PICARRO

L2140-*i* and L2130-*i* Isotopic Water Analyzer and Peripherals Installation and Operation Manual

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Picarro Notices

Thank you for purchasing a Picarro product. Your Picarro system is a quality product that has been designed and manufactured to provide reliable performance.

This User Manual (UM) is an important part of your purchase as it will help familiarize you with the system and explain the numerous features that have been designed into it. Please read this manual thoroughly before using your Picarro system.

Please contact Picarro or your authorized Picarro distributor should you have questions regarding specific applications or if you require additional information.

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READ BEFORE USING THIS MANUAL

This manual includes information on how to install the water analyzer in its most common configuration (analyzer with vaporizer). For other configurations (autosampler, SDM, IM, MCM, CWS), please refer to those manuals directly:

- **A0340 Autosampler User Manual** (PN 40-0094)
- **A0325 Autosampler User Manual** (PN 40025)
- **A0211 High-Precision Vaporizer User Manual** (PN 40-0044)
- **A0214 MCM User Manual** (PN 40022)
- **A0213 Induction Module-CRDS Setup User Manual** (PN 40033)
- **A0101 SDM User Manual** (PN 40-0005)
- **A0217 Continuous Water Sampler Installation and User Manual** (PN 40-0003)

Please note that the High Throughput Vaporizer was discontinued in December 2013. Picarro continues to support these vaporizers in the field, but they are no longer manufactured. If you require installation instructions for the High Throughput Vaporizer, please refer to an earlier version of this manual.

For information on Picarro's measurement technology, see ***APPENDIX E – Introduction to CRDS Technology***.

Be selective when following the manual by only referring to the sections relevant to your configuration of interest. To start, choose one of the setups in the table below based on your configuration.

Refer to Table of Contents to find the location of any of the chapters described below.

SETUP	USE CASE	SETUP CHAPTER
Basic Water Analyzer	This mode is used to measure ambient vapor which does not require any calibration with liquid standards.	See section ***4.5 Basic Water Analyzer Setup***. This setup requires a CRDS analyzer.
Dual Mode	This mode is used for measurement of ambient vapor coupled with automated injection of liquid calibration standards. The measurement mode alternates between analyzing ambient vapor and liquid	See section ***4.6 Dual Mode Setup***. This setup requires A0211 High Precision Vaporizer, A0912 Dual Mode Configuration hardware and software for vapor calibration and an Autosampler. This mode uses high precision method for liquid calibration. Each injection cycle takes 9 minutes.

SETUP	USE CASE	SETUP CHAPTER
	standards based on a user defined sequence.	
Manual Mode	This mode is used for semi-automated measurement of liquid water samples with maximum precision.	See section ***4.7 Manual Mode Setup***. The setup requires an A0211 High Precision Vaporizer. User manually injects samples after prompt. The control of the vaporizer and the analysis of liquid samples are automated. Each injection cycle takes 9 minutes.
Picarro Autosampler and High Precision Vaporizer (A0211)	This setup is used for automated injection of liquid waters. It consists of two modes that utilize the same hardware: High Precision Mode and High Throughput Mode.	See section ***4.8 Picarro Autosampler and High Precision Vaporizer (A0211) Setup***. The setup can operate in five measurement modes: High Precision*, High Throughput*, Standard**, Express**, and Survey**. **High Precision* (same as Standard Mode):** Measures liquid water samples with maximum precision. Liquid samples are automatically injected and analyzed. Each injection cycle takes 9 minutes. **High Throughput*:** Used for faster measurement of liquid water samples with good precision. Liquid samples are automatically injected and analyzed. Each injection cycle takes 4 minutes. High Precision and High Throughput Coordinator Modes operate in the exact same fashion except that the steps of sample preparation and analysis are faster in the high throughput coordinator mode. **Standard** (same as High Precision Mode):** Used to measure liquid water samples with maximum precision. This coordinator must be run in either the “iH2O N2” mode or the “iH2O Air” mode. Automatically injects and analyzes liquid samples. Each injection cycle takes 9 minutes. **Express**:** Used for faster measurement of liquid water samples with good precision. This coordinator must be run in either the “iH2O N2” mode or the “iH2O Air” mode. Automatically injects and analyzes liquid water samples. when using the

SETUP	USE CASE	SETUP CHAPTER
		Express coordinator, we recommend 10 injections, the first 6 injections take 1.5 minutes each, while the last 4 injections take 5 minutes each. The first 7 injections will be discarded to achieve the optimal memory reduction. **Survey**:** Used for super-fast measurements of large sample batches at moderate precision and enables more efficient sample sorting. By manually rearranging samples accordingly, one can reduce the memory effect between adjacent sample. Automatically injects and measures liquid samples. This coordinator must be run in either the "iH2O N2" mode or the "iH2O Air" mode. *****Only available without Coordinator software upgrade ******Only available with Coordinator software upgrade

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1. Introduction

1.1 Intended Use

The L2140-i isotopic water analyzer measures concentrations of $\delta^{18}O$, $\delta^{17}O$, $\delta^{2}H$ and ^{17}O-excess using Picarro's patented Cavity Ring-Down Spectroscopy (CRDS).

