERE:

NEON=NEON

DOM=DOMAIN, e.g. D10

SITE=SITE, e.g. STER

DPL=DATA PRODUCT LEVEL, e.g. DP1

PRNUM = PRODUCT NUMBER =>5 digit number. Set in data products catalog.

TIS = 00000-09999

REV = REVISION, e.g. 001.

TERMS=From NEON's controlled list of terms. Index is unique across products.

HOR = HORIZONTAL INDEX. Semi-controlled; AIS and TIS use different rules.

Examples: Tower=000, DFIR=900.

VER = VERTICAL INDEX. Semi-controlled; AIS and TIS use different rules.

Examples: Ground level=000, second tower level=020.

TMI=TEMPORAL INDEX. Examples: 001=1 minute, 030=30 minute, 999=irregular intervals.

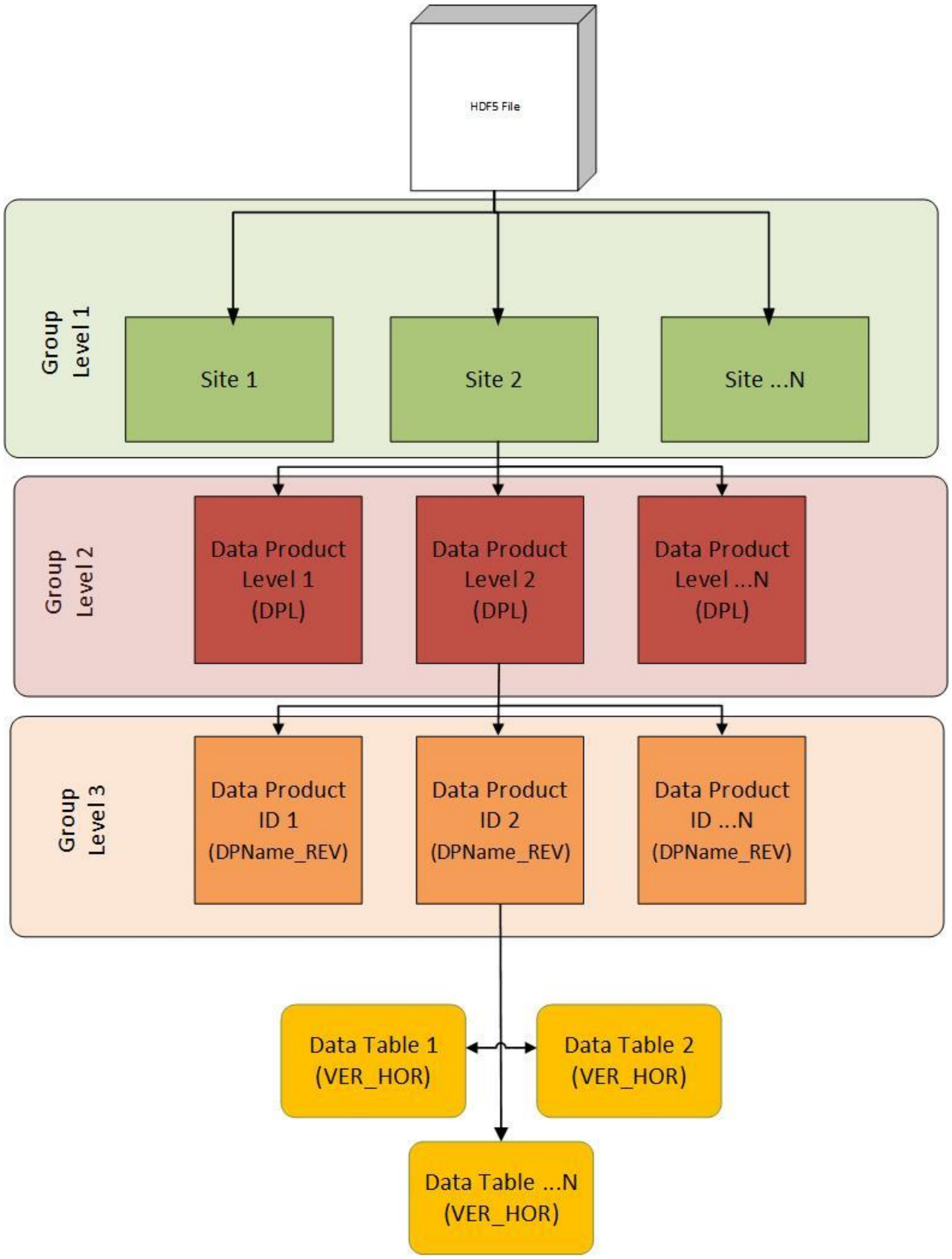

Figure 4. Diagram depicting the NEON HDF5 file structure following the NEON DP naming convention. Note that PRNUM is replaced by the DPName associated with that PRNUM.

One departure from the DP naming convention is the use of the data product name (DPName, i.e. irga) in place of PRNUM in the Data Product ID group level, this change was made to improve readability.

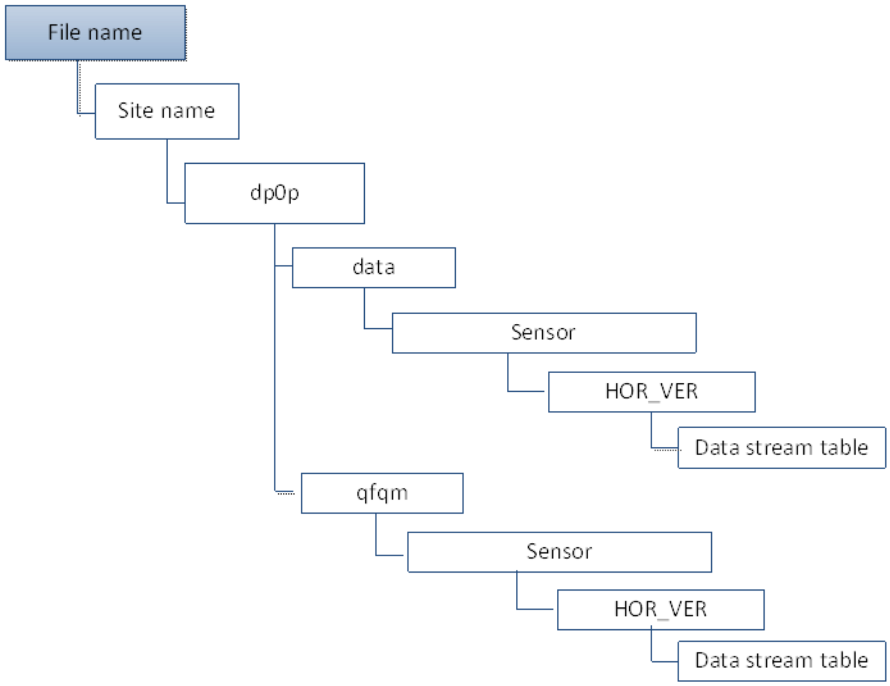

Figure 5. Diagram depicting the general EC L0p HDF5 file structure.

The HDF5 files generated will be comprised of the L0p preprocessed data following the previously discussed algorithmic processes in the structure described above, where one file is generated for each 24 hour period (Figure 5). The files will be generated with a file name describing the subsystem, data product level, 4-letter site code, and the date (ex. ECSE_dp0p_CPER_2016-10-26.h5). The L0p preprocessed data will be provided with the time regularized ISO 8601 timestamp for each data table produced. Under the dp0p, the data will be organized into three separate groups including data and qfqm. Under each of data and qfm, there are a list of all sensors and the data tables are generated for each of horizontal or vertical location of that sensor. In addition, metadata will be packaged with the data as attributes to either a group level or the data table for the L0p preprocessed product. A full list of the metadata to be attached as attributes to the HDF5 file is provided in the Appendix (section 21.1).

