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Ozone Monitor (OZONE) Instrument Handbook

SR Springston
BD Ermold
CJ Flynn
D Chand
JE Shilling

Revised October 2020

ARM

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SR Springston, Brookhaven National Laboratory
D Chand, Pacific Northwest National Laboratory (PNNL)
B Ermold, PNNL
JS Shilling, PNNL
CJ Flynn, University of Oklahoma

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Acronyms and Abbreviations

AAF	ARM Aerial Facility
AGL	above ground level
AMF	ARM Mobile Facility
AMF1	ARM Mobile Facility 1 (includes AOS01 nee MAOS A and MAOS C now sunset)
AMF2	ARM Mobile Facility 2
AMF3	ARM Mobile Facility located at Oliktok Point, Alaska as of September 2020
AOS	aerosol observing system
ARM	Atmospheric Radiation Measurement
ASCII	American Standard Code for Information Interchange
ASI	Ascension Island
atm	atmosphere (unit of pressure)
BNL	Brookhaven National Laboratory
DOE	U.S. Department of Energy
DQPR	Data Quality Problem Report
DQR	Data Quality Report
ENA	Eastern North Atlantic
EPA	Environmental Protection Agency
GUI	Graphical User Interface
IOP	intensive operational period
MAOS	mobile aerosol observing system (an intensively instrumented AOS), renamed AMF1 AOS01
NetCDF	Network Common Data Form
NIST	National Institute of Standards and Technology
NTP	Network Time Protocol
NYS DEC	New York State Department of Environmental Conservation
OLI	Oliktok Point, North Slope of Alaska
OSS	Operations Status System
PFA	perfluoroalkoxy alkane (a fluoropolymer)
QA	quality assurance
QC	quality control
RMS	root mean square
SGP	Southern Great Plains
STP	standard temperature and pressure (273.15 ^{o}C, 1 atm)
UTC	Coordinated Universal Time
UV	ultraviolet
VAC	volts alternating current

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2.0 Contact Information

2.1 Mentor

Stephen R. Springston
Brookhaven National Laboratory, Building 815E
Upton, New York 11973-5000
srs@bnl.gov

2.2 Translators

Duli Chand
Pacific Northwest National Laboratory
902 Battelle Boulevard
P.O. Box 999, MSIN K9-30
Richland, Washington 99352
Duli.Chand@pnnl.gov

John E. Shilling
Pacific Northwest National Laboratory
902 Battelle Boulevard
P.O. Box 999, MSIN K4-28,
Richland, Washington 99352
John.Shilling@pnnl.gov

Connor J. Flynn
University of Oklahoma, School of Meteorology
120 David L Boren Blvd
Norman, Oklahoma 73072
Connor.J.Flynn@ou.edu

2.3 Developer

Brian Ermold
Pacific Northwest National Laboratory
902 Battelle Boulevard
Richland, Washington 99352
Brian.Ermold@pnnl.gov

3.0 Vendor/Developer Contact Information

Thermo Fisher Scientific Inc.
Air Quality Instruments
27 Forge Parkway
Franklin, Massachusetts 02038
www.thermo.com/aqi
508-520-0430

4.0 Instrument Description

The Thermo Fisher Scientific Ozone Analyzer instruments are deployed at multiple ARM surface sites and on the Aerial Facility (AAF) manned aircraft. This covers the ARM Mobile Facility (AMF1) aerosol observing system (AOS01) previously known as MAOS A, ARM Mobile Facility (AMF2) aerosol observing system (AOS02), ARM Mobile Facility (AMF3) aerosol observing system (AOS03), Eastern North Atlantic (ENA) aerosol observing system (AOS06), and the Southern Great Plains (SGP) aerosol observing system (AOS07). The ozone (O_3) instrument is shown in the photograph below.

Figure 1. Model 49i (AAF, AMF1, AMF2, AMF3, ENA, and SGP) (from Ozone Analyzer Manual).

The ozone monitor measures ozone based on absorbance of ultraviolet (UV) light by ozone molecules at a wavelength of 254 nm. The absorbance is directly related to ozone concentration through the Beer-Lambert Law:

$$I/I_0 = e^{-KLC} \quad (1)$$

where

K = molecular absorption coefficient, 308 cm^{-1} (at 0°C and 1 atmosphere)

L = length of cell, 38 cm

C = ozone concentration, in parts per million (ppm)

I = UV light intensity of sample ,with ozone (sample gas)

I_o = UV light intensity of sample, without ozone (reference gas).

This is a classical technique for measuring in situ ozone concentrations. The basic instrument configuration has been the same for at least 20 years with minor enhancements of electronics and the user interface. The dual-cell configuration with selective removal of ozone in the reference cell reduces any response from interfering species. Following each 4-s measurement cycle, the reference and sample cells are reversed, so optical effects (change in lamp output, detector gain, cell cleanliness, etc.) are rejected. In addition, the instrument contains an ozone source to check response and stability over time.

External communication with the monitor is available through an ethernet port configured through the instrument network of the AOS systems. The Model 49i is part of the i-series of Thermo Scientific Instruments. The i-series instruments are designed to interface with external computers through the proprietary Thermo Scientific iPort software. However, this software is somewhat cumbersome and inflexible. Brookhaven National Laboratory has written an interface program in National Instruments LabView that both controls the Model 49i monitor and queries the unit for all measurement and housekeeping data. The LabView virtual interface or "vi" (essentially a program in LabView) ingests all raw data from the instrument and produced output files in a uniform data format, similar to other instruments in the AOS, and described in detail in section 6.0.

Modifications for the instrument include:

1. Addition of a 47-mm x 5-µm Teflon filter on the inlet line.
2. Internal plumbing changes to allow filtered (to remove ozone) ambient air to be used in the photolysis cell (ozone source) for periodic and automatic span checks.

5.0 Measurements Taken

The primary measurement output from the Thermo Scientific Ozone Analyzer is the concentration of the analyte (O_3) reported at 1-s resolution in units of ppbv in ambient air. Note that because of internal pneumatic switching limitations the instrument only makes one independent measurement every 4 seconds. Thus, the same measured concentration is reported repeated roughly four times at the uniform, monotonic 1-s time base used in the AOS systems. Accompanying instrument outputs include sample temperatures, flows, chamber pressure, lamp intensities, and housekeeping information. In addition to the measured fields, there is also a field recording operator comments made at any time while data is being collected.

6.0 ARM AOS Ozone Data

6.1 ARM Data Levels

Data files obtained through the ARM Data Center are distinguished by **data level** denoting specific processing applied by ARM. Data level “00” files are stored *exactly as received* by ARM data collections except that original file names are modified to include a tag identifying the site, facility, source datastream, and the date and time the files were received by the ARM Site Data System. Because the internal content is unchanged, the format of “00”-level files vary widely from data source to data source. In the interest of uniformity and to ensure that critical metadata is provided (even when not available in the native files) ,ARM routinely “ingests” native data into higher data levels stored in NetCDF format. Broadly speaking, ARM data files without ARM standardized QC are termed “a-level”, files with standardized QC with calibration are termed “b-level”, and data files incorporating multiple sources and value-added products are termed “c-level”.

6.1.1 AOS Ozone Native Data (Level 00 or Raw Ozone Data)

The ‘raw’ instrument datastream output includes all parameters reported by the instrument at native frequency of 0.25 to 1 Hz. Metadata are automatically included and saved in hourly ASCII files. The raw data termed level “00” is not relevant for most ARM data users but is archived so that it can be reprocessed if needed.

Metadata are now included in every hourly data file. The metadata are:

Row 1:	Filename
Row 4 (col 1 only):	ARM Climate Research Facility
Row 5:	Site Platform
Row 7:	Last revised date
Row 9:	Instrument
Row 10:	Instrument Serial Number/ARM Inventory Number (WD#)
Row 13:	Instrument Mentor/Affiliation
Rows 14-19:	Comments (operational conditions, calibrations, etc.)
Rows 21-24:	Constants (usually defined in Comments)
Row 35:	Column title
Row 36:	Column units line 1
Row 37:	Column units line 2
Row 40:	First row of data

Data fields in the raw output begin on Row 40 and are:

Date Time	Primary Date/Time stamp yyyy-mm-dd hh:mm:ss as set by the instrument computer and referenced to the site NTP server (or if unavailable, linked to the ‘master’ computer in the AOS)

Inst. Time	Time set on the internal instrument computer hh:mm:ss. This should be equal to the primary Date/Time, but can vary if operator has not set the instrument time. This value is used as a relative number between data lines.
Inst. Date	Date set on the internal instrument computer mm-dd-yyyy. Note this is not a standard format. This value should be equal to the primary Date/Time, but can vary if the operator has not set the instrument time. This value is used only for diagnostic checks.
Flags	%hhhhhhhh (eight hexadecimal digits) showing the state of the instrument. The meaning of individual flags is described in Figure 2 taken from vendor manual, shown below:

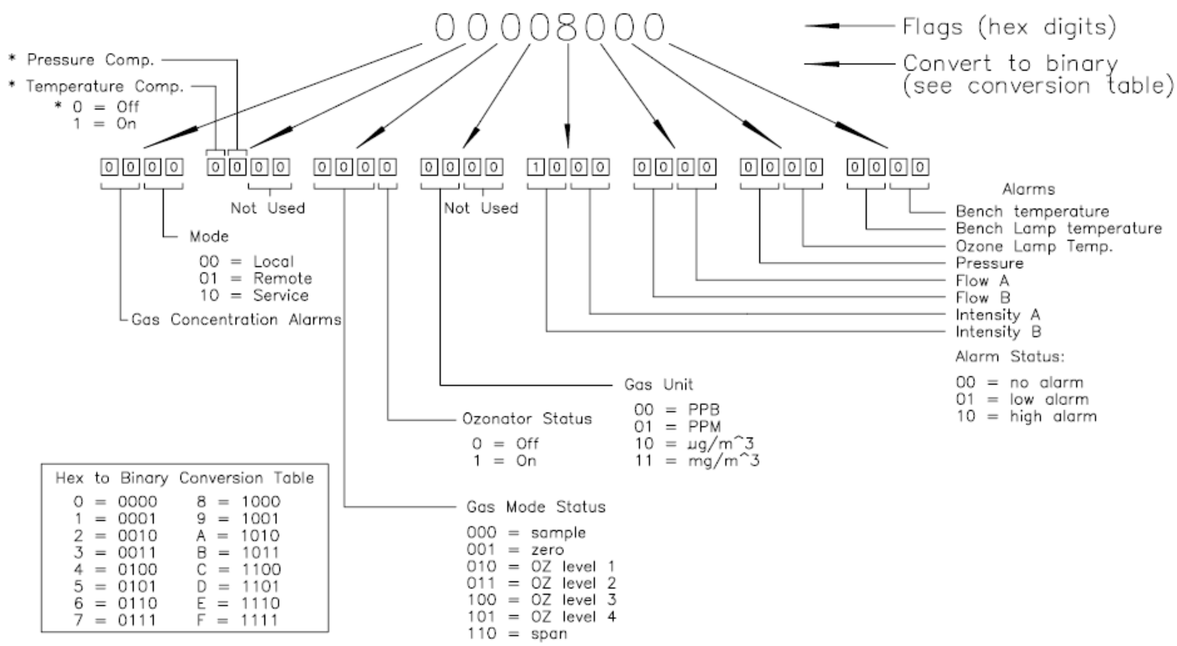

Figure 2. Bit-by-bit meaning of status flag.