The L2130-i isotopic water analyzer measures concentrations of $\delta^{18}O$ and $\delta^{2}H$.

The analyzer can be deployed for monitoring applications in a lab or in the field, allowing in-situ analysis of trace and ambient amounts of isotopic water.

NOTE

In this manual $\delta^{2}H$ is used to represent deuterium. However, δD may be found in the software or result files.

1.2 System Overview

Analyzer

Figure 1 shows the analyzer front and back panels. More detailed information on panel features, functions, and connections are in section ***4, Hardware Installation*** and Setup.

Figure 1: L2140-i, L2130-i Front Panel

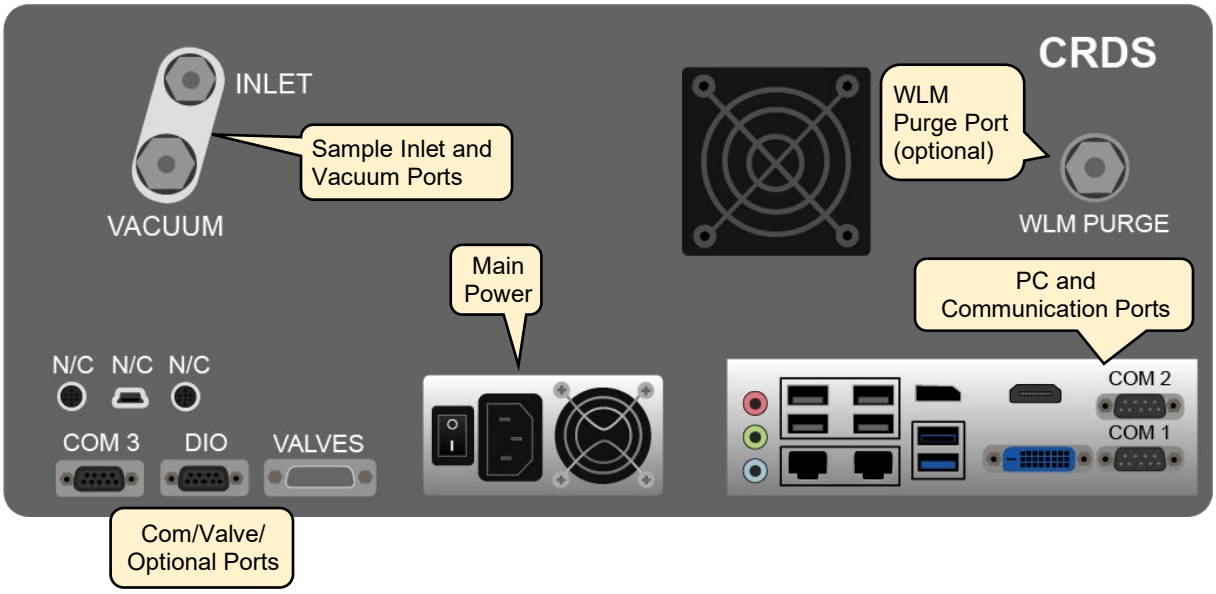


Figure 2: L2140-i, L2130-i Back Panel

A2000 Vacuum Pump

The A2000 vacuum pump (Figure 3) is used to maintain cavity pressure inside the analyzer. The pump should be connected and running whenever the analyzer is in use.