19.3 Algorithm Implementation

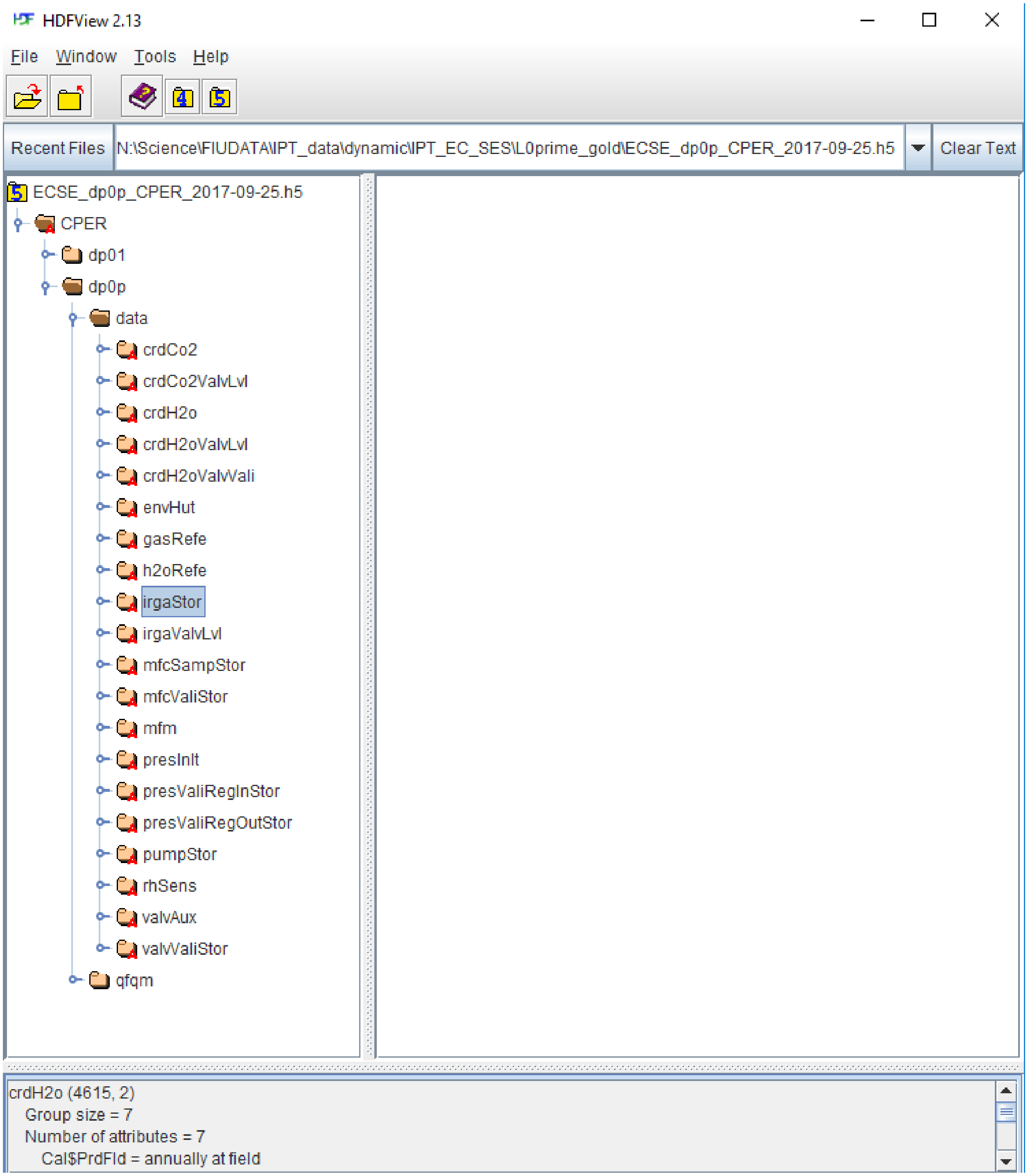

Figure 6. Diagram depicting the ECSE L0p HDF5 file structure.

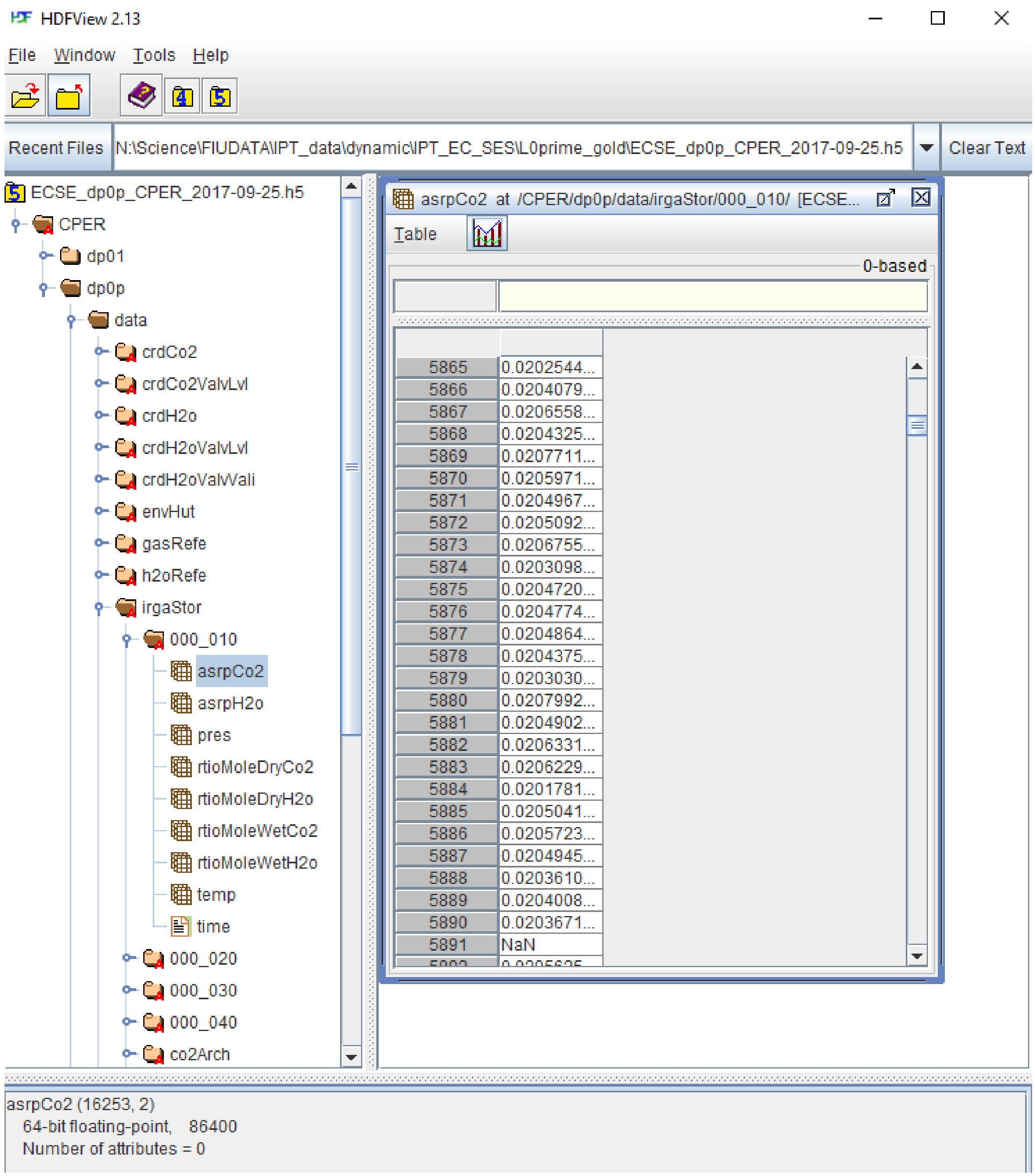

Figure 7. Diagram to show ECSE L0p HDF5 data tables.

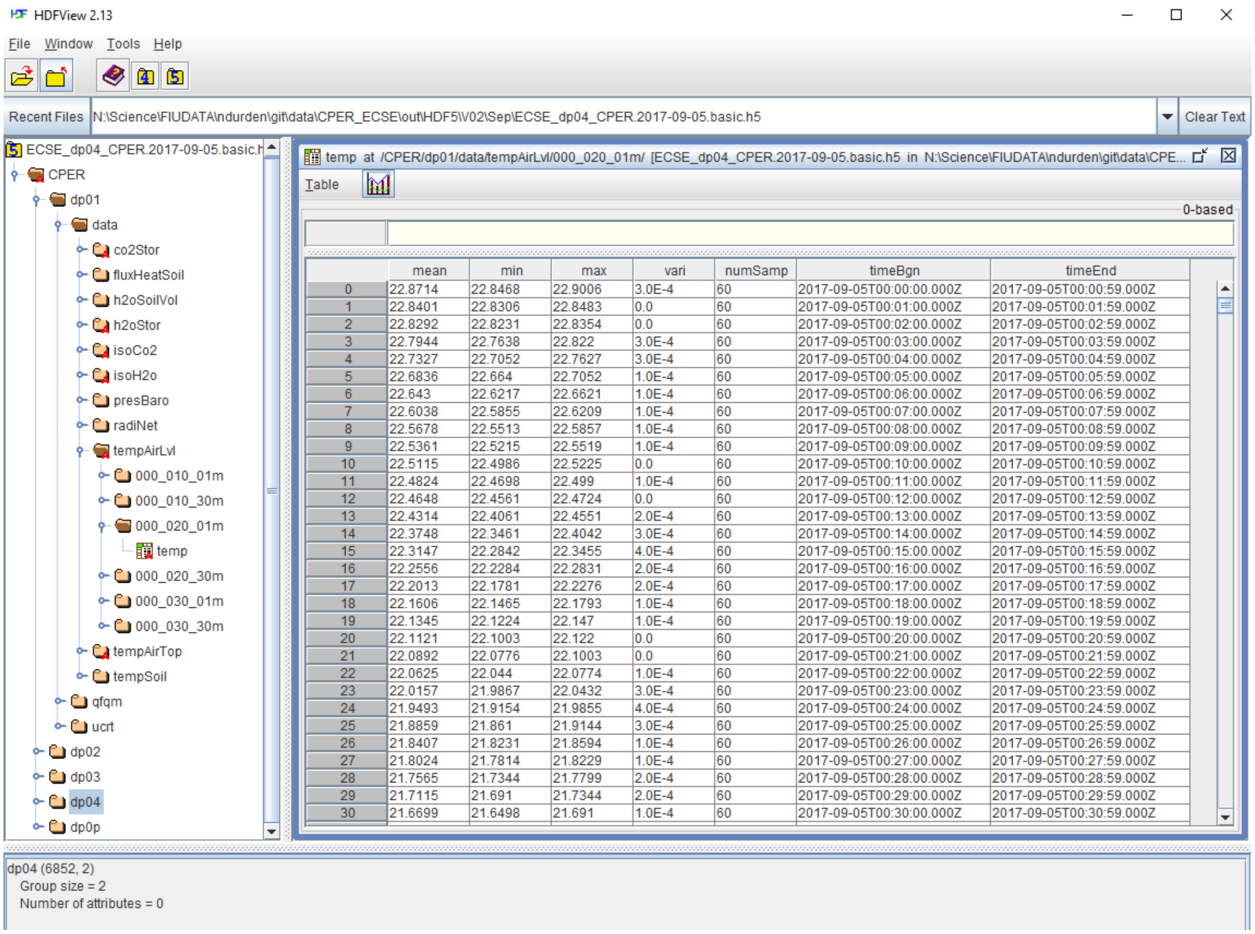

Figure 8. Diagram to show ECSE L1 HDF5 data tables.

