

Atmospheric Observation System for Greenhouse Gases (GHG) Instrument Handbook

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Acronyms and Abbreviations

| | |
|--------|---|
| AMF | ARM Mobile Facility |
| AOSGHG | atmospheric observation system for greenhouse gases |
| ARM | Atmospheric Radiation Measurement |
| CCL | Central Calibration Laboratory |
| CRDS | cavity ringdown spectrometer |
| DQR | Data Quality Report |
| ENA | Eastern North Atlantic |
| GHG | atmospheric observation system for greenhouse gases |
| NOAA | National Oceanic and Atmospheric Administration |
| OLI | Oliktok Point, Alaska |
| QC | quality control |
| RMSE | root-mean-square error |
| TGP | tower gas processing system |
| WMO | World Meteorological Organization |

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1.0 Instrument Title

The atmospheric observation system for greenhouse gases (GHG or AOSGHG).

2.0 Mentor Contact Information

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3.0 Instrument Design

The greenhouse gas (GHG) system, also known as the atmospheric observation system for greenhouse gases (AOSGHG), was deployed for long-term continuous observations of atmospheric trace gases at a single sample height of 10 m above ground level at the two U.S. Department of Energy Atmospheric Radiation Measurement (ARM) user facility observatories at Oliktok Point, Alaska (OLI) as part of the third ARM Mobile Facility (AMF3) deployment and at the Eastern North Atlantic (ENA) site on Graciosa Island, Azores. The GHG system is a combination of two systems in series: (1) a tower gas processing system (TGP), an instrument rack that pulls, pressurizes, and dries air streams from an atmospheric sampling tower through a series of control and monitoring components, and (2) a cavity ringdown spectrometer (CRDS) gas analyzer (Picarro model G2301 series), which measures CO₂ and CH₄ concentrations as primary measurements.

Table 1. GHG system deployments.

| Dates | Site |
|--------------------------|------|
| 2015-06-01 to 2021-06-19 | OLI |
| 2015-07-23 to 2020-01-01 | ENA |

The instrument is located at the base of the tower inside an instrument shelter and the analyzer samples continuously. One measurement of tower sample is a one-minute average of continuous measurements. For calibration, tanks are measured for 10 minutes of which the latter one minute is averaged. The four minutes following the measurements of calibration tanks are discarded before returning to one-minute averaged continuous tower sample measurements, to allow for sufficient transition of air sample in the analyzer cavity.

The TGP is equipped with a cooler (M&C) and a liquid water detector that will stop flow from the tower sample line to the gas analyzer in the event that liquid water is detected in a sample stream. This prevents liquid water from entering the cell cavity of the gas analyzer and potentially damaging it. Prior to entering the gas analyzer, the sample stream is dried by condenser running at 5°C and further dried with Nafion and Drierite dryers. Sample air and calibration cylinder air pressure to the analyzer is controlled at 800 ± 1 Torr. Operating parameters are monitored and logged, and safety cutoffs are actuated by a Campbell CR1000 datalogger. Sample or calibration stream is selected via Valco multi-port valve, and data are logged by the native Picarro software. The CR1000 datastream (aosghgaux) and Picarro data stream (aosghg) are merged post-ingest to form the aosghg.b1 datastream.

3.1 Instrument/Measurement Theory

The method for measuring the primary variables CO_2 and CH_4 is described for the Picarro G2301 series analyzer. The text is adapted from the Picarro documentation “Real-Time Atmospheric Monitoring of Stable Isotopes and Trace Greenhouse Gases.”

The essential CRDS measurement consists of determining the decay time of light in an optical cavity filled with the gas stream to be analyzed. Light from a semiconductor diode laser is directed into a high-finesse optical resonator cavity containing the analyte gas. When the optical frequency matches the resonance frequency of the cavity, energy builds up in the cavity. When the build-up is complete, the laser is shut off. The light circulating in the cavity then decays from the cavity, or “rings down,” with a characteristic decay time. When the wavelength of the injected light does not match an absorption feature of any gas in the cavity, the decay time is dominated by mirror loss. However, when the wavelength of the injected light is resonant with an absorption feature of a species in the cavity, the decay time decreases as the reciprocal of the species concentration.

The instrument’s electronics include a digital signal processing system for determination of the ring-down rate, or optical loss, as a function of wavelength, giving it the speed to measure multiple spectral features and accurately detect multiple species.