Figure 3: A2000 Vacuum Pump – Side Views

1.3 Analyzer Specifications

Table 1: L2140-i, L2130-i Specifications

Parameter	Specification
Measurement Technique	Cavity Ring-Down Spectroscopy (CRDS)
Weight: Analyzer Weight: Pump	20.4 kg (45 lbs.) – Should be lifted by two people. A2000: 6.5 kg (14.4 lbs)
L2130-*i* / L2140-*i* Analyzer Dimensions	Depth: 44.5 cm (17.5”) Width: 43.2 cm (17.0”) Height: 19.1 cm (7.5”) Height without Feet: 17.8 cm (7.0”)
Dimensions – A2000 Pump	Length: 34.5 cm (13.6”) Width: 15.5 cm (6.1”) Height: 22 cm (8.7”)
Ambient Humidity Range	< 85% RH non-condensing
Ambient Temperature Range	Vapor Sample: -10 °C to 45 °C (14 °F to 113 °F) Liquid Sample & System Operation: 10 °C to 35 °C (50 °F to 95 °F) Storage: -10 °C to 50 °C (14 °F to 122 °F)
Maximum Altitude (During operation)	3,048 m (10,000 ft)
Front/Rear Clearance	Front: 15.3 cm (6”); Rear: 15.3 cm (6”)
Sample Pressure	300 to 1000 torr (40 to 133 kPa)
Sample Flowrate	~40 sccm at 760 torr (101 kPa)
Required Accessories	Included: Pump (external), keyboard, mouse Supplied by Customer: LCD monitor
Operating System Data Outputs	Windows 10 RS–232, Ethernet, USB, Analog (optional) 0-10 V
L2130-*i*/L2140-*i* Power Requirements Startup Power Steady-state Power	100 – 240 VAC; 50/60 Hz (auto-sensing) <375 W at start-up, (analyzer and pump) 120 W (analyzer) 150 W (A2000 Pump)
Minimum Rated Circuit Current (Amperes)	10A @ 115 VAC 5A @ 230 VAC
Liquid Ingress Protection	None

1.4 Acronyms

This manual includes various acronyms. For definitions, see below:

Table 2: Acronyms, Formulas, Units, and Symbols

Acronym	Definition
atm.	atmosphere; unit of pressure, equal to atmospheric pressure at sea level. 1 atm. = 14.69595 psi (101.325 kPa)
cm	centimeters
CRDS	Cavity Ring-Down Spectroscopy
CWS	Continuous Water Sampler
DAS	Data Acquisition System (the analyzer)
DIO	Digital Input and Output Between the analyzer and the autosampler. DIO Tells the Autosampler to prepare for an injection, and to perform an injection. Additionally, DIO is the place where the autosampler notifies that an injection has been made.
ft.	Length in feet;1 ft. = 12” or 12 inches (30.48 cm)
GUI	Graphical User Interface
H_2O	Water, Water Vapor
IM	Induction Module
kPa	Kilopascal; unit of pressure; 1 kPa = 0.145 PSI
MCM	Micro-Combustion Module
mm	millimeters
OD	Outside Diameter
ppb	parts per billion
ppm	parts per million
PSI (psi)	Pounds per Square Inch
RH	Relative Humidity
SCCM	Standard cubic centimeters per minute
SDM	Standards Delivery Module
SST	Stainless Steel
UM	User Manual

Acronym	Definition
WLM Purge Port	Wavelength Monitor Purge Port. The Port on the analyzer the dry gas connects to. This keeps the spectroscopy accurate.
“ (as in 1/4”)	Inches
°C	Degrees Celsius
‰	Per mil

1.5 Text Conventions

The following conventions are used in the manual.

- *Italic* text identifies screen names and emphasizes important text or certain features.
- ***Bold Italic*** text identifies section reference links.
- **Bold** text is for actions to take (such as clicking on a UI button), caution and warning statements, and text you should type or select in screens.

2. Safety

2.1 Warning Symbols

Icon notes and warnings are used throughout this manual. The purpose of these icons is to provide a visual convention to alert you of essential information. They indicate dangers to either the operator or to the analyzer, and other important information.

Table 3: Warning/Information Icon Types

Icon	Description
 NOTE	**NOTE** is important information that you should be aware of before proceeding.
 WARNING	**LASER WARNING** alerts you of a laser danger.
 DANGER	**DANGER** indicates an imminently hazardous situation that, if not avoided, will result in death or severe injury.
 WARNING	**WARNING** indicates a potentially hazardous situation which, if not avoided, could result in death or severe injury.
 CAUTION	**CAUTION** alerts user of a potential danger to equipment or to the user.
 WARNING	**HAZARDOUS VOLTAGE** alerts user to areas that may expose a user to electrical energy that is high enough to cause injury or death.
 CAUTION	**HOT SURFACE** alerts user to potential injury from hot surfaces.
 REMINDER	R**EMINDER** is a helpful hint for procedures listed in the text.

2.2 General Safety

CDRH Certification

This Picarro analyzer complies with 21 CFR Chapter 1, sub-chapter J, and is classified as a Class 1 laser system when all panels and covers are on.

CE Certification

This Picarro analyzer complies with European safety standards and the instrument is affixed with a CE label. This CE label is located on the back panel of the instrument.

- **CE:** IEC EN61010-1:2010 (safety) and EN61326-1:2013 (EMC) requirements for electrical equipment for measurement, control, and laboratory use.

WARNING

Using this analyzer in a manner not specified by Picarro may result in damage to the analyzer and render it unsafe to operate.

WARNING

The analyzer is for indoor use only and has an ingress protection rating of IPx-0. It is NOT protected against exposure to water including dripping, spraying, splashing or immersion.