Organizing the L0p preprocessed data and generating the HDF5 file according to the file structure in Figure 6 and Figure 7 consist of the following sequence:

1. Organizing L0p preprocessed data for each sensor, details are provided in section 19.3.1 to 19.3.20.
2. Generate the HDF5 file for 24 hour period following the structure detailed in Figure 6 and Figure 7.
3. Attach metadata to either a group level or the data tables for the L0p preprocessed product, details are provided in the Appendix (section 21.1).

Organizing the existing L1 data and generating the HDF5 file according to the file structure in Figure 8 consist of the following sequence:

1. Organizing existing L1 data for each data product, details are provided in section 19.3.21 to 19.3.27.
2. Generate the HDF5 file for 24 hour period following the structure detailed in Figure 8.

3. Attach metadata to either a group level or the data tables for the existing L1 products, details are provided in the Appendix (section 21.1).

19.3.1 Organizing IRGA L0p preprocessed data

Under the irgaStor node, the data tables are generated for each of horizontal and vertical location of IRGA. In this case measurement location (000_010 to 000_0n0) and validation/calibration gas type (co2Zero, co2Low, co2Med, co2High, and co2Arch) are used to represent the vertical and horizontal location of IRGA, respectively. IRGA data and quality flags will be subset correspond to that measurement location and validation/calibration gas type as following steps:

1. Combine all IRGA L0p preprocessed data and related quality flags (detailed in Table 3-1 in section 3), qfHeat (heater flag generated from section 12), IRGA measurement type (measTypeIrga in section 16), IRGA measurement location (lvlIrga in section 14), and validation gas type (typeGas in section 15).
2. IRGA L0p preprocessed data is subset into data table for each measurement location by:

$$000\_Idx0 = \left| \text{if lvlIrga} = \text{lvlIdx and } \text{measTypeIrga} = \text{samp} \right. \tag{19.1}$$

where Idx is index for the location and equal to 01, 02, 03,…. n

n is the site-specific highest measurement level and can be vary from 04 to 08.

3. Repeat the 2nd step to subset the IRGA quality flags.
4. Inserted missing timestamps and the corresponding data values with NaN which following the procedures detailed in AD[04].
5. Deposit the IRGA data tables and IRGA quality flag data tables which were generated in step 2 to 4 under data/irgaStor and qfqm/irgaStor, respectively.
6. Next, IRGA L0p preprocessed data is subset into data table for each validation gas by

$$X = \left| \text{if typeGas} = X \text{ and } \text{measTypeIrga} = \text{vali or cal} \right. \tag{19.2}$$

where X is co2Zero, co2Low, co2Med, co2High, or co2Arch

7. Repeat the 6th step to subset the IRGA quality flags. However, qfHeat will not include in this subset.
8. Inserted missing timestamps and the corresponding data values with NaN which following the procedures detailed in AD[04].
9. For the IRGA data tables, combine each data table lists below with gas concentration data table (generated in 19.3.19) by:

a. combining data in co2Low data table with gas concentration 712_000 data table,
b. combining data in co2Med data table with gas concentration 713_000 data table,
c. combining data in co2High data table with gas concentration 714_000 data table,
d. combining data in co2Arch data table with gas concentration 710_000 data table. The folder of co2Arch should be remained in HDF5 file to keep consistent file structure even there is no co2Arch data on that day. Fill the data with NaNs.
e. combining data in co2Zero data table with gas concentration for co2Zero data table (see note below).

Note that in section 19.3.19, the gas concentration (709_000) data table for co2Zero is not specified. This is because this zero gas will not provide by CVAL and there will be no L0 data products generated for this gas. To be able to combine the IRGA data table during the validation period of zero gas with co2Zero gas concentration values, the 1 Hz values of dlta13CCo2Refe, rtioMoleDry12CCo2Refe, rtioMoleDry13CCo2Refe, and rtioMoleDryCo2Refe were manually generated as NaN, 0, 0, and 0, respectively for the co2Zero gas concentration values.

10. Deposit the IRGA data tables and IRGA quality flag data tables which were generated in step 6 to 10 under data/irgaStor and qfqm/irgaStor, respectively.

19.3.2 Organizing CRD CO_2 L0p preprocessed data

Under the crdCo2 node, the data tables are generated for each of horizontal and vertical location of CRD CO_2. In this case measurement location (000_010 to 000_0n0) and validation/calibration gas type (co2Low, co2Med, co2High, and co2Arch) are used to represent the vertical and horizontal location of CRD CO_2, respectively. CRD CO_2 data and quality flags will be subset correspond to that measurement location and validation/calibration gas type as following steps:

1. Combine all CRD CO_2 L0p preprocessed data and related quality flags (detailed in Table 4-1 in section 4), qfHeat (heater flag generated from section 12), CRD CO_2 measurement type (measTypeCrdCo2 in section 13), CRD CO_2 measurement location (lvlCrdCo2 in section 14), and validation gas type (typeGas in section 15).
2. CRD CO_2 L0p preprocessed data is subset into data table for each measurement location by:

$$\text{000\_Idx0} = \left| \text{ if lvlCrdCo2} = \text{ lvlIdx and } \text{ measTypeCrdCo2} = \text{samp} \right. \tag{19.3}$$

where Idx is index for the location and equal to 01, 02, 03,…. n

n is the site-specific highest measurement level and can be vary from 04 to 08.

3. Repeat the 2nd step to subset the CRD CO_2 quality flags.

4. Inserted missing timestamps and the corresponding data values with NaN which following the procedures detailed in AD[04].
5. Deposit the CRD CO_2 data tables and quality flags data tables which were generated in step 2 to 4 under data/crdCo2 and qfqm/crdCo2, respectively.
6. Next, CRD CO_2 L0p preprocessed data is subset into data table for each validation gas by:

$$\mathrm{X} = \left| \ \text{if typeGas} = \mathrm{X} \text{ and } \text{measTypeCrdCo2} = \text{vali and lvlCrdCo2} = \text{vali} \right. \tag{19.4}$$

where X is co2Low, co2Med, co2High, or co2Arch

7. Repeat step 6 to subset the CRD CO_2 quality flags. However, qfHeat will not include in this subset.
8. Inserted missing timestamps and the corresponding data values with NaN which following the procedures detailed in AD[04].
9. For the CRD CO_2 data tables, combine each data table lists below with gas concentration data table (generated in 19.3.19) by:
    a. combining data in co2Low data table with gas concentration 712_000 data table,
    b. combining data in co2Med data table with gas concentration 713_000 data table,
    c. combining data in co2High data table with gas concentration 714_000 data table, and
    d. combining data in co2Arch data table with gas concentration 710_000 data table.
10. Deposit the CRD CO_2 data tables and quality flags data tables which were generated in step 6 to 9 under data/crdCo2 and qfqm/crdCo2, respectively.

19.3.3 Organizing CRD H2O L0p preprocessed data

Under the crdH2o node, the data tables are generated for each of horizontal and vertical location of CRD H_2O. In this case measurement location (000_010 to 000_0n0) and validation period (h2oLow, h2oMed, and h2oHigh) are used to represent the vertical and horizontal location of CRD H_2O, respectively. CRD H_2O data and quality flags will be subset correspond to that measurement location and validation H_2O type as following steps:

1. Combine all CRD H_2O L0p preprocessed data and related quality flags (detailed in Table 5-1 in section 5), qfHeat (heater flag generated from section 12), CRD H_2O measurement type (measTypeCrdH2o in section 13), CRD H_2O measurement location (lvlCrdH2o in section 14), and validation H_2O type (typeH2o in section 15).
2. CRD H_2O L0p preprocessed data is subset into data table for each measurement location by:

$$000\_\mathrm{Idx0} = \left| \ \text{if lvlCrdH2o} = \text{lvlIdx and } \text{measTypeCrdH2o} = \text{samp} \right. \tag{19.5}$$

where Idx is index for the location and equal to 01, 02, 03,…. n

n is the site-specific highest measurement level and can be vary from 04 to 08.