O3	Mixing ratio (in ppbv) of ozone at ambient temperature, pressure, and relative humidity.
Pres	Pressure inside the measurement cell (mm Hg).
Bench Temp	Temperature (°C) of the measurement cell. The bench is temperature controlled by a heater in a feedback loop.
O_3 Lamp Temp	Temperature (°C) of the ozone lamp (the lamp used to measure ozone, NOT the other lamp used to generate calibration gas. The lamp block is temperature controlled by a heater in a feedback loop.

Flow A	Flow through cell A (SLPM). This flow is not calibrated. It is useful to indicate a dirty or blocked inlet filter. The reported measurement is not directly affected by flow.
Flow B	Flow through cell B (SLPM). This flow is not calibrated. It is useful to indicate a dirty or blocked inlet filter. The reported measurement is not directly affected by flow.
Noise A	Electronic noise in channel A. This value is normally < 10. Excess values can indicate need to clean the cell or replace the lamp.
Noise B	Electronic noise in channel B. This value is normally < 10. Excess values can indicate need to clean the cell or replace the lamp.
Avg Time	Time in seconds that gas flows through the reference and sample cells before switching the cells. If the instrument is set for fast response (default for AOS systems), the value reported is 2.5X the actual averaging time. Thus all measurements in AOS systems are reported as 10 s when the averaging time is actually 4 s.
Cell A Int	The raw detector value in Hz. This is a measurement of lamp throughput for the system. When the Intensity goes below ~60,000, the lamp voltage must be increased or the lamp replaced.
Cell B Int	Same as Cell A Int except for Cell B.
Lamp temp	Temperature (^oC) for the ozonizer lamp. This temperature is controlled in a feedback loop.
Lamp Volt Bench	Control voltage driving the main (analytical lamp).
Lamp Volt OZ	Control voltage driving the ozonizer (calibration lamp).
Range	This controls the analog output and is not germane to the digital recording.
Lamp	Percentage setting of the ozonizer lamp. Should not be changed.
O_3 Coef	A nominal slope coefficient to the nominal ozone value to a calibrated ozone value. This coefficient should not be changed. Calibrations are done relative to the ‘nominal’ ozone signal output.
O_3 Bkg	A nominal offset to the nominal ozone value to a calibrated ozone value. This offset should not be changed. Calibrations are done relative to the ‘nominal’ ozone signal output.
Diag Volt mb 24	Diagnostic point for the 24V PS on the motherboard.
Diag Volt mb 15	Diagnostic point for the 15V PS on the motherboard.

Diag Volt mb 5	Diagnostic point for the 5V PS on the motherboard.
Diag Volt mb 3.3	Diagnostic point for the 3.3V PS on the motherboard.
Diag Volt mb -3.3	Diagnostic point for the -3.3V PS on the motherboard.
Diag Volt mib 24	Diagnostic point for the 24V PS on the measurement interface board.
Diag Volt mib 15	Diagnostic point for the 15V PS on the measurement interface board.
Diag Volt mib -15	Diagnostic point for the -15V PS on the measurement interface board.
Diag Volt mib 5	Diagnostic point for the 5V PS on the measurement interface board.
Diag Volt mib 3.3	Diagnostic point for the 3.3V PS on the measurement interface board.
L1 – L5	These are levels (in %) to drive the calibration lamp during span checks. These values were set after calibration against the New York State Department of Environmental Conservation (NYS DEC) calibration of the individual instruments.
Pres Comp	On/Off Flag to determine whether pressure compensation is applied. This flag should be on.
Temp Comp	On/Off Flag to determine whether temperature compensation is applied. This flag should be on.
OZ Status	On/Off Flag to determine the ozonizer status.
Gas Units	Units of measurement. Should always be ppb.
Gas Status	Instrument output. Sample, Zero, Levels 1-5.
Comment	This field is the last field in the datastream. It allows operators to enter free-form text from the graphical user interface at any time. Operational notes or disruptions may be entered here.

These data are saved unaltered from what is produced by the instrument. Processing of the raw data must be able to deal with more than 1 record per second and time periods with either no data or only a date/time stamp in the record. If the instrument does not output data, the instrument computer can include a record of empty fields. Since neither the instrument clock nor the instrument computer clock are perfect, minor irregularities (dithering) in the output datastream invariably occur.

6.1.2 Level a1 Ozone Data

The raw (00 level) data are ingested for uniformity to NetCDF format, which is designated the “a1” data level. NetCDF is a platform-independent scientific data format that supports incorporation of scientific data and metadata. The NetCDF is a commonly used scientific format, very compact, and can hold the data in multiple dimensions. All the fields from raw (00) data are processed ingested into an a1. Generally, a1 data are also of less interest to most ARM users as higher levels (e.g., b1, c1) of the data will have additional calibrations and QA/QC applied. As an example, the name of a1 Ozone data file beginning at midnight, October 8 2013 at ENA site (C1) is 'enaaoso3C1.a1.20131008.000000.nc'. Field names of the ingested/translated data along with units and other information are listed in the table below:

Table 1. Field names of ingested/translated data with units and other information.

Variable full name	Variable name used in DOD	Unit
Time of record	time_of_last_state_change	seconds since 1970-1-1 00:00:00
Ozone concentration	o3	ppbv
Ozone pressure	o3_pressure	kPa
Bench temperature	o3_bench_temperature	degC
Ozone lamp temperature	o3_lamp_temperature	degC
Flow in cell A	flow_a	L/min
Flow in cell B	flow_b	L/min
Electric noise in cell A	noise_a	Hz
Electric noise in cell B	noise_b	Hz
Instrument averaging time	averaging_time	s
Intensity in cell A	intensity_a	Hz
Intensity in cell B	intensity_b	Hz
Lamp temperature	lamp_temperature	degC
Lamp bench voltage	lamp_voltage_bench	V
Lamp voltage ozonizer	lamp_voltage_ozonizer	V
Lamp level	lamp_level	%
Instrument range setting	range	ppbv
Instrument ozone coefficient	o3_coefficient	unitless
Ozone background	o3_background	ppbv
Calibration ratio level 1	calibration_level_1	%
Calibration ratio level 2	calibration_level_2	%
Calibration ratio level 3	calibration_level_3	%
Calibration ratio level 4	calibration_level_4	%
Calibration ratio level 5	calibration_level_5	%
Pressure compensation state	pressure_compensation_state	unitless
Temperature compensation state	temperature_compensation_state	unitless
Ozone lamp state	o3_lamp_state	unitless
Gas state	gas_state	unitless

Variable full name	Variable name used in DOD	Unit
Diagnostic +24 volts at motherboard	diagnostic_voltage_mb_24	V
Diagnostic +15 volts at motherboard	diagnostic_voltage_mb_15	V
Diagnostic +5 volts at motherboard	diagnostic_voltage_mb_5	V
Diagnostic +3.3 volt at motherboard	diagnostic_voltage_mb_3p3	V
Diagnostic -3.3 volts at motherboard	diagnostic_voltage_mb_minus_3p3	V
Diagnostic +24 volts at measurement interface board	diagnostic_voltage_mib_24	V
Diagnostic +15 volts at measurement interface board	diagnostic_voltage_mib_15	V
Diagnostic -15 volts at measurement interface board	diagnostic_voltage_mib_minus_15	V
Diagnostic +5 volts at measurement interface board	diagnostic_voltage_mib_5	V
Diagnostic +3.3 volts at measurement interface board	diagnostic_voltage_mib_3p3	V
Ozone flag string	o3_flags	Unitless
North latitude	Lat	degree_N
East longitude	Lon	degree_E
Altitude above mean sea level	Alt	m

6.1.3 Level b0 and b1 Ozone Data

The ingested "a1" level of the data described in section 6.1.2 are further processed to: 1) add more QC checks on data quality, 2) subtract a baseline representing the instrument's ozone reading when presented with zero air, and 3) apply a linear calibration coefficient to account for slight deviations from Equation 1. During normal operations, the instrument is challenged twice a day with zero air that has been scrubbed of ozone. The measurement value during these zero periods represent an instrument baseline that must be removed from sample measurements. Examination of the data showed that this instrument baseline in a1 version drifts slowly in time and that individual measurements were too noisy for direct use. Therefore, we calculate the instrument baseline from data a1 by moving average for 3-6 weeks. The estimation of the zero baseline is saved in data level b0. The b0 data, stored as intermediate records, is needed to calculate the b1 data and is not intended for ARM users.

In addition, we apply a linear calibration coefficient determined by the instrument mentor from a five-point span check measured at the NYS DEC standards laboratory. Several data fields are subjected to automated QC checks and the results of these checks are bit-packed into a single QC variable (qc_ o3), which provides a metric for data reliability. Like the a1 level, the higher-processed b0 and b1 level of the data are also stored in 'nc' format. As an example, the name of b1 level of ozone data file for October 8 2013 at ENA site (C1) is 'enaaoso3C1.b1.20131008.000000.nc'. All the field names in b1 level are the same as a1, except quality check results on field 'ozone concentration' (qc_o3). The qc_o3 is unitless, has bits, as described in the list below. Also, the O_3 concentrations in b1 are calibrated values with revised