WARNING

Do not operate in an explosive atmosphere! Do not operate in the presence of flammable gases or fumes.

CAUTION

This analyzer contains no user-serviceable components except the particulate filter, A0211 Vaporizer injection port septum, CPU fan, and A2000 vacuum pump diaphragms and valves. To order user-replaceable parts and access video replacement instructions, see section *17, Maintenance*.

Do not attempt other repairs; instead, report all problems to Picarro Customer Service or your local distributor. Please contact Picarro if you have any questions regarding the safe operation of this equipment.

CAUTION

Do not replace the mains supply power cord with an inadequately rated cord.

WARNING

If mounting in a 19” rack, this analyzer cannot support itself using a front rack mount kit alone. It must be supported by a shelf, or by user-provided “L” type support brackets.

CAUTION

Equipment Damage: Exceeding gas inlet pressure or temperature specifications could result in damage to the instrument. In the case of higher input pressure or flow, configuring a sampling bypass manifold system is recommended.

Use a 'tee' at the gas inlet and exhaust the remainder of the gas stream appropriately.

WARNING

The inlet gas connector on the back panel of the analyzer, and its immediate vicinity, runs hot during operation of the analyzer. Take care when connecting gas lines or working at the rear of the instrument to wear protective gloves or avoid contact with these surfaces.

CAUTION

Equipment Damage: Do not disconnect the AC power to the analyzer, vacuum line, or the AC power to the External Vacuum Pump while analyzer is operating. Damage may be caused by current surges if power is applied while attaching or removing cables.

WARNING

This analyzer weighs 20.4 kg (45 lbs). Use the technique described below (or follow your local regulations) when lifting the analyzer.

a. **Before lifting, inspect the unit for slippery substances or sharp edges.**
b. **Lift with two people, one on each side of the analyzer.**
c. **Crouch down and stay close to the unit. Always keep your back as straight as possible.**
d. **Position your feet for sturdy balance. Lift with your legs, not your back.**
e. **Do not twist the back while carrying the unit. Rotate direction with hip joints.**
f. **Lower the unit by bending at the knees.**

2.3 Laser Safety

WARNING

This equipment is classified as a Class 1 laser product with an embedded 3B laser in accordance with EN 60825-1:2014. Do not to open the enclosure where this label is placed; there are no user serviceable parts inside.

The following Laser Safety Label is affixed to the outer cover of the analyzer.

Figure 4: Laser Safety Label – Affixed to Outside Cover of Analyzer

WARNING

The laser is a Class 3B when exposed.
Only operate or service this device in accordance with the instructions in this guide, and only open the device in an approved laser safe service area using appropriate laser-safety glasses.

The following **Laser Safety Label** (Figure 5) is affixed to the inside of the analyzer:

Figure 5: Laser Safety Label – Affixed to Inside of Analyzer

WARNING

Use of controls or adjustments or performance of procedures other than those specified herein may result in hazardous radiation exposure.

3. Unpacking

3.1 Inspect the Shipping Boxes

Picarro products are inspected and tested before leaving the factory. Their packing containers have been designed to keep the equipment safe from damage during transit.

Inspect the condition of the boxes upon arrival. The larger box includes the analyzer and most of the accessories. Even if the outer box shows damage, the inner box holding the analyzer will protect the instrument under most circumstances.

If the equipment is damaged, photograph the damage and contact Picarro (email pictures if possible) as soon as possible.

NOTE

Keep all packing materials so the instrument can easily be returned Picarro (if necessary) or transported to another location.

3.2 Unpack Components

While unpacking each shipping box:

- Inspect each item to ensure it is not damaged.
- If items are missing, contact Picarro.
- Keep the shipping materials to reuse when transporting the analyzer.
- Contact Picarro for options on transporting systems to remote labs.

WARNING

The analyzer weighs 20.4 kg (45 lbs). Use the technique outlined on Page 23 when lifting or moving the analyzer.

