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Precise Gas System (PGS) Instrument Handbook

S Biraud   K Reichl

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ARM

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K Reichl
Both at Lawrence Berkeley National Laboratory

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Acronyms and Abbreviations

ARM	Atmospheric Radiation Measurement
C1	SGP Central Facility
CCL	Central Calibration Laboratory
CRDS	cavity ring-down spectroscopy
DQR	Data Quality Report
IR	infrared
IRGA	infrared gas analyzer
NDIR	non-dispersive, infrared
NOAA	National Oceanic and Atmospheric Administration
PGS	precise gas system
QC	quality control
RMSE	root-mean-square error
SGP	Southern Great Plains
TGP	tower gas processing system
WMO	World Meteorological Organization

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The precise gas system (PGS)

2.0 Mentor Contact Information

Lead mentor: Sébastien Biraud
Lawrence Berkeley National Laboratory
Berkeley, California 94720
ph: 510-759-2914
email: scbiraud@lbl.gov

Associate mentor: Andrew Moyes
Lawrence Berkeley National Laboratory
Berkeley, California 94720
ph: 510-486-6246
email: abmoyes@lbl.gov

Associate mentor: Ken Reichl
Lawrence Berkeley National Laboratory
Berkeley, California 94720
ph: 805-813-1488
email: kreichl@lbl.gov

3.0 Instrument Description

The PGS is deployed for long-term, continuous observations of atmospheric trace gases at four sample heights of 2 m, 4 m, 25 m, and 60 m above ground level. The PGS has evolved over the data collection record starting in April 2001, and is a combination of two systems in series: (1) the 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 gas analyzer, which measures CO_2 and CH_4 concentrations as the primary measurements of the PGS system.

Table 1. PGS system configuration from deployment to present day. Note that CH_4 measurements were added to the datastream starting in 2010 after transition from Licor to Picarro gas analyzer.

Dates	Analyzer Deployed	System Note
2001-04-11 to 2011-04-11	Licor LI-6252 CO_2 Analyzer	Prototype I gas processing system
2010-10-06 to 2014-05-23	Picarro G1301 CO_2 and CH_4 Analyzer	Prototype II gas processing system
2015-12-02 to present	Picarro G2301 CO_2 and CH_4 Analyzer	TGP integrated

The instrument is located at the base of the 60-m tower at the Atmospheric Radiation Measurement (ARM) user facility's Southern Great Plains (SGP) Central Facility (C1), inside an instrument shelter, and

the analyzer is sampling continuously. One measurement of each of four tower sample heights is measured in sequence for five minutes (10 minutes for calibration tanks), of which the latter one minute is average.

Table 2.   PGS measurement method changes over the data record.

Dates	Measurement Window (minutes)	Averaging Window (minutes)
2001-04-11 to 2010-10-05	3	0.5
2010-10-06 to present	5	1

3.1   Instrument/Measurement Theory

For data collected prior to October 2010, the trace gas analyzer measurement is performed by the Licor LI-6252. The infrared gas analyzer (IRGA) was run in differential mode, where the difference between absorption in the sample cell and absorption in the reference cell is measured. The text is adapted from the LI-COR documentation "LI-6252 CO_2 Analyzer Instruction Manual." The LI-6252 is a differential, non-dispersive, infrared (NDIR) gas analyzer. The CO_2 measurements are based on the difference in absorption of infrared (IR) radiation passing through two gas sampling cells. The reference cell is used for a gas of known CO_2 concentration, and the sample cell is used for a gas of unknown concentration. Infrared radiation is transmitted through both cell paths, and the output of the analyzer is proportional to the difference in absorption between the two. The lead selenide detectors operate approximately as a linear quantum counter; that is, over much of its range the detector signal output is proportional to the number of photons reaching the detector. The output voltage that is used to compute CO_2 mole fraction is proportional to the difference between the signals generated by the detector when it sees the sample cell and when it sees the reference cell. The reference gas used was at around 360 ppm CO_2 through the reference cell at all times. Every 15 minutes, the reference gas was passed through the sample cell as well, to correct for gain (zero drift) in the system.

For data collected after October 2010, the trace gas analyzer measurement is performed by a Picarro cavity ring-down spectrometer. Although two analyzer models were used during this period; the G1301 followed by the G2301, the operating principles are the same. The method for measuring the primary variables CO_2 and CH_4 is described for the Picarro G2301 series deployments starting in 2010 and up to present. The text is adapted from the Picarro documentation "Real-Time Atmospheric Monitoring of Stable Isotopes and Trace Greenhouse Gases." The essential cavity ring-down spectroscopy (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. To optimize the tower gas sample handling by minimizing the effects of dilution by water vapor, and protect the analyzer from liquid water entering the sample line, an upgraded TGP system was developed and deployed in 2015. Prior to this, an earlier sample gas and calibration tank handling method was used, as described below.

3.1.1   Prototype I Gas Processing System (2001 to 2010)

The analyzer used during this period was the Licor L1-6252 up to 2010. This early sample processing system consisted of the following components:

- Sample was dried with a cooling unit and a Nafion membrane drier.

- Flow was regulated with mass flow controller, pumps, and valves.

- A 1-liter buffer volume is used to dampen very-short-term variation in CO_2 concentration.