3. Repeat the 2nd step to subset the CRD H_2O quality flags.
4. Inserted missing timestamps and the corresponding data values with NaN which following the procedures detailed in AD[04].
5. Deposit the CRD H_2O data tables and quality flags data tables which were generated in step 2 to 4 under data/crdH2o and qfqm/crdH2o, respectively.
6. Next, CRD H_2O L0p preprocessed data is subset into data table during the validation period by:

$$\mathrm{X} = \left| \text{ if typeH2o} = \mathrm{X} \text{ and measTypeCrdH2o} = \text{vali and lvlCrdH2o} = \text{vali} \right. \quad (19.6)$$

where X is h2oLow, h2oMed, or h2oHigh

7. Repeat step 6 to subset the CRD H_2O quality flags. However, qfHeat will not include in this subset.
8. Inserted missing timestamps and the corresponding data values with NaN which following the procedures detailed in AD[04].
9. For CRD H_2O data table, combine each data table lists below with the water concentration 700_000 data table (generated in 19.3.20) by:
   a. combining data in h2oLow data table with water concentration 712_000 data table (select only dlta2HH2oRefeLow and dlta18OH2oRefeLow),
   b. combining data in h2oMed data table with gas concentration 713_000 data table (select only dlta2HH2oRefeMed and dlta18OH2oRefeMed), and
   c. combining data in h2oHigh data table with gas concentration 714_000 data table (select only dlta2HH2oRefeHigh and dlta18OH2oRefeHigh).
10. Deposit the CRD H_2O data tables and quality flags data tables which were generated in step 6 to 9 under data/crdH2o and qfqm/crdH2o, respectively.

19.3.4 Organizing temperature sensor in the hut L0p preprocessed data

Under the envHut node, the data tables are generated for horizontal and vertical location (HOR_VER) of hut temperature which is 700_000.

1. Retrieve all hut temperature L0p preprocessed data and related quality flags (detailed in Table 6-1 in section 6)
2. Generate data table individually for hut temperature data and quality flags.
3. Deposit the Hut temperature data table and quality flags data table under data/envHut and qfqm/envHut, respectively.

19.3.5 Organizing gas cylinder pressure sensors preprocessed data

Under the presValiRegInStor node, the data tables are generated for each of horizontal and vertical location (HOR_VER) of gas cylinder pressure sensor which is including of 709_000, 710_000, 711_000, 712_000, 713_000, and 714_000.

1. For each location, retrieve all gas cylinder pressure L0p preprocessed data and related quality flags (detailed in Table 7-1 in section 7).
2. Generate data table individually for gas cylinder pressure data and quality flags.
3. Deposit the gas cylinder pressure data tables and quality flags data tables will under data/presValiRegInStor and qfqm/presValiRegInStor, respectively.

19.3.6 Organizing delivery pressure sensors preprocessed data

Under the presValiRegOutStor node , the data tables are generated for each of horizontal and vertical location (HOR_VER) of delivery pressure sensor, including 709_000, 710_000, 711_000, 712_000, 713_000, and 714_000.

1. For each location, retrieve all delivery pressure L0p preprocessed data and related quality flags (detailed in Table 7-1 in section 7).
2. Generate data table individually for delivery pressure data and quality flags.
3. Deposit the delivery pressure data tables and quality flags data tables under data/presValiRegOutStor and qfqm/presValiRegOutStor, respectively.

19.3.7 Organizing inlet absolute pressure transducers preprocessed data

Under the presInlt node, the data tables are generated for each of horizontal and vertical location (HOR_VER) of inlet pressure transducer, including 000_010, 000_020, 000_030,…, 000_0n0, where n is the site-specific highest measurement level and can be vary from 4 to 8.

1. For each location, retrieve all inlet pressure L0p preprocessed data and related quality flags (detailed in Table 8-1 in section 8).
2. Generate data table individually for inlet pressure data and quality flags.
3. Deposit inlet pressure data tables and quality flags data tables under data/presInlt and qfqm/presInlt, respectively.

19.3.8 Organizing mass flow meter L0p preprocessed data

Under the mfm node, the data tables are generated for each of horizontal and vertical location (HOR_VER) of mass flow meter, including 700_010, 700_020, 700_030,…, 700_0n0, where n is the site-specific highest measurement level and can be vary from 4 to 8.

1. For each location, retrieve all mass flow meter L0p preprocessed data and related quality flags (detailed in Table 9-1 in section 9).
2. Generate data table individually for mass flow meter data and quality flags.
3. Deposit mass flow meter data tables and quality flags data tables under data/mfm and qfqm/mfm, respectively.

19.3.9 Organizing mass flow controller for field validation gases L0p preprocessed data

Under the mfcValiStor node, the data tables are generated for horizontal and vertical location (HOR_VER) of mass flow controller which is 700_000.

1. Retrieve all field validation gases mass flow controller L0p preprocessed data and related quality flags (detailed in Table 10-1 in section 10).
2. Generate data table individually for mass flow controller data and quality flags.
3. Deposit mass flow controller data table and quality flags data table under data/mfcValiStor and qfqm/mfcValiStor, respectively.

19.3.10 Organizing mass flow controller for IRGA L0p preprocessed data

Under the mfcSampStor node, the data tables are generated for horizontal and vertical location (HOR_VER) of IRGA mass flow controller which is 700_000.

1. Retrieve all IRGA mass flow controller L0p preprocessed data and related quality flags (detailed in Table 10-1 in section 10).
2. Generate data table individually for mass flow controller data and quality flags.
3. Deposit mass flow controller data table and quality flags data table under data/ mfcSampStor and qfqm/ mfcSampStor, respectively.

19.3.11 Organizing pumps L0p preprocessed data

Under the pumpStor node, the data tables are generated for each of horizontal and vertical location (HOR_VER) of pump, including of 700_000, 700_010, 700_020, 700_030,…, 700_0n0, where n is the highest measurement level which is site specific and can be vary from 4 to 8.

1. For each location, retrieve all pump's L0p preprocessed data and related quality flags (detailed in Table 11-1 in section 11).
2. Generate data table individually for pump data and quality flags.
3. Deposit pump data tables and quality flags data tables under data/pumpStor and qfqm/pumpStor, respectively.

19.3.12 Organizing IRGA sample manifold L0p preprocessed data

Under the irgaValvLvl node, the data tables are generated for horizontal and vertical location (HOR_VER) of IRGA sample manifold which is 701_000.

1. Retrieve all IRGA sample manifold L0p preprocessed data (detailed in Table 14-1 in section 14).
2. Generate sample manifold data table.
3. Deposit the data table under data/irgaValvLvl.

19.3.13 Organizing CRD CO_2 sample manifold L0p preprocessed data

Under the crdCo2ValvLvl node, the data tables are generated for horizontal and vertical location (HOR_VER) of CRD CO_2 sample manifold which is 702_000.

1. Retrieve all CRD CO_2 sample manifold L0p preprocessed data (detailed in Table 14-1 in section 14).
2. Generate sample manifold data table.
3. Deposit the data table under data/crdCo2ValvLvl.

19.3.14 Organizing CRD H_2O sample manifold L0p preprocessed data

Under the crdH2oValvLvl node, the data tables are generated for horizontal and vertical location (HOR_VER) of CRD H_2O sample manifold which is 704_000.

1. Retrieve all CRD H_2O sample manifold L0p preprocessed data (detailed in Table 14-1 in section 14).
2. Generate sample manifold data table.
3. Deposit the data table under data/crdH2oValvLvl.

19.3.15 Organizing validation manifold L0p preprocessed data

Under the valvValiStor node, the data tables are generated for horizontal and vertical location (HOR_VER) of validation manifold which is 703_000.

1. Retrieve all validation manifold L0p preprocessed data (detailed in Table 15-1 in section 15).
2. Generate validation manifold data table.
3. Deposit the data table under data/valvValiStor.

19.3.16 Organizing auxiliary valves L0p preprocessed data

Under the valvAux node, the data tables are generated for horizontal and vertical location (HOR_VER) of auxiliary valves which is 700_000.

1. Retrieve all auxiliary valves L0p preprocessed data and related quality flags (detailed in Table 13-1 in section 13).
2. Generate data table individually for auxiliary valves data and quality flags.
3. Deposit auxiliary valves data table and quality flags data table under data/valvAux and qfqm/valvAux, respectively.

19.3.17 Organizing vaporizer 3-way valve L0p preprocessed data

Under the crdH2oValvVali node, the data tables are generated for horizontal and vertical location (HOR_VER) of validation manifold which is 700_000.

1. Retrieve all crdH2oValvVali L0p preprocessed data (detailed in Table 15-1 in section 15).
2. Generate crdH2oValvVali data table.
3. Deposit the data table under data/crdH2oValvVali.

19.3.18 Organizing inlet heater L0p preprocessed data

Under the rhSens node, the data tables are generated for horizontal and vertical location (HOR_VER) of relative humidity sensor, including of 000_0n0, and 003_000, where n is the highest measurement level which is site specific and can be vary from 4 to 8.

1. For each location, retrieve all rhSens's L0p preprocessed data and qfSens (detailed in Table 12-1 in section 12).
2. Generate data table individually for rhSens data and qfSens.
3. Deposit rhSens data tables and quality flags data tables under data/rhSens and qfqm/rhSens, respectively.

19.3.19 Organizing gas cylinder concentration L0p preprocessed data

Under the gasRefe node, the data tables are generated for each of horizontal and vertical location (HOR_VER) of gas concentration, including of 710_000, 712_000, 713_000, and 714_000.