3.2 Instrument System Functional Diagram

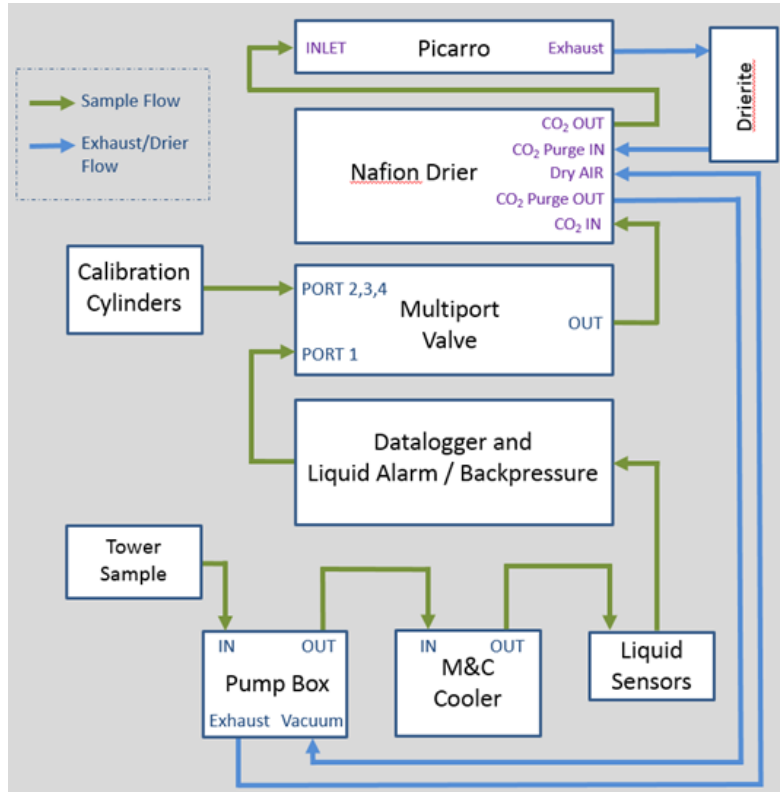


Figure 1. Tower sample and calibration cylinders plumbing diagram for GHG.

3.3 Calibration

Measurements of CO₂ and CH₄ are calibrated by measuring the low- and high-span cylinders every 11 hours and 35 minutes (to prevent any possibility of diurnal systematic bias), with a measurement of a Target cylinder in the middle. Each calibration cylinder is measured for 10 minutes with the latter one-minute averaged to yield one measurement. With the completion of measurements of span cylinder pairs, linearly interpolated gain and offset coefficients are applied to the b0-level tower data and Target cylinder measurements to generate b1-level data.

Calibration coefficients are determined by linear regression by measuring known values of species for a set of low- and high-span calibration tanks. For linear calibration, gain and offset coefficients are calculated for each species. The linear calibration goes as:

$$\chi_{\text{corr}} = (\chi' - b) / a$$

where χ' is the measured concentration of each species CO₂, CH₄ from the tower sample or Target calibration cylinder, b is the offset coefficient, a is the gain coefficient, and χ_{corr} is the calibrated concentration of each species.

3.4 Uncertainty

Overall instrument uncertainty is characterized by the variability in the calibration residual from measurements of Target cylinders compared to the known secondary values of each species, across the record from each site.

This allows for the estimate to encompass components of uncertainty that are caused by systematic and/or operational errors that may or may not be characterized and that come from the actual operation of the system.

The Target calibration residual is defined as: $\text{Residual} = (\text{Calibrated, Measured}) - (\text{Known Value})$. The table below represents uncertainty metrics used by mentors to assess instrument performance, where columns are defined as:

- MEAN = mean of difference measured and known quantities as, $\chi_{\text{resid}} = \chi_{\text{meas}} - \chi_{\text{known}}$, where χ are subscripted as measured calibrated or known values of species CO₂, CH₄
- STDERR = the standard error of the mean of residuals
- RMSE = the root-mean-square error calculated as, $\sqrt{(\sum \chi_{\text{resid}}^2 / N)}$, where the summation occurs over the square of residual from of N Target tank measurements used in the assessment.