QCs in each b1 file. Some of the fields (e.g., instrument pressure warnings), are specified by the mentor uniquely for each site and or intensive operational period (IOP). The quality flags qc_o3(time):int] and its inputs are listed below:

qc_o3(time):int
long_name = Quality check results on field: ozone concentration
units = unitless
description = This field contains bit-packed integer values, where each bit represents a QC test on the data. Non-zero bits indicate the QC condition given in the description for those bits; a value of 0 (no bits set) indicates the data has not failed any QC tests.
pressure_min_warning:float
pressure_max_warning:float
bench_temp_min_alarm:float
bench_temp_max_alarm:float
lamp_temp_min_alarm:float
lamp_temp_max_alarm:float
flow_a_min_alarm:float
flow_a_max_alarm:float
flow_b_min_alarm:float
flow_b_max_alarm:float
noise_a_min_alarm:float
noise_a_max_alarm:float
noise_b_min_alarm:float
noise_b_max_alarm:float
intensity_a_min_alarm:float
intensity_a_max_alarm:float
intensity_b_min_alarm:float
intensity_b_max_alarm:float
lamp_voltage_bench_min_alarm:float
lamp_voltage_bench_max_alarm:float
lamp_voltage_ozonizer_min_alarm:float
lamp_voltage_ozonizer_max_alarm:float
o3_coefficient_min_warning:float
o3_coefficient_max_warning:float
o3_background_min_warning:float
o3_background_max_warning:float
o3_lamp_temperature_min_alarm:float
o3_lamp_temperature_max_alarm:float
lead_alarm:float
lag_alarm:float
flag_method = bit
bit_1_description = Value is equal to missing_value (least significant bit)
bit_1_assessment = Bad
bit_2_description = Value is less than the valid_min.
bit_2_assessment = Bad
bit_3_description = Value is greater than the valid_max.
bit_3_assessment = Bad
bit_4_description = pressure < pressure_min_warning OR pressure > pressure_max_warning
bit_4_assessment = Indeterminate

bit_5_description = bench_temperature < bench_temp_min_alarm OR bench_temperature > bench_temp_max_alarm
bit_5_assessment = Bad
bit_6_description = lamp_temperature < lamp_temp_min_alarm OR lamp_temperature > lamp_temp_max_alarm
bit_6_assessment = Bad
bit_7_description = flow_a < flow_a_min_alarm OR flow_a > flow_a_max_alarm
bit_7_assessment = Bad
bit_8_description = flow_b < flow_b_min_alarm OR flow_b > flow_b_max_alarm
bit_8_assessment = Bad
bit_9_description = noise_a < noise_a_min_alarm OR noise_a > noise_a_max_alarm
bit_9_assessment = Bad
bit_10_description = noise_b < noise_b_min_alarm OR noise_b > noise_b_max_alarm
bit_10_assessment = Bad
bit_11_description = intensity_a < intensity_a_min_alarm OR intensity_a > intensity_a_max_alarm
bit_11_assessment = Bad
bit_12_description = intensity_b < intensity_b_min_alarm OR intensity_b > intensity_b_max_alarm
bit_12_assessment = Bad
bit_13_description = lamp_voltage_bench < lamp_voltage_bench_min_alarm OR lamp_voltage_bench > lamp_voltage_bench_max_alarm
bit_13_assessment = Bad
bit_14_description = lamp_voltage_ozonizer < lamp_voltage_ozonizer_min_alarm OR lamp_voltage_ozonizer > lamp_voltage_ozonizer_max_alarm
bit_14_assessment = Bad
bit_15_description = o3_coefficient < o3_coefficient_min_warning OR o3_coefficient > o3_coefficient_max_warning
bit_15_assessment = Indeterminate
bit_16_description = o3_background < o3_background_min_warning OR o3_background > o3_background_max_warning
bit_16_assessment = Indeterminate
bit_17_description = o3_lamp_temperature < o3_lamp_temperature_min_alarm OR o3_lamp_temperature > o3_lamp_temperature_max_alarm
bit_17_assessment = Bad
bit_18_description = pressure_compensation_state = 0 OR temperature_compensation_state = 0 OR o3_lamp_state = 0 OR gas_state not = 1
bit_18_assessment = Bad
bit_19_description = non-equilibrium conditions, (time - time_of_last_state_change) > lead_alarm AND (time - time_of_last_state_change) < lag_alarm
bit_19_assessment = Bad
bit_20_description = Scheduled calibration
bit_20_assessment = Bad
operational_qc_bits:int = 19, 20
operational_qc_explanation = These tests will frequently be flagged during normal operation and should be ignored by DQO metrics

6.1.4 Filename Conventions and File Structure

The first data retrieved from the instrument have been processed from the ‘raw’ datastream (level 00). In general, the raw data from site are processed in 1-month chunks (for the AAF, the files are by each flight). For each month (or other period), three files are produced from the raw data.

The raw data are processed to get a1 files and a1 files are further processed to get the b0 and b1 level of the data files. The a1 and b0 levels of the data are updated and processed daily, but since b1 data use the estimated baseline from moving averages, the b1 file availability will be delayed in time. The naming conventions of raw (00) and processed (a1 and b1) are listed below:

[site][platform][subsite].[species].[resolution].[level].[date].[time].[processing level].[delimiter]{.log.txt | .plots.pdf}

[site][platform][species][subsite].[level **xx**].[date].[processing info].[nc}

Where:

[site]	The site of the measurement (usually the 3-letter specifier of the nearest airport)
[platform]	The structure used for the instrument (aos)
[subsite]	The subsite of the sampling site (M1 : main site | S1 : supplemental site | E13 : extended site)
[species]	Species measured – for this instrument this is ‘o3’
[resolution]	[xxs] (xx: two significant figures, s: time units string – s = seconds, m = minutes, h = hours, d = day, w = week, M = month) Typically this is always s or m
[level]	Level of this data. Always use the highest-level number with this name
[date]	Date of first point in file (yyyymmdd)
[time]	Time of first point in file (hhmmss)
[processing level]	This is either ‘raw’ for ‘raw’ data or ‘m02’ for mentor-QA/QCd data with only ambient measurements (zeros and calibrations removed), vetted and all appropriate calibration factors used in processing.
[processing info]	000000, 000001, 000002 etc.
[delimiter]	Typically this is ‘tsv’ for tab-separated values, but could be ‘csv’ for comma separated values.
{.log.txt | .plots.pdf}	Optional extension. In addition to the data file, the mentor prepares a .log.txt file containing explanations of processing unique for this time period and a plots.pdf file with time series plots of processed data.
[level xx]	“a1” or “b0, or “b1”. Quality assurance increase from a1 to b1. The b1 data are calibrated and quality assured at highest-quality level.

The 00 ozone data from all AMF/AMF instruments follow the file structure used for most U.S. Department of Energy/Brookhaven National Laboratory/AOS instruments:

File Structure:

Row 1:	Filename
Row 4 (col 1 only):	ARM Climate Research Facility
Row 5:	Site Platform
Row 7:	Last revised date
Row 9:	Instrument
Row 13:	Instrument Mentor/Affiliation
Rows 14-19:	Comments (operational conditions, calibrations, etc.)
Rows 21-24:	Constants (usually defined in Comments)
Row 35:	Column title
Row 36:	Column units line 1
Row 37:	Column units line 2
Row 40:	First row of data

Beginning in 2014, raw data have all the metadata described above. Data are given in an arbitrary number of columns. The first column is date/time.

Time - Time is reported in UTC as set by an NTP server. Following convention, the time is the beginning of the period. The parameter reported at this time is the average of all points >= the time and < the next time. Data are reported at 1- s resolution. All non-operational periods have been removed (empty field or NAN). As per convention, data are reported as tab-delimited ASCII files. Files are formatted such that they are self-documenting.

Data Columns (for mentor-QA/QC data):

Column 1: Date Time – All times are in UTC as yyyy-mm-dd hh:mm:ss{.ss} and are the beginning of the time period. All data reported here correspond to data from samples taken >= this time and < than this time + the data increment.

Column 2: [Ozone] – Mixing volume of O_3 in ambient air (no water vapor correction). This is this instrument's primary measurement.

The a0 data are ingested to get the a1 data; a1 data are processed to add the QCs and calibration in the b1-level data. The QCs for data b1 are defined in section previous section (6.1.3).

6.2 Data Ordering

Ozone data collected are distributed through the ARM Data Center and are presently updated daily or weekly intervals (a1 and b1) and monthly (a0). All the ARM data can be downloaded at the ARM website https://www.arm.gov/data. At this website, the ARM Discovery box 'Get ARM Data' can be used to select and filter the desired data sets in ASCII-CSV and NetCDF formats.

6.3 Data Plots

6.3.1 Level 'a0' Data Plots

The mentor-edited monthly data plots of O3 raw data (Figure 3, 4), housekeeping (Figure 5, 6), and final data sets (Figure 7), typical plots, and explanations are shown in the section below. More plots and quicklooks routinely O3 produced by ARM can be downloaded from the Data Quality Office (DQO) at the web link https://dq.arm.gov/dq-plotbrowser/).

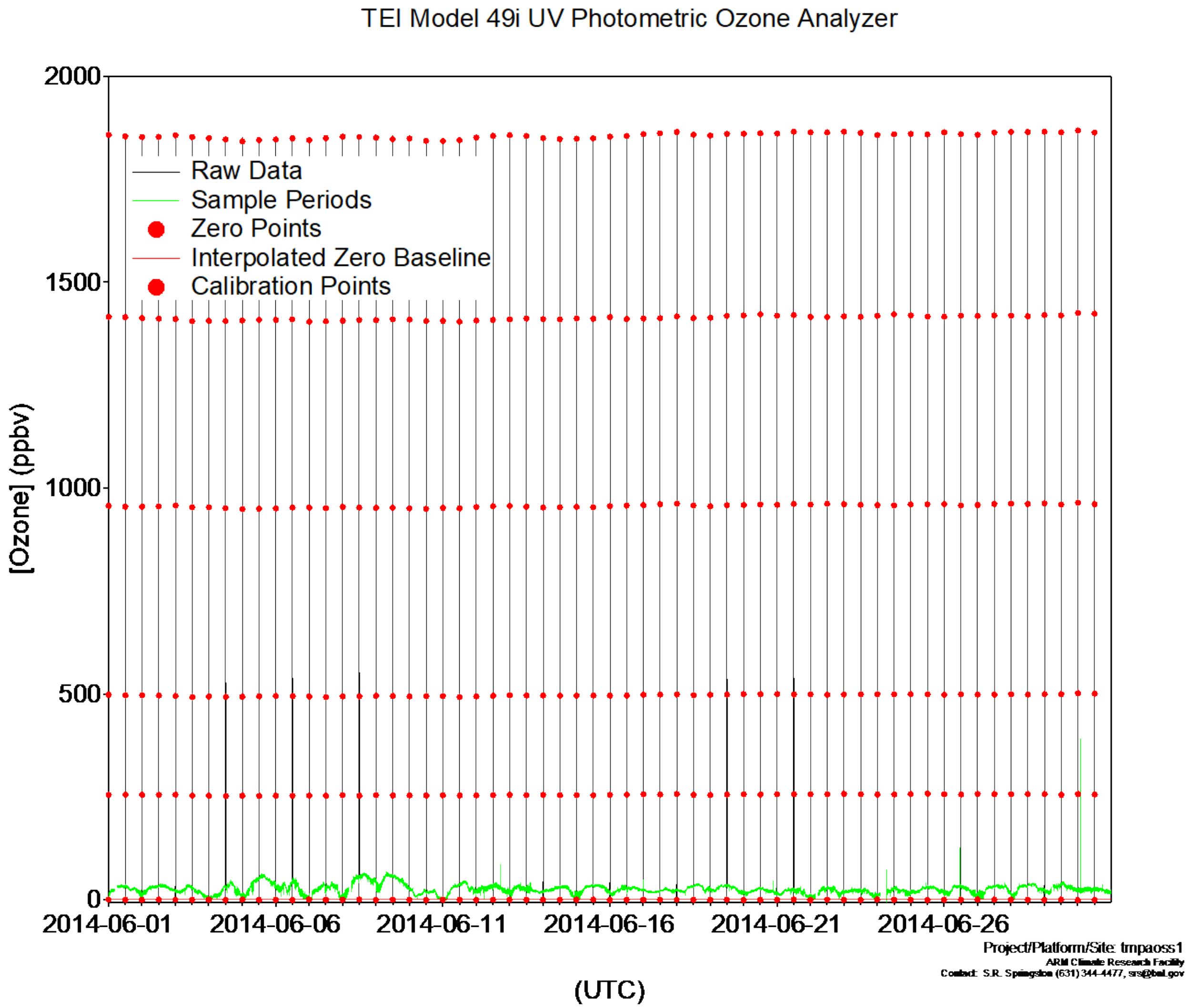

Figure 3. Raw ozone data for one month.