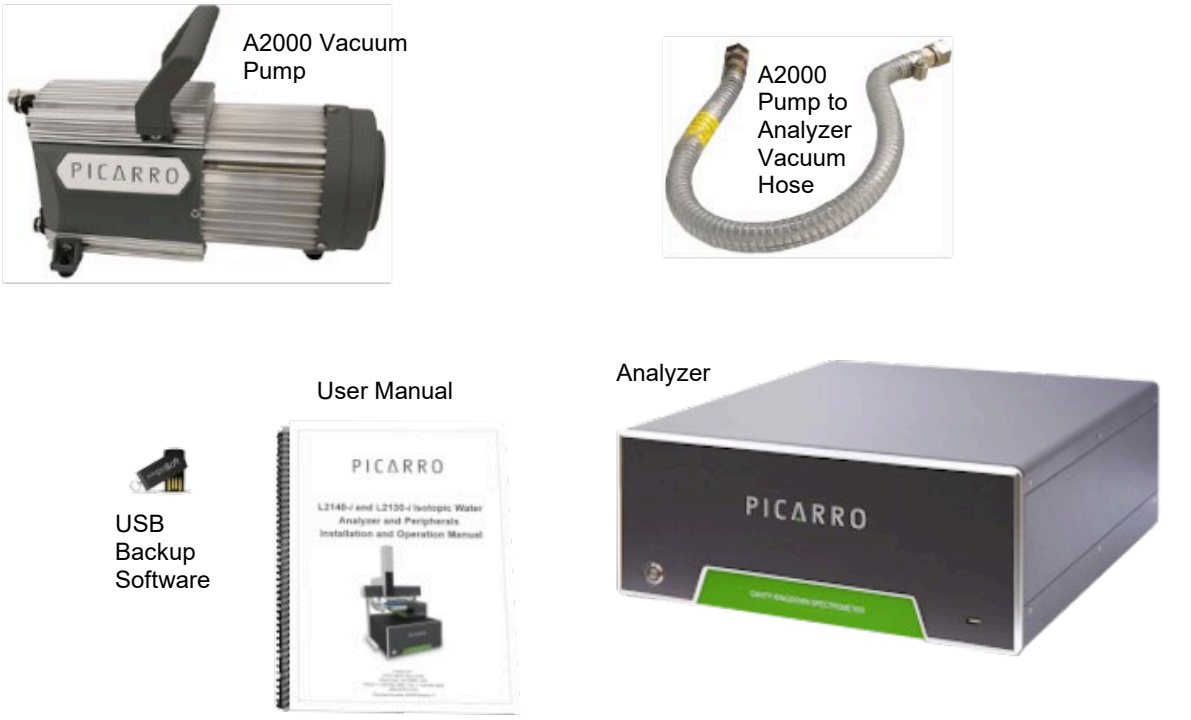


Figure 6: L2140-i, L2130-i Shipping Box Contents

Table 4: Box One: Analyzer and Accessories

Item (qty)	Description
Analyzer (1)	Includes all the data acquisition, control, and communications hardware and firmware to perform all gas handling, spectral collection, and analysis.
AC Power Cable (1)	A power cable with connectors appropriate to your country is provided. **Note:** The analyzer automatically adjusts to local voltage.
Nut (1) and Ferrules (2)	For connecting input line to analyzer gas INPUT.
Vacuum Hose (1)	Hose to connect the pump to the analyzer.
Keyboard and Mouse (1)	Set, Keyboard & Mouse Combo (Monitor not included)
USB Flash Drive (1)	Contains backup software.
Spare Fuses (3)	5x20, 6A, 250V
Document Packet (1)	Includes this user manual and certificate of compliance.

Table 5: Box Two: A2000 Vacuum Pump and Accessories

Item (qty)	Description
A2000 Vacuum Pump (1)	Provides vacuum required for sample gas sequencing into and out of the analyzer.
AC Power Cable (1)	A power cable with connectors appropriate to your country is provided. **Note:** The vacuum pump voltage must be selected. See ***Pump Voltage Setting*** in section ***4.4***.
Pump Manual (1)	Detailed instructions for pump.

4. Hardware Installation and Setup

4.1 Items/Tools Required

- Analyzer and accessories included in shipment
- Pump and accessories included in shipment
- Peripherals and accessories included in the shipment according to your order
- 5/8” open end wrench
- 11/16’’ open end wrench
- Power cords for analyzer, pump, and peripherals

4.2 Installation Safety

Read this safety section in its entirety before proceeding.

WARNING

Two-person lift required: The analyzer weighs 20.4 kg (45 lbs). When lifting the analyzer, use the technique described on page 23 (or follow your local regulations).

CAUTION

When the analyzer is being integrated to an external system, the safety of that system is the responsibility of the assembler of that system.

WARNING

Equipment Damage: Do not attach electrical power to or start the analyzer until after attaching and turning on the External Vacuum Pump. Do not disconnect the vacuum line while the analyzer is running. Failure to do so could result in damage to the optics.

WARNING

Picarro sells certain USB enabled devices, such as GPS, which are approved for use. Do not connect USB hubs or unauthorized USB devices (except flash drives, mice, and keyboards) to the USB ports. Unauthorized USB devices may interfere with the normal functioning of the analyzer.

Warning

When using compressed gases, follow all appropriate safety conventions, including use of eye protection, physical restraint of cylinders, etc.

CAUTION

Lines connected to the 1/4" Swagelok sample inlet connector must not exceed 5 PSIG of pressure. Picarro recommends 2 to 3 PSIG of pressure.