Table 2. Target calibration residual statistics on N Target calibration tank measurements from the entirety of OLI and ENA deployments.

| | MEAN | STDERR | RMSE | N |
|-----------------------|-------|--------|------|------|
| ENA | | | | |
| CO ₂ (ppm) | 0.03 | 0.00 | 0.07 | 1817 |
| CH ₄ (ppb) | -0.15 | 0.01 | 0.31 | 2891 |
| OLI | | | | |
| CO ₂ (ppm) | 0.04 | 0.00 | 0.07 | 3856 |
| CH ₄ (ppb) | -0.03 | 0.00 | 0.29 | 3896 |

3.4.1 Culling Data for Residuals Statistics

Not all Target cylinder measurements are used in the assessment of instrument uncertainty. In addition to the diagnostic quality control (QC) tests the measurements undergo (section 4.2), specified periods of measurements of the Target tank are excluded from statistics using machine-readable documentation describing possible or confirmed periods of instrument instability coincident with those measurements. This machine-readable documentation is a mentor-compiled .csv file of all of the Data Quality Reports (DQRs) associated with the datastream and is used as a configuration file in the data ingest process. Examples of criteria for manually identified periods of instrument instability include:

- Target calibration residuals are outside of mentor-defined standards for one or more gas species

- Calibration coefficient outliers or periods of systematic deviation from expected values; significant outliers suggest the instrument was not in optimal condition and may be coincident with the previous criteria.

For the case of coefficients, when data is being reprocessed and coefficients are recalculated; the QC state of coefficients corresponding to the DQR entries are overwritten as “missing value” to then be excluded from linear interpolation of coefficients upon all future data reprocessing.

4.0 Definitions and Relevant Information

The b1-level datastreams are:

- for OLI: oliaosghgM1.b1
- for ENA: enaaosghgC1.b1

Auxiliary and input datastreams associated with b1-level datastreams;

- for OLI:
 - oliaosghgM1.a1
 - oliaosghgauxM1.a1
 - oliaosghgM1.b0
 - oliaosghgcoeffM1.b1
- for ENA:
 - enaaosghgC1.a1
 - enaaosghgauxC1.a1
 - enaaosghgC1.b0
 - enaaosghgcoeffC1.b1

4.1 Primary Variables

At b1 level, primary variable names are:

- CO2_DRY_AVG_CORR
- CH4_DRY_AVG_CORR

Associated QC variables:

- QC_CO2_DRY_AVG_CORR
- QC_CH4_DRY_AVG_CORR

Note:

- The “best data” are those with QC_* values of 0 for tower sample or Target measurements
- Tower sample data correspond to VALCOPOSITION variable equal to integer 1.

4.2 QC Bit Definitions

```

flag_method = "bit" ;
bit_1_description = "Value is equal to missing_value -9999."; 1
bit_2_description = "Value is less than the valid_min."; 2
bit_3_description = "Value is greater than the valid_max."; 4
bit_4_description = "Value for *_dry_slope is missing value"; 8
bit_5_description = "Value for *_dry_slope_err is missing value"; 16
bit_6_description = "Value for *_dry_slope is below valid_min."; 32
bit_7_description = "Value for *_dry_slope is above valid_max."; 64
bit_8_description = "Value for *_dry_slope is significant with respect to a slope of zero
(abs(ch4_dry_slope)-(ch4_dry_slope_err) > 0)"; 128
bit_9_description = "QC state for at least one of the mentor-defined auxiliary variables is not equal to 0" ;
256

```

Note: bit_1, 2, 3, and 9 are for tower sample measurements while all pertain to calibration tank measurements

4.3 Calibration Database

To achieve and maintain compatibility of our observations with different laboratories and observation networks, our measurements are traceable to the World Meteorological Organization /Global Atmosphere Watch scales.

Calibration tank values are transcribed to a machine-readable configuration file used in ARM user facility ingest processing. The file is updated by the mentor each time the calibration tanks are changed out – about once every two years. The values are provided by the World Meteorological Organization (WMO)’s Central Calibration Laboratory (CCL) at the U.S. National Oceanic and Atmospheric Administration’s (NOAA) Earth System Research Laboratory. The calibration scales used for each species are given below in Table 3.

Table 3. WMO CCL scale spans for each species. Contact the mentor for access to calibration certificates of each species.

| | Calibration Scale |
|-----------------|-----------------------------|
| CO ₂ | WMO-CO ₂ -X2019 |
| CH ₄ | WMO-CH ₄ -X2004A |

5.0 Citable References

Contact instrument mentors for up-to-date references.

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