The raw data plot shows all signal data recorded from the instrument. Processing software is used to parse the data into sampling and zero/calibration periods. Every midnight and noon, the instrument goes into an automatic zero and span check. A blow-up of one of these periods is shown in Figure 4.

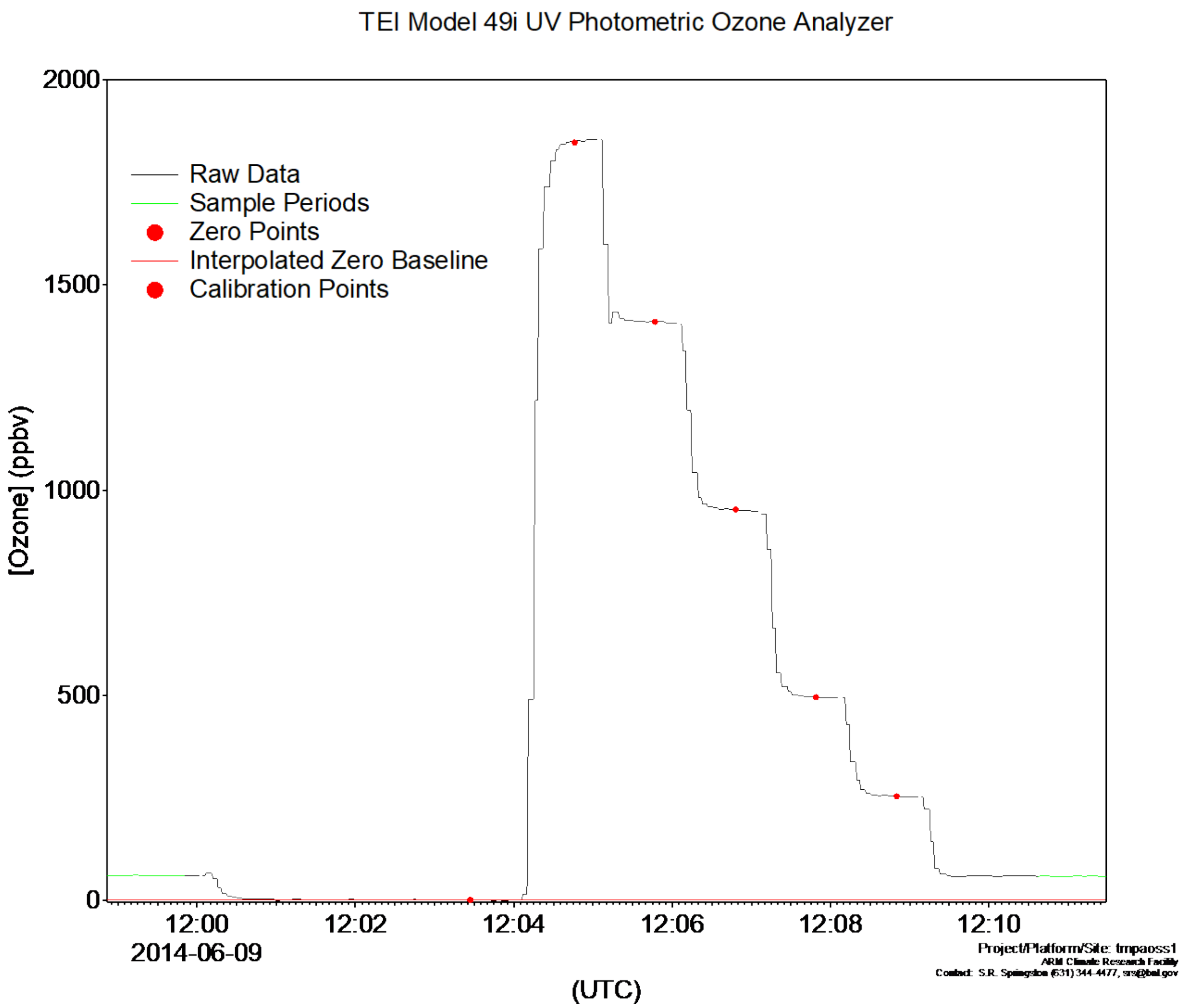

Figure 4. Typical zero, span check.

Sample periods are automatically delineated with time allowed for measurements to re-stabilize. The centroids (numerical averages) of zeros and span checks are shown by the red circles in Figure 4.

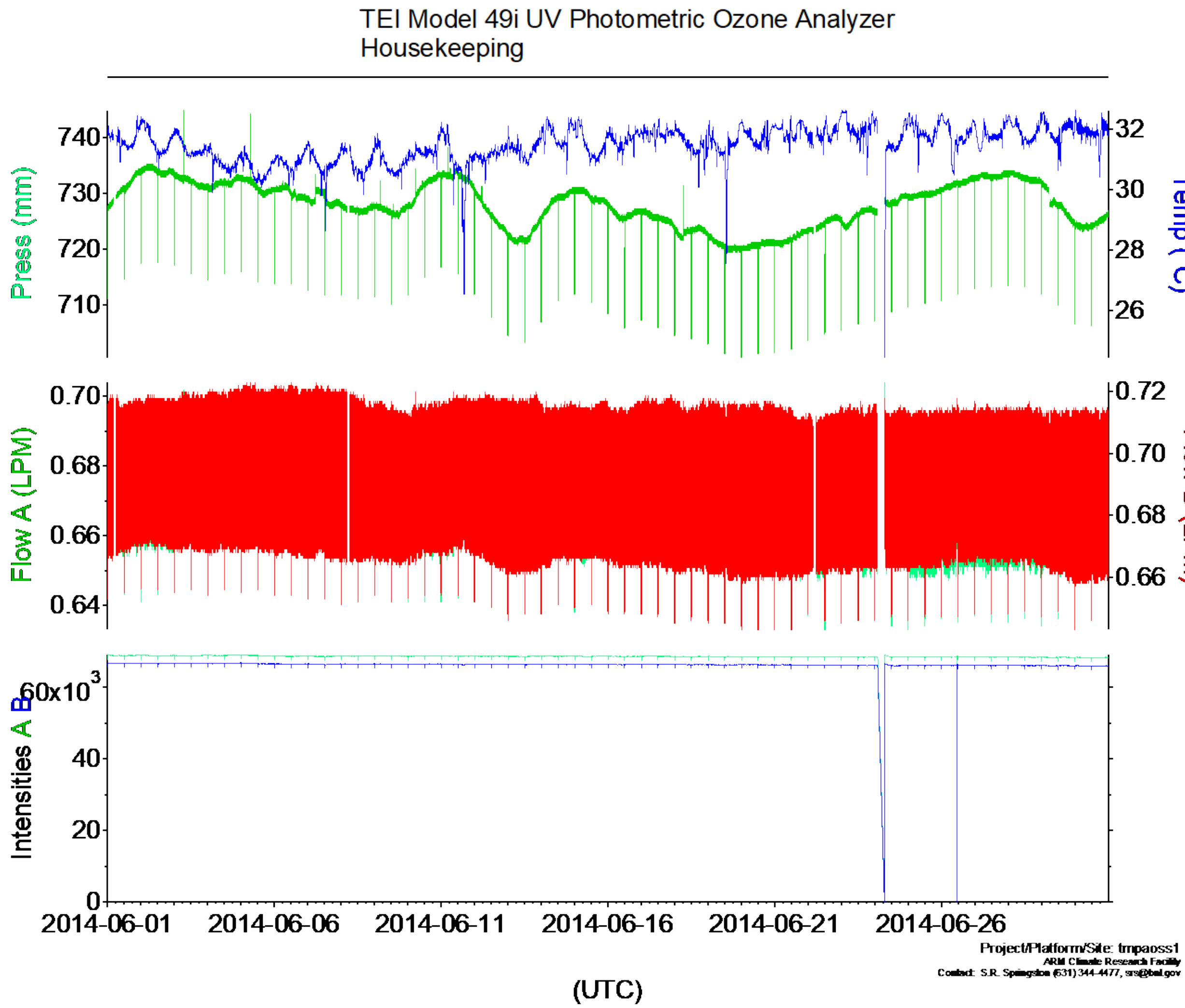

Figure 5. Housekeeping data for one month.

The sample cell pressure and temperature are shown in the top panel. These values are used internally by the instrument to report ozone concentrations at STP (1 atm, 0ºC). The twice-daily negative spikes in pressure are momentary and due to flow interruptions proximate to the zero/span checks. The flows in the two cells are shown in the middle panel. While this technique is fundamentally a concentration-sensitive detector (independent of flow rate), the flows do affect the concentration of ozone generated for the span checks. The raw lamp intensities for the two channels are shown in the bottom panel. When these reduce to below 60,000 Hz, the lamp intensity is raised by the mentor to 110-120,000 Hz. Generally, the intensity does not affect the instrument response.