CAUTION

During installation, do not position the analyzer so that it is difficult to operate the electrical disconnecting device (such as an emergency off (EMO) switch or breaker).

CAUTION

When working with hazardous gases, remove the pump exhaust muffler, adapt a tube to the vacuum pump exhaust port and direct the exhaust to a safe place for venting the mixture of sample gases. For instructions, see *APPENDIX C – Setting up Contained Exhaust Flow*.

CAUTION

Use the AC power cables supplied with the analyzer or a similarly rated cable. Check with Picarro technical support if you have questions about power cable replacement. An inadequately rated power cable can result in equipment damage.

CAUTION

Cords shall be RATED for the maximum current for the equipment and the cable used shall meet the requirements of IEC 60227 or IEC 60245. Cords certified or approved by a recognized testing authority are regarded as meeting this requirement. The connector type used should be: IEC320 C13.

CAUTION

Equipment Damage: It is imperative that the analyzer have adequate ventilation and/or cooling to maintain the ambient temperature below 35 °C when operating. Do not place the pump or the instrument in any enclosure without providing adequate forced air flow.

Do not plug or block any perforations in the chassis of the instrument. Do not put anything near the instrument that will impede the air flow. Failure to provide adequate airflow, especially clearance at the front and rear panels, to ensure proper airflow and/or cooling to the analyzer will result in overheating of the analyzer causing a shutdown and potential damage. There should be 6" (15 cm) of clearance in the front and back of the analyzer.

To determine if the ventilation is adequate in an enclosure, monitor the temperature of the air near the instrument and adjust ventilation so that the ambient temperature is within specification. As a guide, the ambient temperature of the air around the instrument cannot exceed the specifications listed below.

Thermal Specifications	Min	Max	Description
Ambient Operating Temperature	10 °C	35 °C	Worst-case environmental limits (unless otherwise specified)

CAUTION

If the analyzer has been stored at less than 10 °C (50 °F), allow the components to equalize to room temperature before starting the installation process.

4.3 Ventilation Considerations

The instrument and pump require adequate ventilation in order to function properly. Do not plug or block any perforations in the chassis of the instrument. Don't place anything near the instrument that will impede the air flow.

4.4 Pump Voltage Setting

Set the A2000 vacuum pump input voltage to the correct level for your area by rotating the voltage selector switch located on the side of the pump next to the fuse holder (Figure 7).

Figure 7: Vacuum Pump Voltage Selection

4.5 Basic Water Analyzer Setup

This basic water analyzer mode is used to measure ambient vapor which does not require any calibration with liquid standards. This setup includes an L21x0-*i* analyzer, A2000 pump, and related accessories.

Refer to Figure 8 through Figure 10 below.

1. Remove the analyzer and the external vacuum pump from their respective shipping containers.
2. Place the analyzer on a cart or table.
3. Place the external vacuum pump near the analyzer on a cart, table, or on the floor.
4. Unpack the analyzer accessories (vacuum line, manual, and certificate of compliance).

   Store the certificate of compliance in a safe place. It may be required if you contact Picarro for service or questions.

5. Remove the caps from the analyzer **SAMPLE** inlet and **VACUUM** connection ports. Save the caps so they can be reinstalled when the analyzer is stored, moved or shipped.
6. Remove the caps from the pump vacuum inlet. Save the caps for reuse in case the analyzer and pump is stored, moved, or shipped.
7. Connect the provided vacuum line between the analyzer port labeled VACUUM and the pump vacuum inlet (Refer to Figure 8).

   Hand tighten the nut, then make an additional 1/4 turn with an 11/16" wrench.
8. The exhaust port of the external vacuum pump has a muffler attached for noise reduction. If desired, attach a tube to the pump exhaust port and direct it to a safe place for venting the mixture of sample gases for air/N_2 and H_20. For instructions, see ***APPENDIX C – Setting up Contained Exhaust Flow***
9. Connect a monitor to the HDMI monitor port on the analyzer's back panel. Once powered up, the analyzer will detect the connection and adjust the resolution to match the monitor.
10. Connect a mouse and keyboard to a pair of USB ports.
11. Check that the A2000 pump voltage input switch is set correctly.
12. *Ensure the power switch on both the analyzer pump are set to OFF*.
13. Attach the power cable to the analyzer and pump.

    This completes the basic analyzer installation.

NOTE

The analyzer has a universal power supply that automatically adjusts to power sources ranging from 100-240 VAC, 47 to 63 Hz, 10 A max.

NOTE

The A2000 pump does not automatically adjust to power sources. If using the A2000 vacuum pump, ensure its input voltage is set to the correct level for your area by rotating the voltage selector switch located on the side of the pump next to the fuse holder (see Figure 7).