- System was controlled and conditions logged by a Campbell Scientific datalogger CR23x.

3.1.2   Prototype II Gas Processing System (2011 to 2014)

The sample processing system was modified to accommodate the change in analyzer, when the LI-6252 analyzer was replaced with the Picarro G1301 series analyzer.

- Vacuum pump was added for Picarro analyzer operation.

- Valves used for sample/calibration tank selection were replaced with Valco multi-position selector valve.

During this first deployment of the Picarro in 2014, liquid water had entered the sample stream and damaged the analyzer, prompting analyzer upgrade to a Picarro G2301 and redesign of the gas processing system to prevent liquid water from entering the gas analyzer.

3.1.3   Tower Gas Processing System (2015 to Present)

The TGP is equipped with a liquid water detector that will stop pressurized flow from the tower sample line to the Picarro analyzer if liquid water is detected in a sample stream. This prevents liquid water from entering the cell cavity of the Picarro instrument. Prior to entering the Picarro analyzer, the sample stream is dried with by condenser running at 5 C and further dried with Nafion and Drierite dryers. Sample air and calibration cylinder air pressure to the analyzer are 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 (pgsaux) and Picarro datastream (pgs) are merged during ingest to form the pgs.b1 datastream.

3.2 Instrument System Functional Diagram
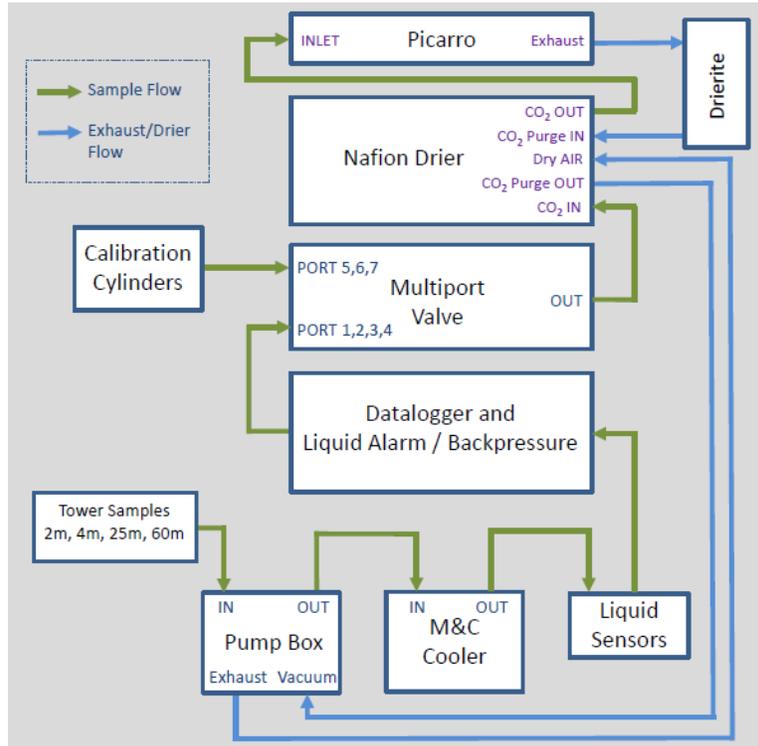
Figure 1. Tower sample and calibration cylinders plumbing diagram for PGS as of the 2015 ARM baselining.

3.3 Calibration

Measurements of CO_2 and CH_4 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. Refer to Table 3 for a description of how the calibration method varied dependent on the time period.

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 for data from December 2015 to present goes as:

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

where χ' is the measured concentration of each species CO_2, CH_4 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.

Table 3.   PGS calibration method by periods of system configuration.

Dates	# of Span Tanks	Frequency (hrs)	Calibration Method
2001-04-11 to 2011-04-11	4	4	Polynomial*
2010-10-06 to 2014-05-23	2	23	Linear
2015-12-02 to present	2	11.58	Linear with Target calibration check

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 December 2015 to present (as of the date of this handbook).

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: Residual = (Calibrated, Measured) – (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,

$$\chi_{resid} = \chi_{meas} - \chi_{known}$$

where χ are subscripted as measured calibrated or known values of species CO_2, CH_4

STDERR = the standard error of the mean of residuals

RMSE = the root-mean-square error calculated as,

$$\sqrt{(\sum \chi_{resid}^2 / N)}$$

where the summation occurs over the square of residual from of N Target tank measurements used in the assessment.

Table 4.   Target calibration residual statistics on N Target calibration tank measurements from the SGP deployment December 2015 to July 2024.

	MEAN	STDERR	RMSE	N
CO_2 (ppm)	-0.03	0.00	0.06	5454
CH_4 (ppb)	-0.06	0.00	0.34	5456

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 that 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, periods of systematic deviation from expected values, or 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 datastream is: sgppgsC1.b1

Auxiliary and input datastreams associated with b1-level datastreams;

for SGP:
- sgppgsC1.a1
- sgppgsauxC1.a1
- sgppgsC1.b0
- sgppgscoeffC1.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 integers 1, 2, 3, or 4, for the four tower sample heights respectively.

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 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 (NOAA)'s Earth System Research Laboratory. The calibration scales used for each species are given below in Table 5.

Table 5.   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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