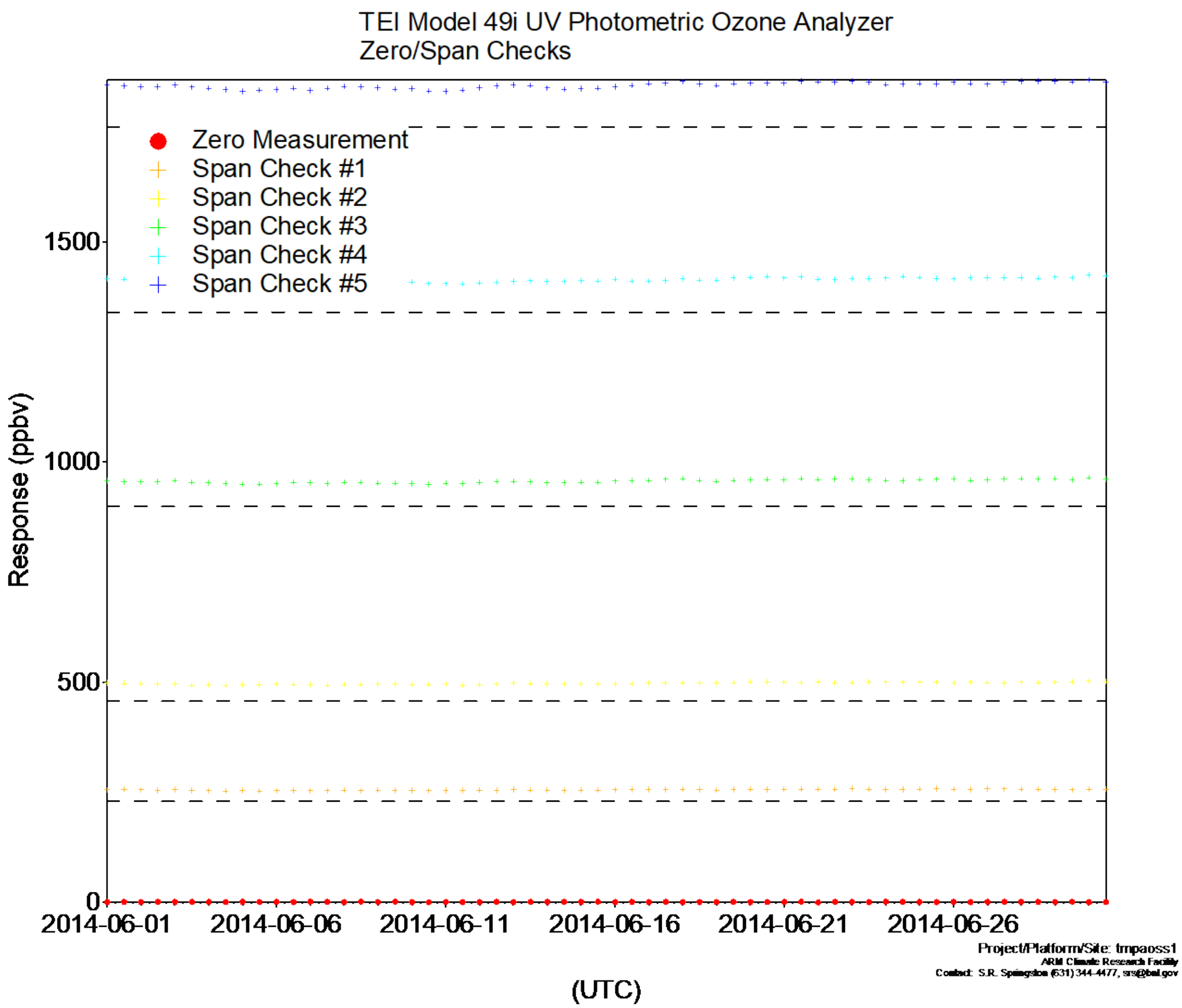

Figure 6. Zero and span check stability over one month.

A one-month record of zero and span checks is shown in Figure 6. The dotted lines are the responses for the five span checks measured at the NYS DEC standards laboratory after receipt of the instrument. The difference between the measured span and the calibrated span value is usually less than 5%. This difference is judged to be instability and drift in the photolysis lamp and NOT in the measurement cell. Drift in the span response is monitored over long periods (> 1 year) and drifts of more than 5% indicate need for recalibration at the NYS DEC laboratory.

A monthlong data set is shown in Figure 7: here the ambient ozone concentrations are adjusted for any baseline drift. Here the peaks in O_3 are as a result of diurnal variations (local photochemistry) and/or transport from adjacent areas.

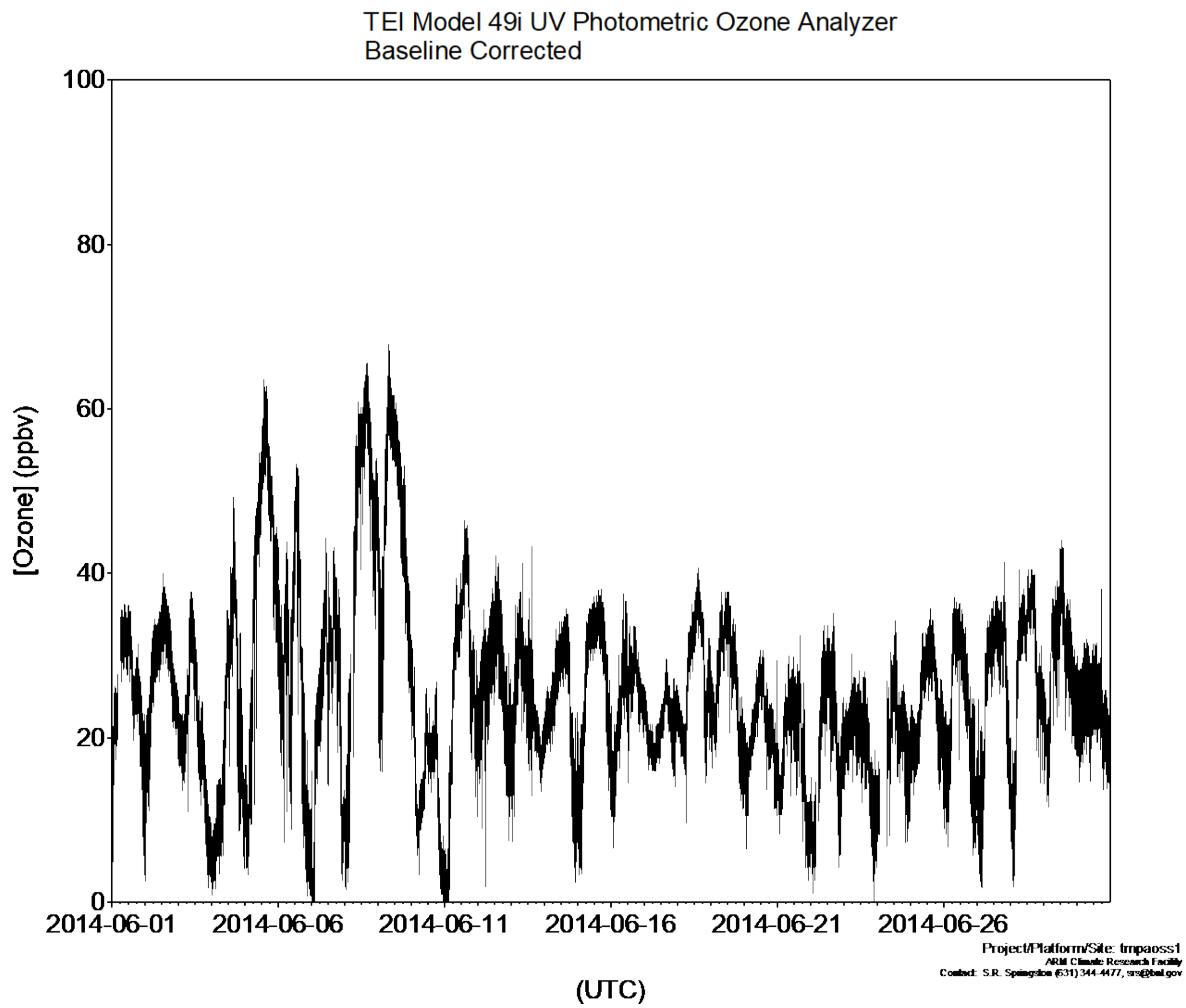

Figure 7. Processed data for one month.

Figure 7 shows a typical month's ambient data record. A diurnal pattern is (usually) present since ambient ozone is predominantly produced by photochemistry. Night-time removal of ozone occurs by dry deposition, dilution, and reaction with other trace gases.

6.3.2 Level 'a1' Data Plots

Ozone and some other selected fields from a1-level data are plotted from ARM ENA site for 2013-10-12. The wide range of the O_3 calibration has compressed the fine O_3 variability on y-axis in the top left panel of Figure 8.

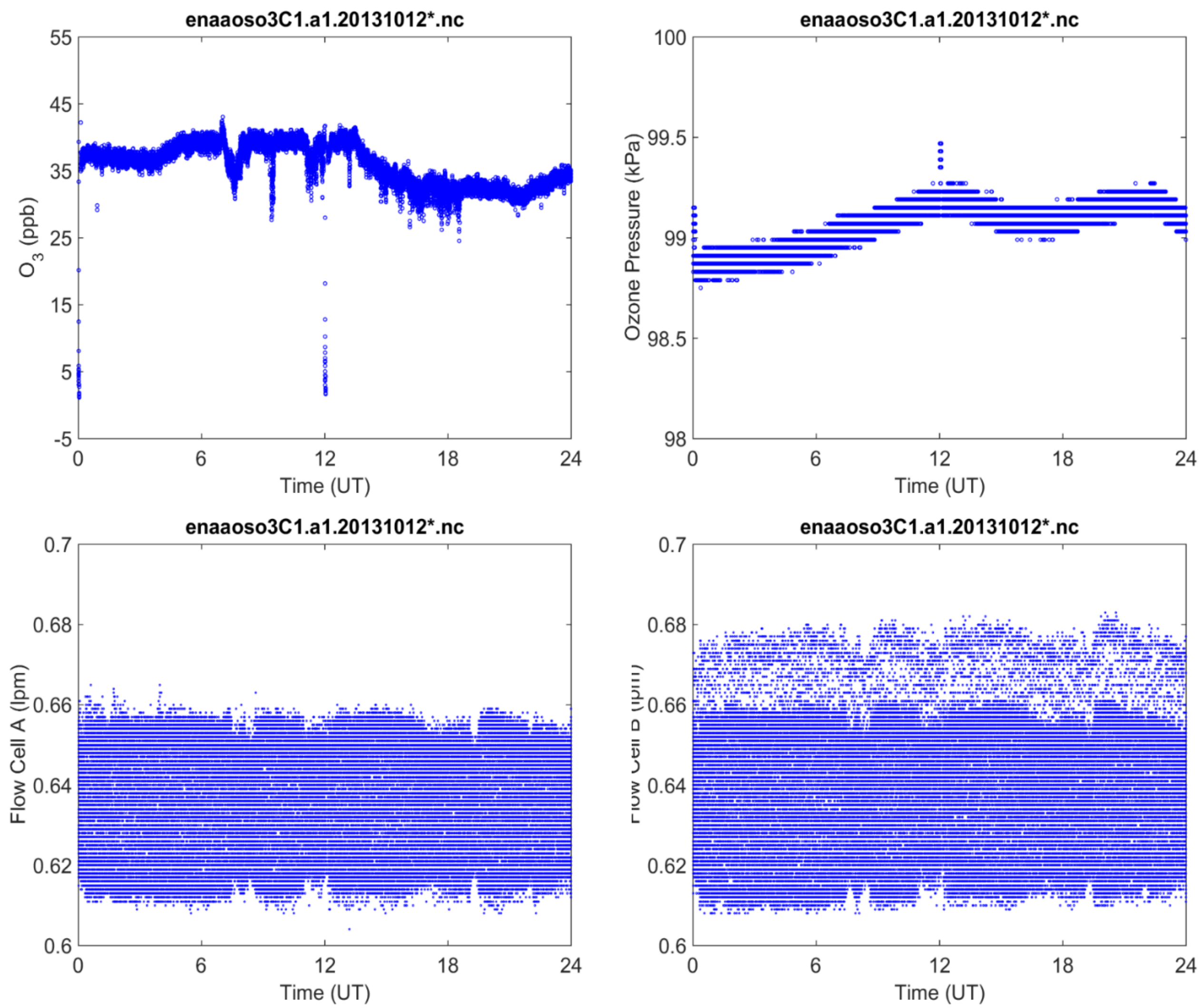

Figure 8. Ozone concentration (top left), cell pressure (top right) and sample flow in cell-A and B (lower panels) for October 12 2013 at ENA site. The O_3 dips in top left panel are the zero calibrations made at 00 and 12 UTC. The O_3 spans often > 60 ppb, are out of scale and not shown on the top left panel.