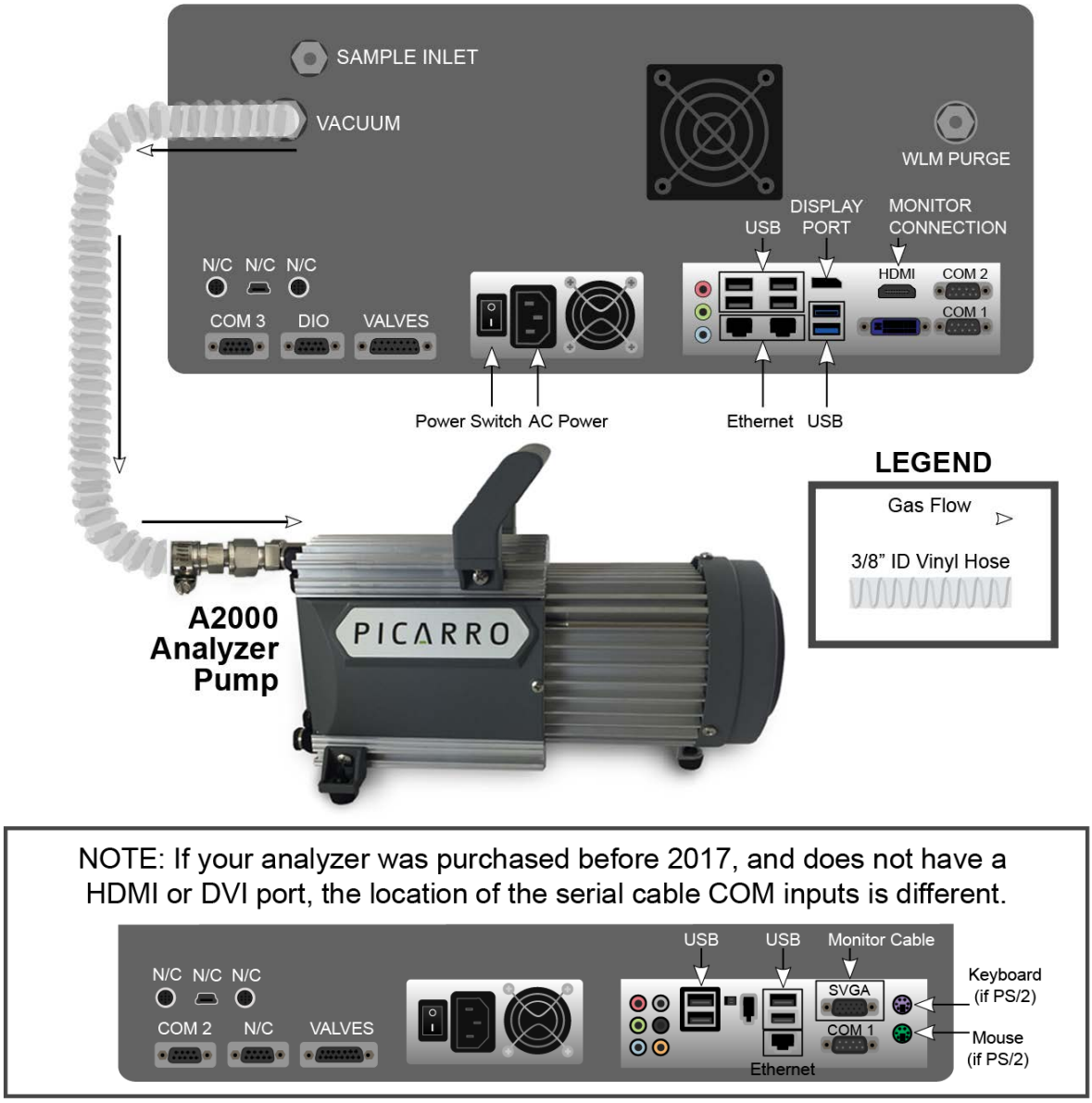


Figure 8: Basic Water Analyzer Setup with A2000 Pump

Sample Gas Inlet Connection (SST Tubing)

If your analyzer is supplied with connectors for stainless steel tubing, follow these steps.

1. Use 1/4" OD SST tubing and connector sets to connect from sample source to the sample inlet.
2. Place the two ferrules inside the nut as shown below.