1. For each location, retrieve all gas concentration L0p preprocessed data (detailed in Table 17-1 in section 17).
2. Generate gas concentration data tables.
3. Deposit the data table under data/gasRefe.

19.3.20 Organizing water standard L0p preprocessed data

Under the h2o90Refe node, the data tables are generated for horizontal and vertical location (HOR_VER) of water standard which is 700_000.

1. Retrieve all water standard L0p preprocessed data (detailed in Table 18-1 in section 18).

2. Generate water standard data table.
3. Deposit the data table under data/h2o90Refe.

19.3.21 Organizing single aspirated air temperature sensor (SAATS) existing L1 data

Under the "tempAirLvl" node in HDF5 file, the data tables are generated for each of horizontal and vertical location (HOR_VER) of SAATS, including of 000_010, 000_020, 000_030,…, 000_0n0, where n is the second-highest measurement level which is site specific and can be vary from 3 to 7. "_1m" or "_30m" indicates the aggregation over 1 min or 30 min time period.

1. For each location under "data" folder, retrieve following SAATS existing L1 data from expanded data set and put them into corresponding columns of "temp" data table in the HDF5 file. Do this for both 1 min and 30 min data. This step will be identical to generate basic HDF5 file or expanded HDF5 file.

Table 19-1: Mapping between fieldName for tempAirLvl existing L1 data stream and fieldname (column) in HDF5 data table.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table
tempSingleMean	temp	mean
tempSingleMinimum	temp	min
tempSingleMaximum	temp	max
tempSingleVariance	temp	vari
tempSingleNumPts	temp	numSamp
startDateTime	temp	timeBgn
endDateTime	temp	timeEnd

2. Under "data" folder, add attributes to data product group and each data table group according to the info in the example HDF5 file provided by science team
3. For each location under "qfqm" folder, retrieve following SAATS existing L1 data from expanded data set and put them into corresponding columns of "temp" data table in the HDF5 file to generate **basic** HDF5 file. Do this for both 1 min and 30 min data.

Table 19-2: Mapping between quality flag fieldName for tempAirLvl existing L1 data stream and fieldname (column) in hdf5 data table for generating basic hdf5 file.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table
finalQF	temp	qfFinl
startDateTime	temp	timeBgn
endDateTime	temp	timeEnd

4. For each location under "qfqm" folder, retrieve following SAATS existing L1 data from expanded data set and put them into corresponding columns of "temp" data table in the HDF5 file to generate **expanded** HDF5 file. Do this for both 1 min and 30 min data. For the qfSci, it is a science review flag. If it does not exist yet by the time the HDF5 file is generated, fill qfSci as 0.

Table 19-3: Mapping between quality flag fieldName for tempAirLvl existing L1 data stream and fieldname (column) in hdf5 data table for generating expaned hdf5 file.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table
alphaQM	temp	qfAlph
betaQM	temp	qfBeta
	temp	qfSci
finalQF	temp	qfFinl
startDateTime	temp	timeBgn
endDateTime	temp	timeEnd

5. For each location under "ucrt" folder, retrieve following SAATS existing L1 data from expanded data set and put them into corresponding columns of "temp" data table in the HDF5 file. Do this for both 1 min and 30 min data. This step will be identical to generate basic HDF5 file or expanded HDF5 file.

Table 19-4: Mapping between uncertainty fieldName for tempAirLvl existing L1 data stream and fieldname (column) in hdf5 data table.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table
tempSingleExpUncert	temp	ucrtCal95

tempSingleStdErMean	temp	se
startDateTime	temp	timeBgn
endDateTime	temp	timeEnd

19.3.22 Organizing triple redundancy aspirated air temperature sensors (TRAATS) existing L1 data

Under the tempAirTop node, the data tables are generated for horizontal and vertical location (HOR_VER) of TRAATS which is 000_0n0, where n is the highest measurement level at a site, which is site specific and can vary from 4 to 8. "_1m" or "_30m" indicates the aggregation over 1 min or 30 min time period.

1. For each location under "data" folder, retrieve following TRAATS existing L1 data from expanded data set and put them into corresponding columns of "temp" data table in the HDF5 file. Do this for both 1 min and 30 min data. This step will be identical to generate basic HDF5 file or expanded HDF5 file.

Table 19-5: Mapping between fieldName for tempAirTop existing L1 data stream and fieldname (column) in hdf5 data table.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table
tempTripleMean	temp	mean
tempTripleMinimum	temp	min
tempTripleMaximum	temp	max
tempTripleVariance	temp	vari
tempTripleNumPts	temp	numSamp
startDateTime	temp	timeBgn
endDateTime	temp	timeEnd

2. Under "data" folder, add attributes to data product group and each data table group according to the info in the example HDF5 file provided by science team
3. For each location under "qfqm" folder, retrieve following TRAATS existing L1 data from expanded data set and put them into corresponding columns of "temp" data table in the HDF5 file to generate **basic** HDF5 file. Do this for both 1 min and 30 min data.

Table 19-6: Mapping between quality flag fieldName for tempAirTop existing L1 data stream and fieldname (column) in hdf5 data table for generating basic hdf5 file.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table
finalQF	temp	qfFinl
startDateTime	temp	timeBgn
endDateTime	temp	timeEnd

4. For each location under "qfqm" folder, retrieve following TRAATS existing L1 data from expanded data set and put them into corresponding columns of "temp" data table in the HDF5 file to generate **expanded** HDF5 file. Do this for both 1 min and 30 min data. For the qfSci, it is a science review flag. If it does not exist yet by the time the HDF5 is generated, fill qfSci as 0.

Table 19-7: Mapping between quality flag fieldName for tempAirTop existing L1 data stream and fieldname (column) in hdf5 data table for generating expaned hdf5 file.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table
alphaQM	temp	qfAlph
betaQM	temp	qfBeta
	temp	qfSci
finalQF	temp	qfFinl
startDateTime	temp	timeBgn
endDateTime	temp	timeEnd

5. For each location under "ucrt" folder, retrieve following TRAATS existing L1 data from expanded data set and put them into corresponding columns of "temp" data table in the HDF5 file. Do this for both 1 min and 30 min data. This step will be identical to generate basic HDF5 file or expanded HDF5 file.

Table 19-8: Mapping between uncertainty fieldName for tempAirTop existing L1 data stream and fieldname (column) in hdf5 data table.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table

tempTripleExpUncert	temp	ucrtCal95
tempTripleStdErMean	temp	se
startDateTime	temp	timeBgn
endDateTime	temp	timeEnd

19.3.23 Organizing Shortwave and longwave radiation (net radiometer) existing L1 data

Under the radiNet node, the data tables are generated for horizontal and vertical location (HOR_VER) of net radiometer which is 000_0n0, where n is the highest measurement level at a site, which is site specific and can vary from 4 to 8. "_1m" or "_30m" indicates the aggregation over 1 min or 30 min time period.

1. For each location under "data" folder, retrieve following net radiometer existing L1 data from expanded data set and put them into corresponding columns of data tables in the HDF5 file (see table below. Do this for both 1 min and 30 min data. This step will be identical to generate basic HDF5 file or expanded HDF5 file.

Table 19-9: Mapping between fieldName for radiNet existing L1 data stream and fieldname (column) in hdf5 data table.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table
inSWMean	radiSwIn	mean
inSWMinimum	radiSwIn	min
inSWMaximum	radiSwIn	max
inSWVariance	radiSwIn	vari
inSWNumPts	radiSwIn	numSamp
startDateTime	radiSwIn	timeBgn
endDateTime	radiSwIn	timeEnd
outSWMean	radiSwOut	mean
outSWMinimum	radiSwOut	min
outSWMaximum	radiSwOut	max

outSWVariance	radiSwOut	vari
outSWNumPts	radiSwOut	numSamp
startDateTime	radiSwOut	timeBgn
endDateTime	radiSwOut	timeEnd
inLWMean	radiLwIn	mean
inLWMinimum	radiLwIn	min
inLWMaximum	radiLwIn	max
inLWVariance	radiLwIn	vari
inLWNumPts	radiLwIn	numSamp
startDateTime	radiLwIn	timeBgn
endDateTime	radiLwIn	timeEnd
outLWMean	radiLwOut	mean
outLWMinimum	radiLwOut	min
outLWMaximum	radiLwOut	max
outLWVariance	radiLwOut	vari
outLWNumPts	radiLwOut	numSamp
startDateTime	radiLwOut	timeBgn
endDateTime	radiLwOut	timeEnd

2. Under "data" folder, add attributes to data product group and each data table group according to the info in the example HDF5 file provided by science team
3. For each location under "qfqm" folder, retrieve following net radiometer existing L1 data from expanded data set and put them into corresponding columns of data tables in the HDF5 file to generate **basic** HDF5 file. Do this for both 1 min and 30 min data.