6.3.3 Level "b1" Data Plots

Calibrated ozone concentrations from 'b1'-level data are plotted from the ARM SGP, Oliktok Point (OLI), and ENA sites for multiple months, as shown in Figure 9. The blue symbols are calibrated O_3 from ARM automatic production and the red symbols are mentor-edited (labor-intensive) data. The ARM algorithm-generated data are within 1% of the mentor-edited data. Overall, the comparison looks reasonable except a small difference at OLI (the ARM production systematically overestimates around 1 ppbv of O_3). This is likely due to the difference in offsets (zeros). Taking mentor-edited data as the gold standard, the small difference in automated processed data from ARM O_3 may be due to the O_3_zero fit calculation from the moving average in ARM production. There are some challenges running the instruments 24/7 at the OLI site, so routine switching on/off may cause some shift in O_3 zero.

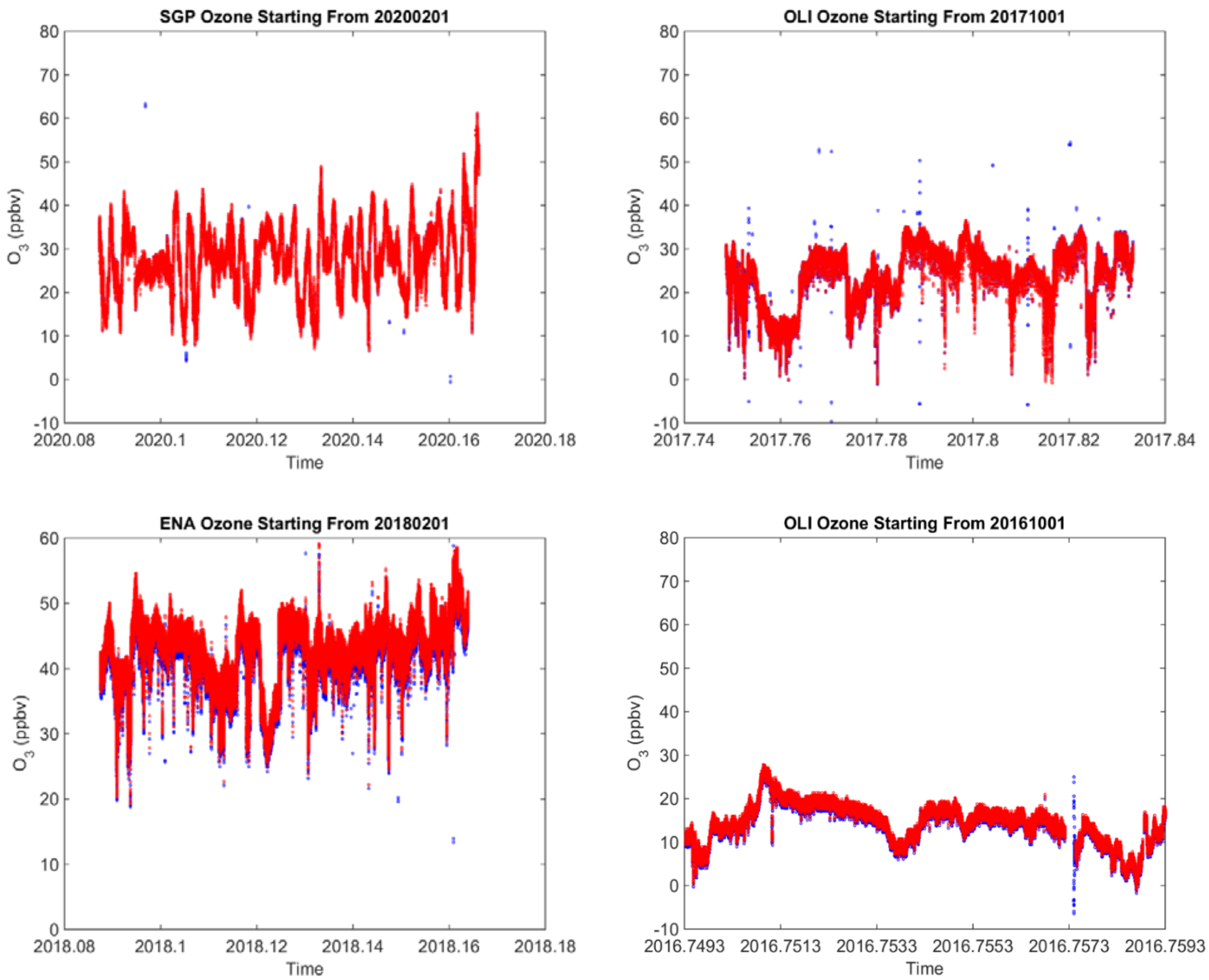

Figure 9. Ozone concentration at SGP (top left), ENA (bottom left), and OLI (right panels) for multiple months or years. The blue symbols are calibrated O_3 from ARM routine production and the red symbols are mentor-edited (manual) data.

6.4 Data Quality Checks

The level of b0 and b1 O_3 data quality is automatic flagging of data when the instrument changes states during zero and span checks. Normally this eliminates the first 105 seconds after the zero is actuated and then the first 30 seconds after each span level. The zero sampling time period can vary with flow; we use the zero and spans when the O_3 signal is stable with time, for example, an average of ~30 seconds once a stable level has been achieved for each span/state.

The second level of data quality is inspection of the 2X daily zeros and span checks. Data are assessed for possible short-term (few weeks) and long-term (years) drifts with a defined relative standard deviation and minimal drift (<2%). Values greater than this drift indicate a need for instrument recalibration at the NY DEC. At present, there is no capability within ARM to deliver a calibration source for ozone to remote field sites, but we bring the instruments back to the laboratory and calibrate them from time to time.

Instrument flow rates do not directly affect the instrument response but do affect the span check values. Under normal operation two factors can change the instrument flow rate: dirt accumulation on the inlet filter or degradation of the internal diaphragm pump. Given the two-week filter change schedule, dirt accumulation is not observed to reduce flow. Drastic changes in flow, pressure, temperature, and other instrumental conditions are stored with different quality fields, as shown in Figure 10. Pump life under continuous operation is 2-3 years.

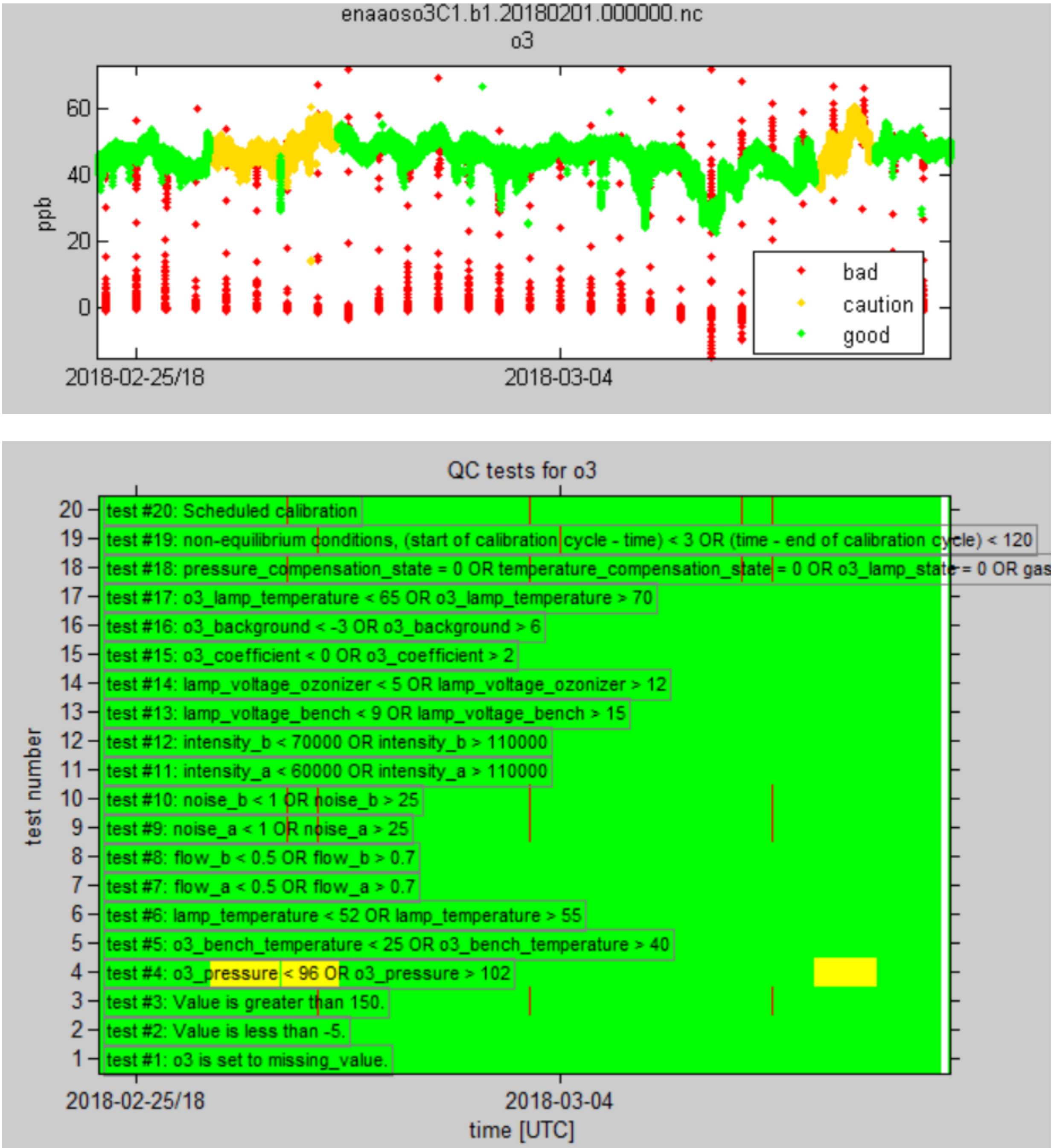

Figure 10. An example of ozone concentration at ENA (top), and the QCs bit test (bottom panel). Green color means everything is good, yellow is a warning sign, and red means abnormal operations.