Table 19-10: Mapping between quality flag fieldName for radiNet existing L1 data stream and fieldname (column) in hdf5 data table for generating basic hdf5 file.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table
inSWfinalQF	radiSwIn	qfFinl
startDateTime	radiSwIn	timeBgn
endDateTime	radiSwIn	timeEnd
outSWfinalQF	radiSwOut	qfFinl
startDateTime	radiSwOut	timeBgn
endDateTime	radiSwOut	timeEnd
inLWfinalQF	radiLwIn	qfFinl
startDateTime	radiLwIn	timeBgn
endDateTime	radiLwIn	timeEnd
outLWfinalQF	radiLwOut	qfFinl
startDateTime	radiLwOut	timeBgn
endDateTime	radiLwOut	timeEnd

4. For each location under “qfqm” folder, retrieve following net radiometer existing L1 data from expanded data set and put them into corresponding columns of data table in the HDF5 file to generate **expanded** HDF5 file. Do this for both 1 min and 30 min data. For the qfSci, it is a science review flag. If it does not exist yet by the time the HDF5 file is generated, fill qfSci as 0.

Table 19-11: Mapping between quality flag fieldName for radiNet existing L1 data stream and fieldname (column) in hdf5 data table for generating expaned hdf5 file.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table
inSWAlphaQM	radiSwIn	qfAlph
inSWBetaQM	radiSwIn	qfBeta
	radiSwIn	qfSci
inSWfinalQF	radiSwIn	qfFinl

startDateTime	radiSwIn	timeBgn
endDateTime	radiSwIn	timeEnd
outSWAlphaQM	radiSwOut	qfAlph
outSWBetaQM	radiSwOut	qfBeta
	radiSwOut	qfSci
outSWfinalQF	radiSwOut	qfFinl
startDateTime	radiSwOut	timeBgn
endDateTime	radiSwOut	timeEnd
inLWAlphaQM	radiLwIn	qfAlph
inLWBetaQM	radiLwIn	qfBeta
	radiLwIn	qfSci
inLWfinalQF	radiLwIn	qfFinl
startDateTime	radiLwIn	timeBgn
endDateTime	radiLwIn	timeEnd
outLWAlphaQM	radiLwOut	qfAlph
outLWBetaQM	radiLwOut	qfBeta
	radiLwOut	qfSci
outLWfinalQF	radiLwOut	qfFinl
startDateTime	radiLwOut	timeBgn
endDateTime	radiLwOut	timeEnd

5. For each location under "ucrt" folder, retrieve following net radiometer existing L1 data from expanded data set and put them into corresponding columns of data table in the HDF5 file. Do this for both 1 min and 30 min data. This step will be identical to generate basic HDF5 file or expanded HDF5 file.

Table 19-12: Mapping between uncertainty fieldName for radiNet existing L1 data stream and fieldname (column) in hdf5 data table.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table
inSWExpUncert	radiSwIn	ucrtCal95
inSWStdErMean	radiSwIn	se
startDateTime	radiSwIn	timeBgn
endDateTime	radiSwIn	timeEnd
outSWExpUncert	radiSwOut	ucrtCal95
outSWStdErMean	radiSwOut	se
startDateTime	radiSwOut	timeBgn
endDateTime	radiSwOut	timeEnd
inLWExpUncert	radiLwIn	ucrtCal95
inLWStdErMean	radiLwIn	se
startDateTime	radiLwIn	timeBgn
endDateTime	radiLwIn	timeEnd
outLWExpUncert	radiLwOut	ucrtCal95
outLWStdErMean	radiLwOut	se
startDateTime	radiLwOut	timeBgn
endDateTime	radiLwOut	timeEnd

19.3.24 Organizing soil heat flux plate existing L1 data

Under the "fluxHeatSoil" node in HDF5 file, the data tables are generated for each of horizontal and vertical location (HOR_VER) of soil heat flux plate, including of 001_501, 003_501, 005_501. "_1m" or "_30m" indicates the aggregation over 1 min or 30 min time period.

1. For each location under "data" folder, retrieve following soil heat flux plate existing L1 data from expanded data set and put them into corresponding columns of "fluxHeatSoil" data table in the HDF5 file. Do this for both 1 min and 30 min data. This step will be identical to generate basic HDF5 file or expanded HDF5 file.

Table 19-13: Mapping between fieldName for fluxHeatSoil existing L1 data stream and fieldname (column) in hdf5 data table.

fieldName for existing L1 data stream	**HDF5 data table**	**fieldName (column) in HDF5 data table**
SHFMean	fluxHeatSoil	mean
SHFMinimum	fluxHeatSoil	min
SHFMaximum	fluxHeatSoil	max
SHFVariance	fluxHeatSoil	vari
SHFNumPts	fluxHeatSoil	numSamp
SHFInSituCorFactor	fluxHeatSoil	calFld
startDateTime	fluxHeatSoil	timeBgn
endDateTime	fluxHeatSoil	timeEnd

2. Under "data" folder, add attributes to data product group and each data table group according to the info in the example HDF5 file provided by science team
3. For each location under "qfqm" folder, retrieve following soil heat flux plate existing L1 data from expanded data set and put them into corresponding columns of "fluxHeatSoil"data table in the HDF5 file to generate **basic** HDF5 file. Do this for both 1 min and 30 min data.

Table 19-14: Mapping between quality flag fieldName for fluxHeatSoil existing L1 data stream and fieldname (column) in hdf5 data table for generating basic hdf5 file.

fieldName for existing L1 data stream	**HDF5 data table**	**fieldName (column) in HDF5 data table**
finalQF	fluxHeatSoil	qfFinl
startDateTime	fluxHeatSoil	timeBgn
endDateTime	fluxHeatSoil	timeEnd

4. For each location under "qfqm" folder, retrieve following soil heat flux plate existing L1 data from expanded data set and put them into corresponding columns of "fluxHeatSoil"data table in the HDF5 file to generate **expanded** HDF5 file. Do this for both 1 min and 30 min data. For the qfSci, it is a science review flag. If it does not exist yet by the time the HDF5 file is generated, fill qfSci as 0.

Table 19-15: Mapping between quality flag fieldName for fluxHeatSoil existing L1 data stream and fieldname (column) in hdf5 data table for generating expaned hdf5 file.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table
alphaQM	fluxHeatSoil	qfAlph
betaQM	fluxHeatSoil	qfBeta
	fluxHeatSoil	qfSci
finalQF	fluxHeatSoil	qfFinl
startDateTime	fluxHeatSoil	timeBgn
endDateTime	fluxHeatSoil	timeEnd

5. For each location under "ucrt" folder, retrieve following soil heat flux plate existing L1 data from expanded data set and put them into corresponding columns of "fluxHeatSoil"data table in the HDF5 file. Do this for both 1 min and 30 min data. This step will be identical to generate basic HDF5 file or expanded HDF5 file.

Table 19-16: Mapping between uncertainty fieldName for fluxHeatSoil existing L1 data stream and fieldname (column) in hdf5 data table.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table
SHFExpUncert	fluxHeatSoil	ucrtCal95
SHFStdErMean	fluxHeatSoil	se
startDateTime	fluxHeatSoil	timeBgn
endDateTime	fluxHeatSoil	timeEnd

19.3.25 Organizing soil temperature existing L1 data

Under the tempSoil node, the data tables are generated for each of horizontal and vertical location (HOR_VER) of soil temperature, including of 00n_501, 00n_502, 00n_503,…, 00n_509, where n is the soil plot number, which varies from 1 to 5. "_1m" or "_30m" indicates the aggregation over 1 min or 30 min time period.

1. For each location under "data" folder, retrieve following soil temperature existing L1 data from expanded data set and put them into corresponding columns of data tables in the HDF5 file (see table below. Do this for both 1 min and 30 min data. This step will be identical to generate basic HDF5 file or expanded HDF5 file.

Table 19-17: Mapping between fieldName for tempSoil existing L1 data stream and fieldname (column) in hdf5 data table.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table
soilTempMean	tempSoil	mean
soilTempMinimum	tempSoil	min
soilTempMaximum	tempSoil	max
soilTempVariance	tempSoil	vari
soilTempNumPts	tempSoil	numSamp
startDateTime	tempSoil	timeBgn
endDateTime	tempSoil	timeEnd

2. Under "data" folder, add attributes to data product group and each data table group according to the info in the example HDF5 file provided by science team
3. For each location under "qfqm" folder, retrieve following soil temperature existing L1 data from expanded data set and put them into corresponding columns of data tables in the HDF5 file to generate **basic** HDF5 file. Do this for both 1 min and 30 min data.

Table 19-18: Mapping between quality flag fieldName for tempSoil existing L1 data stream and fieldname (column) in hdf5 data table for generating basic hdf5 file.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table

finalQF		qfFinl
startDateTime		timeBgn
endDateTime		timeEnd

4. For each location under "qfqm" folder, retrieve following soil temperature existing L1 data from expanded data set and put them into corresponding columns of data table in the HDF5 file to generate **expanded** HDF5 file. Do this for both 1 min and 30 min data. For the qfSci, it is a science review flag. If it does not exist yet by the time the HDF5 file is generated, fill qfSci as 0.

Table 19-19: Mapping between quality flag fieldName for tempSoil existing L1 data stream and fieldname (column) in hdf5 data table for generating expaned hdf5 file.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table
alphaQM	tempSoil	qfAlph
betaQM	tempSoil	qfBeta
	tempSoil	qfSci
finalQF	tempSoil	qfFinl
startDateTime	tempSoil	timeBgn
endDateTime	tempSoil	timeEnd

5. For each location under "ucrt" folder, retrieve following soil temperature existing L1 data from expanded data set and put them into corresponding columns of data tables in the HDF5 file. Do this for both 1 min and 30 min data. This step will be identical to generate basic HDF5 file or expanded HDF5 file.

Table 19-20: Mapping between uncertainty fieldName for tempSoil existing L1 data stream and fieldname (column) in hdf5 data table.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table
soilTempExpUncert	tempSoil	ucrtCal95
soilTempStdErMean	tempSoil	se

startDateTime	tempSoil	timeBgn
endDateTime	tempSoil	timeEnd

19.3.26 Organizing soil water content and water salinity existing L1 data

Under the h2oSoilVol node, the data tables are generated for each of horizontal and vertical location (HOR_VER) of soil water content and water salinity, including of 00n_501, 00n_502, 00n_503,…, 00n_508, where n is the soil plot number, which varies from 1 to 5. "_1m" or "_30m" indicates the aggregation over 1 min or 30 min time period.

1. For each location under "data" folder, retrieve following soil water content and water salinity existing L1 data from expanded data set and put them into corresponding columns of data tables in the HDF5 file (see table below. Do this for both 1 min and 30 min data. This step will be identical to generate basic HDF5 file or expanded HDF5 file.

Table 19-21: Mapping between fieldName for h2oSoilVol existing L1 data stream and fieldname (column) in hdf5 data table.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table
VSWCMean	h2oSoilVol	mean
VSWCMinimum	h2oSoilVol	min
VSWCMaximum	h2oSoilVol	max
VSWCVariance	h2oSoilVol	vari
VSWCNumPts	h2oSoilVol	numSamp
startDateTime	h2oSoilVol	timeBgn
endDateTime	h2oSoilVol	timeEnd
VSICMean	ionSoilVol	mean
VSICMinimum	ionSoilVol	min
VSICMaximum	ionSoilVol	max
VSICVariance	ionSoilVol	vari

VSICNumPts	ionSoilVol	numSamp
startDateTime	ionSoilVol	timeBgn
endDateTime	ionSoilVol	timeEnd

2. Under "data" folder, add attributes to data product group and each data table group according to the info in the example HDF5 file provided by science team
3. For each location under "qfqm" folder, retrieve following soil water content and water salinity existing L1 data from expanded data set and put them into corresponding columns of data tables in the HDF5 file to generate **basic** HDF5 file. Do this for both 1 min and 30 min data.

Table 19-22: Mapping between quality flag fieldName for h2oSoilVol existing L1 data stream and fieldname (column) in hdf5 data table for generating basic hdf5 file.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table
VSWCFinalQF	h2oSoilVol	qfFinl
startDateTime	h2oSoilVol	timeBgn
endDateTime	h2oSoilVol	timeEnd
VSICFinalQF	ionSoilVol	qfFinl
startDateTime	ionSoilVol	timeBgn
endDateTime	ionSoilVol	timeEnd

4. For each location under "qfqm" folder, retrieve following soil water content and water salinity existing L1 data from expanded data set and put them into corresponding columns of data table in the HDF5 file to generate **expanded** HDF5 file. Do this for both 1 min and 30 min data. For the qfSci, it is a science review flag. If it does not exist yet by the time the HDF5 file is generated, fill qfSci as 0.

Table 19-23: Mapping between quality flag fieldName for h2oSoilVol existing L1 data stream and fieldname (column) in hdf5 data table for generating expaned hdf5 file.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table
VSWCAlphaQM	h2oSoilVol	qfAlph

VSWCBetaQM	h2oSoilVol	qfBeta
	h2oSoilVol	qfSci
VSWCFinalQF	h2oSoilVol	qfFinl
startDateTime	h2oSoilVol	timeBgn
endDateTime	h2oSoilVol	timeEnd
VSICAlphaQM	ionSoilVol	qfAlph
VSICBetaQM	ionSoilVol	qfBeta
	ionSoilVol	qfSci
VSICFinalQF	ionSoilVol	qfFinl
startDateTime	ionSoilVol	timeBgn
endDateTime	ionSoilVol	timeEnd

5. For each location under "ucrt" folder, retrieve following soil water content and water salinity existing L1 data from expanded data set and put them into corresponding columns of data tables in the HDF5 file. Do this for both 1 min and 30 min data. This step will be identical to generate basic HDF5 file or expanded HDF5 file.

Table 19-24: Mapping between uncertainty fieldName for h2oSoilVol existing L1 data stream and fieldname (column) in hdf5 data table.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table
VSWCExpUncert	h2oSoilVol	ucrtCal95
VSWCStdErMean	h2oSoilVol	se
startDateTime	h2oSoilVol	timeBgn
endDateTime	h2oSoilVol	timeEnd
VSICExpUncert	ionSoilVol	ucrtCal95
VSICStdErMean	ionSoilVol	se

startDateTime	ionSoilVol	timeBgn
endDateTime	ionSoilVol	timeEnd

19.3.27 Organizing barometric pressure existing L1 data

Under the "presBaro" node in HDF5 file, the data table is generated for site-specific horizontal and vertical location (HOR_VER) of barometric pressure, which is on the tower between ML1 and ML2 (HOR_VER will be 000_015) or between ML2 and ML3 (HOR_VER will be 000_025), or between ML3 and ML4 (HOR_VER will be 000_035). The vertical index varies from site to site. "_1m" or "_30m" indicates the aggregation over 1 min or 30 min time period.

1. For each location under "data" folder, retrieve following barometric pressure existing L1 data from expanded data set and put them into corresponding columns of "presAtm" and "presCor" data tables in the HDF5 file. Do this for both 1 min and 30 min data. This step will be identical to generate basic HDF5 file or expanded HDF5 file.

Table 19-25: Mapping between fieldName for presBaro existing L1 data stream and fieldname (column) in hdf5 data table.

fieldName for existing L1 data stream	**HDF5 data table**	**fieldName (column) in HDF5 data table**
staPresMean	presAtm	mean
staPresMinimum	presAtm	min
staPresMaximum	presAtm	max
staPresVariance	presAtm	vari
staPresNumPts	presAtm	numSamp
startDateTime	presAtm	timeBgn
endDateTime	presAtm	timeEnd
corPres	presCor	mean
startDateTime	presCor	timeBgn
endDateTime	presCor	timeEnd

2. Under "data" folder, add attributes to data product group and each data table group according to the info in the example HDF5 file provided by science team

3. For each location under "qfqm" folder, retrieve following barometric pressure existing L1 data from expanded data set and put them into corresponding columns of "presAtm" data table in the HDF5 file to generate **basic** HDF5 file. Do this for both 1 min and 30 min data.

Table 19-26: Mapping between quality flag fieldName for presBaro existing L1 data stream and fieldname (column) in hdf5 data table for generating basic hdf5 file.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table
staPresFinalQF	presAtm	qfFinl
startDateTime	presAtm	timeBgn
endDateTime	presAtm	timeEnd

4. For each location under "qfqm" folder, retrieve following barometric pressure existing L1 data from expanded data set and put them into corresponding columns of "presAtm" and "presCor" data tables in the HDF5 file to generate **expanded** HDF5 file. Do this for both 1 min and 30 min data. For the qfSci, it is a science review flag. If it does not exist yet by the time the HDF5 file is generated, fill qfSci as 0.

Table 19-27: Mapping between quality flag fieldName for presBaro existing L1 data stream and fieldname (column) in hdf5 data table for generating expaned hdf5 file.

fieldName for existing L1 data stream	HDF5 data table	fieldName (column) in HDF5 data table
staPresAlphaQM	presAtm	qfAlph
staPresBetaQM	presAtm	qfBeta
	presAtm	qfSci
staPresFinalQF	presAtm	qfFinl
startDateTime	presAtm	timeBgn
endDateTime	presAtm	timeEnd
corPresTempQF	presCor	qfTemp
corPresDewPtQF	presCor	qfDew
	presCor	qfSci

corPresFinalQF	presCor	qfFinl
startDateTime	presCor	timeBgn
endDateTime	presCor	timeEnd

5. For each location under "ucrt" folder, retrieve following barometric pressure existing L1 data from expanded data set and put them into corresponding columns of "presAtm" and "presCor" data tables in the HDF5 file. Do this for both 1 min and 30 min data. This step will be identical to generate basic HDF5 file or expanded HDF5 file.

Table 19-28: Mapping between uncertainty fieldName for presBaro existing L1 data stream and fieldname (column) in hdf5 data table.

fieldName for existing L1 data stream	**HDF5 data table**	**fieldName (column) in HDF5 data table**
staPresExpUncert	presAtm	ucrtCal95
staPresStdErMean	presAtm	se
startDateTime	presAtm	timeBgn
endDateTime	presAtm	timeEnd
corPresExpUncert	presCor	ucrtCal95
startDateTime	presCor	timeBgn
endDateTime	presCor	timeEnd

19.3.28 QA/QC Procedure

NA

19.4 Uncertainty

NA

20 FUTURE PLANS AND MODIFICATION

This ATBD will be version controlled, i.e. future developments might results in modifications to this ATBD, which will be documented accordingly.