The third level of data quality and assessment deals with visual inspection of the output datastream. Periods when the instrument is not operating properly are identified and flagged. Either an instrument failure or an inlet failure causes such periods. In some cases, operators note problems with the instrument, but more often it is up to the mentor to recognize nonsensical values and determine the cause(s). The complete recording of all instrument and inlet housekeeping aids in this diagnosis. Except for pump/inlet failures and several instances where the inlet filter was replaced with an impermeable spacer (documented below), mentors have not experienced any pattern of failures that could be algorithmically identified. Failures, their identification and remedy, and the mentor write-up in the DQPR/DQR system tend to be unique individual events.

One phenomenon requiring visual inspection involves short aberrations in the output signal. These are primarily of 4-s duration (one measurement cycle) and can be positive or negative. Because of the mixing ratio in the inlet, sample lines, and instrument dead volume, a step function in actual atmospheric concentrations on this time scale is nonsensical. However, a 20-40 ppbv spike dramatically affects daily max/min readings. So, these excursions are flagged. Note that these instrumental spikes are visually quite distinguishable from negative peaks of 30-s to 10-min duration from local internal combustion sources that produce nitric oxide (NO) which then titrates (reduces) the local ambient ozone. Note that negative peaks from titration represent real changes in the ambient ozone concentration and are not flagged. Distinguishing ambient (negative) ozone spikes from spurious instrumental spikes requires a certain amount of experience and judgment. Local sources can in some instances be identified by referring to the wind direction measured at the point of sampling. but identification of local interference is quite subjective.

6.5 Calibration Database

The Thermo Scientific ozone monitors are calibrated for response upon receipt from the manufacturer. This is done by the mentor at the NYS DEC testing laboratory at Albany. These results are tabulated by the mentor and put into ARM’s Operations Status System (OSS). The DEC reference standard is used only for calibration of ozone instruments and is certified by the U.S. Environmental Protection Agency (EPA) with a National Institute of Standards and Technology (NIST)-traceable reference. All the calibration data (zero, spans, and NYS DEC testing data sets) are used to make the b1 level of the O_3 datastream.

7.0 Technical Specification

7.1 Units

The measured quantity of interest is the mixing volume of analyte. This is reported in units of parts per billion (ppbv) or million (ppmv) by the instrument. There is no correction for ambient water vapor. The ‘v’ stands for volume in the O_3 units.

7.2 Range

The upper range of this model is somewhat arbitrary. It extends well past conceivable ambient levels. Linearity up to 2000 ppbv is demonstrated with the automatic span checks done twice daily. The zero baseline is assessed in two ways. First, the instrument cycles alternately between reference and sample cells with switching solenoid valves. The only difference is removal of ambient ozone by a proprietary catalyst (presumably a Hopcalite-type substance that is a mixture of copper and manganese oxides). Second, the zero level is further checked twice daily with a charcoal removal catalyst. All zero and span checks are done through the ambient inlet filter, so should buildup on the filter cause ozone destruction, it would be obvious in the span checks.

7.3 Accuracy

Calibrations are done twice a day with an internal zero and 5-level span checks. These reveal short-term (daily) and long-term (annual) drifts. However, the stability of the span check source itself is known to be inferior to the stability of the absorbance photometer. After instruments are received from the manufacturer, the internal calibration is checked against the NYS DEC standard. At the same time, the internal span source is also checked. All the calibration (O_3 zero and spans) data are assessed for short and long trends and necessary corrections are applied to data of the best quality. The initial (on receipt) calibration is within 1-2% accuracy. However, field conditions vary substantially. Variation from the original measurement standard would appear to be ~5%.

7.4 Repeatability

Precision (repeatability) is given here as the noise of the 1-s signal (which is actually a 4-s measurement). Under quiet ambient conditions, this has been measured as:

$[O_3]$ $\sigma = 2$ ppbv

Therefore, for normally distributed noise, $\pm 2\sigma$ encompasses 95% of the points. The precision of the instrument under average ambient conditions is then given as:

$[O_3]$ 95% Confidence Interval = ± 4 ppbv

Note that these Confidence Intervals represent repeatability over a relatively short period. Day-to-day and month-to-month repeatability has a larger confidence interval and approaches the accuracy uncertainties given in the previous section. The manufacturer reports zero noise as 0.25 ppb RMS (for a 60-s average), which is slightly better (smaller) than the values observed under field conditions and reported above.

7.5 Sensitivity

Sensitivity as a lower detectable limit is reported as 95% confidence interval above baseline, which in this case would be 4 ppbv for data as reported to ARM (1 value per second, but each value represents 4 repetitive reports of a 4-s integration time). Assuming the noise decreases inversely with the square of the integration time, the measurement sensitivity under field conditions is similar to the 1.0 ppb ‘Lower detectable limit’ reported by the manufacturer.

7.6 Uncertainty

Uncertainty is an integral of all errors. It is a combined measurement of accuracy and precision (repeatability) discussed above.

7.7 Output Values

Described in section 6.0.

8.0 Instrument System Functional Diagram

Based on experience, the ozone monitor is modified upon receipt. These changes are shown here in Figures 11-12.

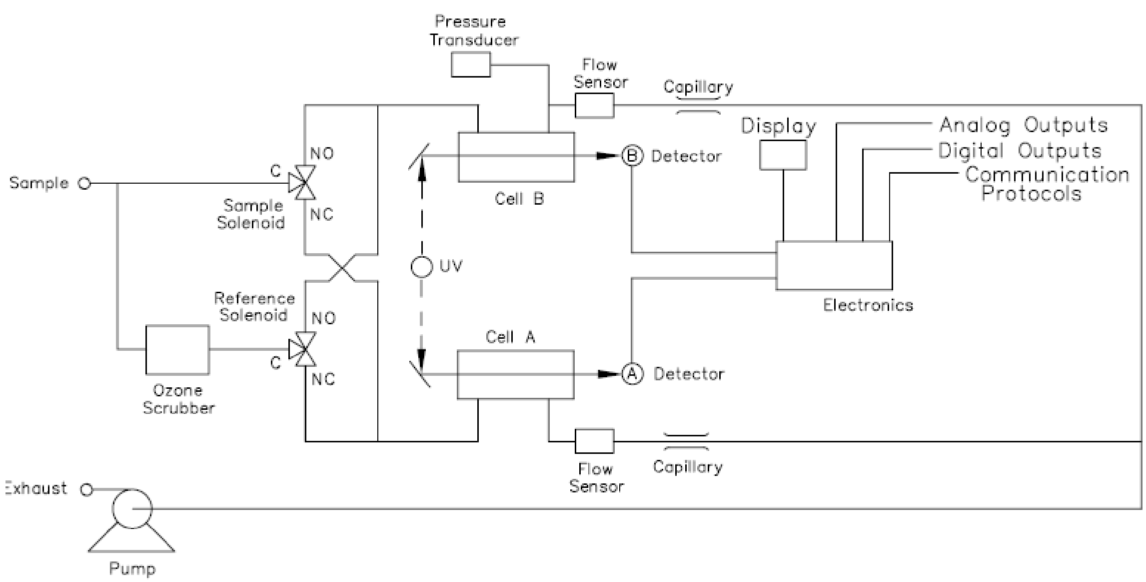

Figure 11. Diagram of flow schematic (from Thermo Scientific Manual).

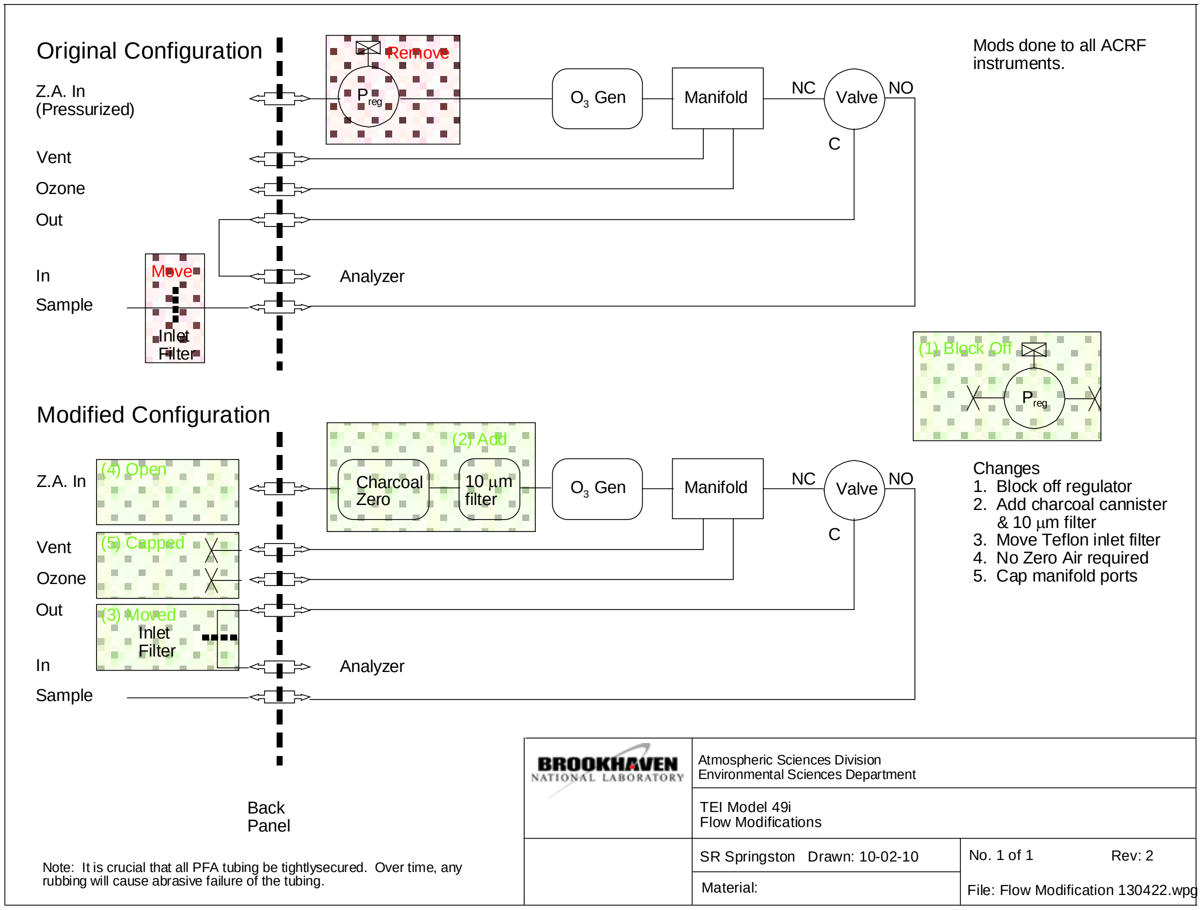

Figure 12. Modifications to the TEI Model 49i by the mentor.

In Figure 12, the red boxes indicate components that are removed and green boxes indicate components added. The original (as received) configuration is shown in the top and the current configuration is shown in the bottom panel. The changes in Figure 12 are summarized as:

1. The 5-µm Teflon filter (47-mm diam) is moved so that ambient sample AND zeros/spans go through the same flow stream (as recommended by the manufacturer).

2. Instead of supplying zero air to the ozone span generator, the instrument pump draws ambient air through a zeroing charcoal canister and metal filter. This means that the pressure in the ozone generator varies with atmospheric pressure and the output concentration can vary (since it is a function of both pressure and residence time, the variation is with the inverse square of the ambient pressure). However, the supplied pressure regulator only supplies consistent gauge pressure, not absolute pressure and the affect is similar.

Figure 13 shows the trace-gas sampling/inlet used in the AOS systems. It consist of a high-flow ½” OD PFA tubing sampling from under the aerosol inlet rain hat at ~10-m AGL. Air is pulled into the container at 30 LPM as controlled by a rotometer. The residence time to the back of the instrument is ~1-2 s.

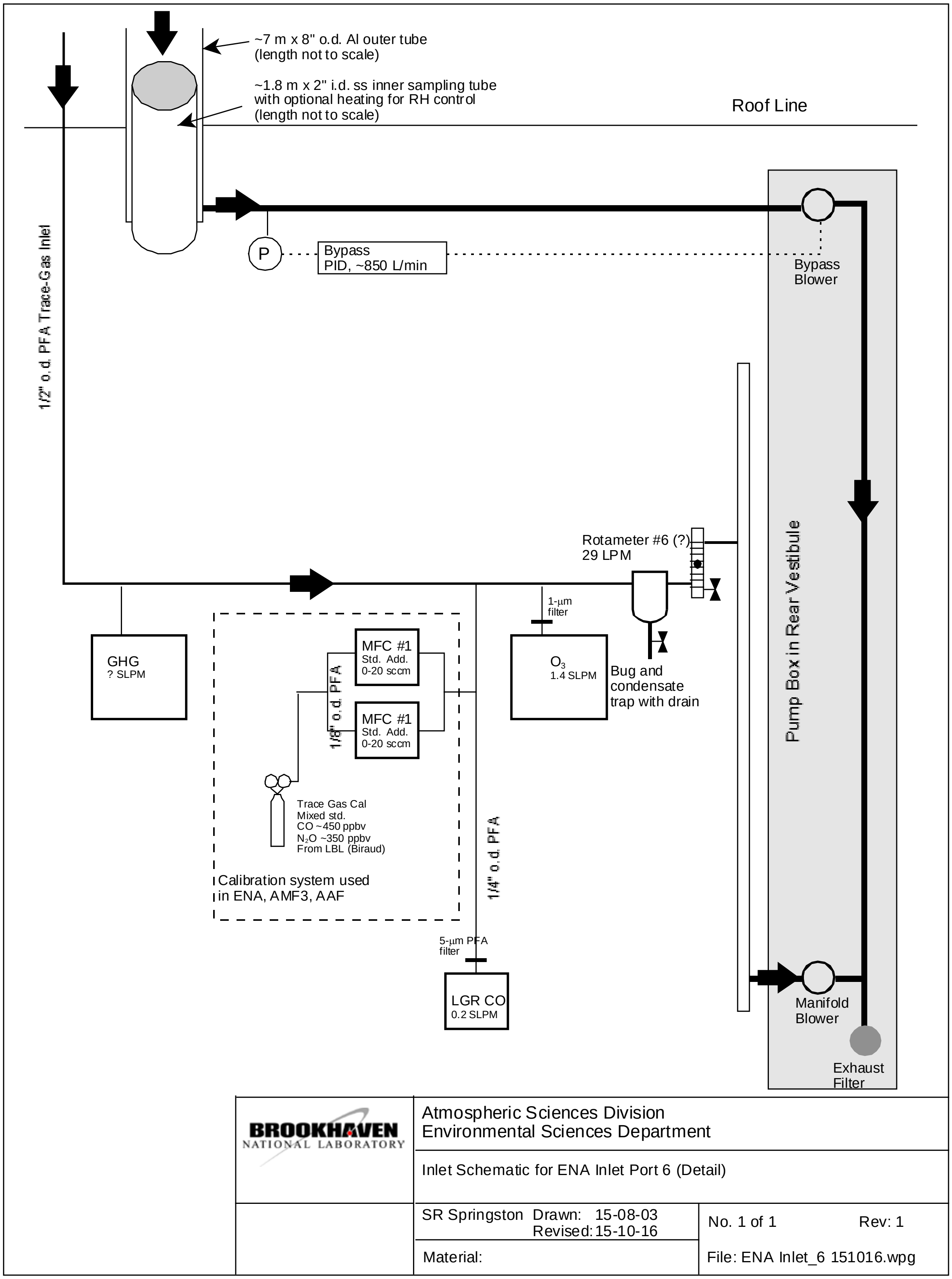

Figure 13. Ground inlet schematic.

9.0 Instrument/Measurement Theory

The following description is taken from the Thermo Scientific Manual:

"The sample is drawn into the Model 49i through the sample bulkhead and is split into two gas streams, as shown in Figure 13. One gas stream flows through an ozone scrubber to become the reference gas (Io). The reference gas then flows to the reference solenoid valve. The sample gas (I) flows directly to the sample solenoid valve. The solenoid valves alternate the reference and sample gas streams between cells A and B every 10 seconds. When cell A contains reference gas, cell B contains sample gas and vice versa. The UV light intensities of each cell are measured by detectors A and B. When the solenoid valves switch the reference and sample gas streams to opposite cells, the light intensities are ignored for several seconds to allow the cells to be flushed. The Model 49i calculates the ozone concentration for each cell and outputs the average concentration to the front panel display, the analog outputs, and also makes the data available over the serial or ethernet connection."

10.0 Setup and Operation of Instrument

The instrument is permanently installed in the AOS systems. This includes:

1. Physical mounting of the instrument in a shock-isolated 19" instrument rack.
2. Plumbing of the sample line into the fast flow ½" PFA trace gas manifold line with the associated 47-mm PFA filter and filter holder.
3. Connection of the RJ-45 ethernet output to the AOS Instrument Network switch.
4. Connection of the 110 VAC power line to the appropriate Power Distribution Unit outlet.

Initialization involves only making sure the ½" PFA trace gas manifold line runs up the aerosol stack to under the 14" rain hat and turning on the power.

After power is turned on, the instrument goes through self-checks and commences putting out data. Note that after extended shut down, this warm-up period can be 10 minutes or more.

11.0 Software

A graphical user interface (GUI) has been written for the instrument computer ('brick') acquiring data from the ozone monitor. This GUI is similar to other AOS instrument GUIs. The zero and span checks are controlled on a predetermined schedule by the instrument computer.

12.0 Calibration

Calibration procedures are described in earlier sections. These include two daily zero and span checks. The instruments are checked and cross-calibrated at the Brookhaven National Laboratory standards facility after they are returned from ARM sites.

13.0 Maintenance

Maintenance is minimal for this instrument. The mentor advises changing the inlet particle filter every two weeks. The filter is a 47-mm-diam. 5-µm PFA membrane filter Type LS (Millipore Catalog # LSWPO4700). Note that the filter is not directional (either side up). The filter is white and is packed in a stack separated by blue plastic spacers. DO NOT USE THE SPACER! USE THE WHITE FILTER. (This error has been made multiple times.)

Figure 14. 47-mm PFA filter holder.

Figure 15. 47-mm filter holder wrenches.

The green filter holder wrenches were delivered with the instrument. One end goes over the orange locking ring and the other (smaller) end goes over the PFA body. When opening the holder, note (and report) if the previous filter appears damaged. The filter being replaced should have at most a faint circle of trapped dirt. If the circle is visibly dark, increase the change frequency and notify the mentor.

The ¼” PFA fittings on the ends of the filter have an integral ferrule in the nut (no separate ferrule needed). These are finger tightened, but should be quite snug on the ¼” PFA tubing. The old filter may be disposed of in regular garbage.

14.0 Safety

This unit has no safety concerns during normal operation. The unit has separate mercury PenRay lamps in the photometer and the ozone span source. Both lamps emit light at 254 nm and should not be viewed directly. The internal instrument pump has an exposed shaft that drives the diaphragm on one end and a hard plastic fan on the other end. Both sides are open inside of the enclosure and pose a hazard to fingers. Older versions of this instrument had exposed electrical terminals on the pump motor. The current ARM version does not seem to have any exposed terminals with 110 VAC, but normal electrical procedures and cautions should be used. The instrument should not be operated with the cover off without proper training, precautions, and approvals.

It has been observed that the PFA tubing inside the instrument can abrade even when rubbing against another PFA tube. Thus, all tubing must be strain relieved (with tie wraps) to prevent any rubbing.

15.0 Citable References

N/A

16.0 Data Tools for ARM NetCDF

The ozone and related data can be downloaded from ARM Discovery/search (https://adc.arm.gov/discovery/). The data can be downloaded in multiple ways (Globus, Thredds, Dropbox) using NetCDF and ASCII-csv formats. The NetCDF data can viewed using several scientific software programs, including Python, Matlab, idl, etc. additional info on NetCDF visualization software can also be found at the University Corporation for Atmospheric Research (UCAR) website: (https://www.unidata.ucar.edu/software/netcdf/). There are a broad variety of tools (freely available and commercial) accessible through this website to view a NetCDF file. However, some NetCDF tools expect NetCDF files having a particular convention. The ARM-Tested Tools website contains descriptions and links for tools that have been specifically tested to work well with the ARM data format. The Matlab functions within the “anc_tools” directory of the publicly available repository https://github.com/ConnorJFlynn/mlib by Connor Flynn extend built-in Matlab NetCDF support for ARM-convention NetCDF files.

17.0 Infrastructure/Developer Links

https://www.arm.gov/
Enter "aoso3" in the search field at https://pcm.arm.gov/pcm/ to see the structure of ARM AOS ozone NetCDF files for all data levels.

18.0 Summary and History of Changes

This handbook is revised from its previous version of March 2016 with the following updates:

1. Multiple editing clarifications and corrections.
2. Descriptions of the QC flags and bits are added and demonstrated for the b1 level of the data.
3. The b1 level of data is described for the first time. This level of the data applies a baseline correction and a calibration factor correction to the O_3 observations given in the a1 files.
4. Examples of the intermediate (a1) level and the calibrated (b1) level of the data from various ARM sites are shown in this report.
5. Data used for zero and O_3 spans (b0 and bcal) are processed and saved separately (for producing b1 data).

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