21 APENDIX

21.1 HDF5 metadata

Table 21-1: List of metadata to be compiled and packaged in the HDF5 files.

fieldName	Field Description	HDF5 Site Group	HDF5 DP Group	Data table specific
		L0p (dp0p)		
LatTow	The Latitude of the tower Reference point	X		
LonTow	The Longitude of the tower Reference point	X		
LvlMeasTow	A list containing the identifier number associated with the meaurement level heights	X		
DistZaxsLvlMeasTow	A list containing approximate tower measurement level heights (m) associted with the tower measurement levels (sensor measurement heights should be calculated using Z provided for each sensor)	X		
TypeEco	The ecosystem type as described by the National Land Cover Database (NLCD)	X		
DistZaxsCnpy	The average height (m) of the canopy above the ground surface	X		
TimeTube	ECSE: transit time (s) for air parcel travels in gas tube at different tower measurement levels	X		
Mfr	Name of the sensor manufacturer		X	
Modl	Sensor model		X	
VersFmw	Firmware version that the sensor is running.		X	
FreqSamp	The frequency the data is being collected in Hertz (Hz)		X	
Cal$PrdFld	The time period interval for field calibration (i.e. daily calibration)		X	
Val$PrdFld	The time period interval for sensor field validation		X	

PrdLvlSamp	ECSE: Time spent on each level for measurements (min)		X	
RtioMoleDryCo2	Calibration gas standard coefficients for CO2 concentration			X
RtioMoleDry12CCo2	Calibration gas standard coefficients for 12CO2 concentration			X
RtioMoleDry13CCo2	Calibration gas standard coefficients for 13CO2 concentration			X
Dlta13CCo2	Calibration gas standard coefficients for isotope δ13C			X
dlta2HH2oLow	Ratio of stable isotopes 2H:1H in low H2O reference standard			X
dlta18OH2oLow	Ratio of stable isotopes 18O:16O in low H2O reference standard			X
dlta2HH2oMed	Ratio of stable isotopes 2H:1H in intermediate H2O reference standard			X
dlta18OH2oMed	Ratio of stable isotopes 18O:16O in intermediate H2O reference standard			X
dlta2HH2oHigh	Ratio of stable isotopes 2H:1H in high H2O reference standard			X
dlta18OH2oHigh	Ratio of stable isotopes 18O:16O in high H2O reference standard			X
sd	Calibration standard coefficient for repeatability (Standard deviation)			X
dfUcrtRaw	Degrees of Freedom for calculating combined uncertainty using raw data			X
ucrtRaw	Calibration standard coefficient for combined uncertainty using raw data			X
ucrtAve	Calibration standard coefficient for combined uncertainty using averaged data			X

dfUcrtAve	Degrees of Freedom for calculating combined uncertainty using averaged data			X
Dspk$Br86$MaxReso	Brock (1986) de-spiking resolution threshold; spike if deviation larger than measurement resolution x Dspk$Br86$MaxReso			X
Dspk$Br86$NumBin	Brock (1986) de-spiking number of initial PDF bins			X
Dspk$Br86$NumWndw	Brock (1986) de-spiking window width of median filter in number of data points; needs to be an odd number			X
Pers$DiffMin	Value threshold for the persistence test, which indicates whether there is a realistic fluctuation of values over a designated period of time			X
Pers$TimeDiff	Time step for the persistence test, which indicates whether there is a realistic fluctuation of values over a designated period of time			X
Rng$Max	Upper threshold for the range test, which indicates whether a datum exceeds a realistic value			X
Rng$Min	Lower threshold for the range test, which indicates whether a datum exceeds a realistic value			X
Step$DiffMax	Threshold for the step test, which indicates whether unusual jumps in the data exist			X
Name	Name of each reported variable			X
Unit	The units of each reported variable			X
L1 (dp01)				
PrdIncrAgrDflt	Step-size by which period aggregation.		X	
PrdWndwAgrDflt	Defining the time-block resolution for which outputs are being reported.		X	
Mfr*	Name of the sensor manufacturer		X	

Modl*	Sensor model		X	
VersFmw*	Firmware version that the sensor is running.		X	
FreqSamp*	The frequency the data is being collected in Hertz (Hz)		X	

*Apply only existing L1 DPs.

22 BIBLIOGRAPHY

Balslev-Clausen, D. M. (2011) Application of cavity ring down spectroscopy to isotopic bio- geo- & climate-sciences & the development of a mid-infrared CRDS analyzer for continuous measurements of N_2O isotopomers (Doctoral dissertation), University of Copenhagen, Denmark.

Bowling, D.R., Tans, P.P. & Monson R.K. (2011) Partitioning net ecosystem carbon exchange with isotopic fluxes of CO_2. *Global Change Biology*, **7**, 127–145.

Busch, K. W. & Busch, M. A. (1997) Cavity ringdown spectroscopy: an ultratrace absorption measurement technique. *ACS Symposium Series,* **720**, 20-33.

Crosson, E. R. (2008) A cavity ring-down analyzer for measuring atmospheric levels of methane, carbon dioxide and water vapor. *Applied Physics*, **92**, 403-408.

Gerald, C. F., and Wheatley, P. O. (1998) Applied numerical analysis. Addison-Wesley, New York. 6th ed. ISBN 10: 020187072X

Griffis, T. J. (2013) Tracing the flow of carbon dioxide and water vapor between the biosphere and atmosphere: a review of optical isotope techniques and their application. *Agricultural and Forest Meteorology*, **174–175**, 85-109.

Hu, Z., Wen, X., Sun, X., Li, L., Yu, G., Lee, X., & Li, S. (2014) Partitioning of evapotranspiration through oxygen isotopic measurements of water pools and fluxes in a temperate grassland. *Journal of Geophysical Research - Biogeosciences*, **119**, 358–372.

Iannone, R. Q., Romanini, D., Cattani, O., Meijer, H. A. J., & Kerstel, E. R. Th. (2010) Water isotope ratio (d2 H and d18O) measurements in atmospheric moisture using an optical feedback cavity enhanced absorption laser spectrometer. *Journal of Geophysical Research*, **115**, D10111, doi:10.1029/2009JD012895.

Korkiakoski, M. (2014) Water vapor correction functions for CO_2 and CH_4 in cavity ring-down spectroscopy (Master's thesis). University of Helsinki, Finland.

LI-COR, Inc. (2016) LI-840A CO2/H2O Gas Analyzer Instruction Manual. https://www.licor.com/documents/y10gor2jal2p3t8ev4hm

Ohkubo, S., Kosugi, Y., Takanashi, S., Matsuo, N., Tani, M. & Nik, A. R. (2008) Vertical profiles and storage fluxes of CO2, heat and water in a tropical rainforest at Pasoh, Peninsular Malaysia. *Tellus B*, **60**, 569–582. DOI: 10.1111/j.1600-0889.2008.00367.x

Randerson, J. T., Still, C. J., Balle´, J. J., Fung, I. Y., Doney, S. C., Tans, P. P., Conway, T. J., White, J. W. C., Vaughn, B., Suits, N. & Denning, A. S. (2002a). Carbon isotope discrimination of arctic and boreal biomes inferred from remote atmospheric measurements and a biosphere-atmosphere model. *Global Biogeochemistry Cycles,* **13**, doi; 10.1029/2001GB001435.

Randerson, J. T., Collatz, G. J., Fessenden, J. E., Munoz, A. D., Still, C. J., Berry, J. A., Fung, I. Suits, N. & Denning, A.S. (2002b) A possible global covariance between terrestrial gross primary production and ^{13}C discrimination: consequences for the atmospheric ^{13}C budget and its response to ENSO. *Global Biogeochemistry Cycles*, **16,** doi:10.1029/2001GB001845.

Wahl, E.H., Fidric, B., Rella, C.W., Koulikov, S., Kharlamov, B., Tan, S., Kachanov, A.A., Richman, B.A., Crosson, E.R., Paldus, B.A., Kalaskar, S. & Bowling, D.R. (2006) Applications of cavity ring-down spectroscopy to high precision isotope ratio measurement of $^{13}C/^{12}C$ in carbon dioxide. *Isotopes Environ Health Studies*, **42**, 21-35.

Werner, C. & Gessler, A. (2011) Diel variations in the carbon isotope composition of respired CO_2 and associated carbon sources: a review of dynamics and mechanisms. *Biogeosciences*, **8**, 2437-2459, doi:10.5194/bg-8-2437-2011.

Wheeler, M., Newman, S., Orr-Ewing, A. & Ashfold, M. (1998) Cavity ring-down spectroscopy. *Journal of the Chemical Society, Faraday Transactions*, **94**, 337-351.

Yakir, D. & Wang, X.F. (1996) Fluxes of CO_2 and water fluxes between terrestrial vegetation and the atmosphere estimated from isotope measurements. *Nature*, **380**, 515–517.

Yepez, E. A. , Williams, D. G. , Scott, R. L. & Lin, G. (2003) Partitioning overstory and understory evapotranspiration in a semiarid savanna woodland from the isotopic composition of water vapor. *Agricultural and forest meteorology*, **119**, 53-68.

Zare, R. N., Kuramoto, D. S., Haase, C., Tan, S. M., Crosson, E. R. & Saad, N. M. R. (2009) High-precision optical measurements of $^{13}C/^{12}C$ isotope ratios in organic compounds at natural abundance. *Proceeding of the National Academy of Sciences of the United States of America*, **106**, 10928-10932, doi:10.1073/pnas.0904230106.