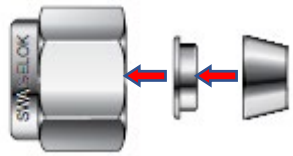


Figure 9: Orientation of Inlet Nut and Ferrules

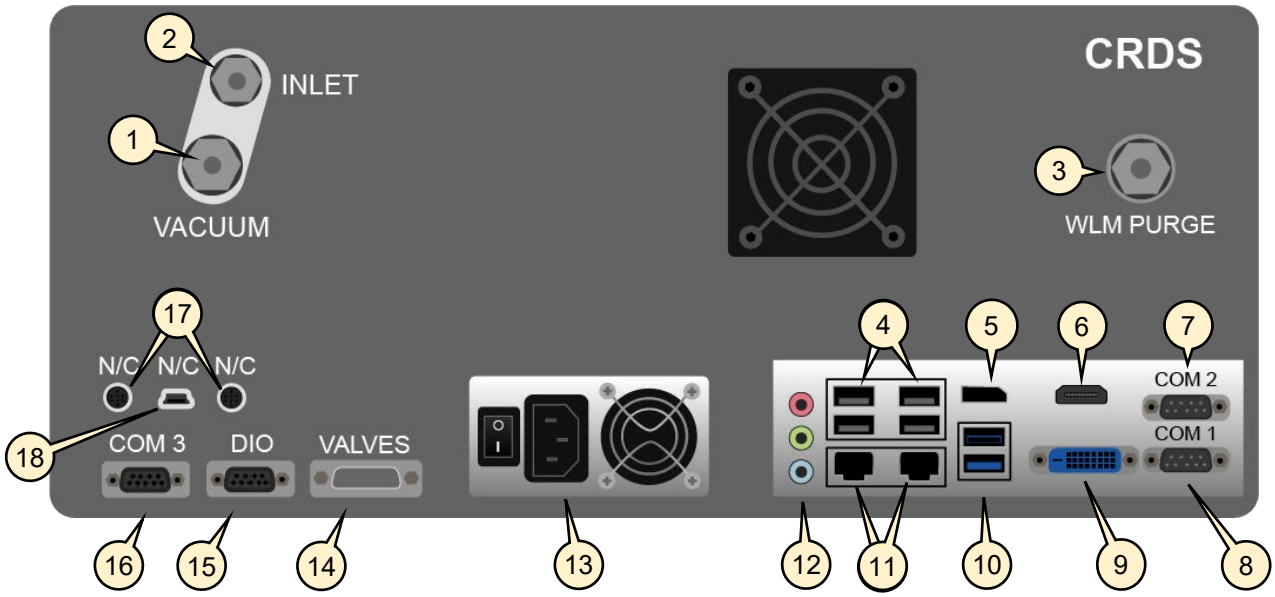
3. Loosely connect the nut to the INLET on the back panel of the analyzer, being careful not to let the ferrules fall out.
4. Insert the tubing into the back of the nut and through the ferrules, feeding it in as far as possible without deforming the tubing.
5. Hand tighten the nut.
6. Using a 9/16" wrench (not included), tighten the nut 1-1/4 turns.

When reconnecting SST tubing:

1. Inspect the ferrules. If you see any damage, replace the ferrules and follow the directions above for making a new connection.
2. If there is no damage, hand tighten the connector to the analyzer sample inlet.
3. Using a 9/16" wrench, tighten the nut 1/6 of a turn (60°).

Electrical Connections

Refer to Figure 10 and its callout list below for connection points.



1. External Vacuum Pump Port	**10.** USB 3.0 Ports (2 qty.)
2. Gas Sample Inlet	**11.** Ethernet Ports – RJ-45 (2 ea)
3. WLM Purge Port (optional)	**12.** Audio In/Out Ports
4. USB 3.0 Ports (4 qty.)	**13.** AC Power Input and Power ON Switch
5. Display Port	**14.** Valve Control Port (Solenoid valves)
6. HDMI 2.0 Monitor Port	**15.** DIO (Only for PAL autosampler connection)
7. COM 2 Port	**16.** COM 3 Port (Connected but typically not used.)
8. COM 1 Port	**17.** Analog EIC Output (Optional upgrade)
9. DVI-I Video Monitor Port	**18.** USB for Logic Board (Not connected)

Figure 10: Annotated Back Panel Diagram

4.6 Dual Mode Setup

Refer to **Figure 11**, **Figure 12**, and **Figure 13** below.

Dual mode is used for measurement of ambient vapor coupled with automated injection of liquid calibration standards. The measurement mode alternates between analyzing ambient vapor and liquid standards based on a user defined sequence.

Dual Mode setup requires an **A0211 High Precision Vaporizer**, an **A0340 (or A0325) Autosampler**, and **A0912 Dual Mode Configuration hardware and software for vapor calibration**. Dual mode uses a high-precision method for liquid calibration. Each injection cycle takes 9 minutes.

1. Carefully unpack the peripheral boxes and prepare the facility.
2. Review the section, ***Installation Safety*** before proceeding .
3. Install the analyzer and its external vacuum pump per the instructions in sections ***4.1*** through ***4.5***).
4. Install the Autosampler and Vaporizer.

   Refer to the Installation chapter in the A0340 Autosampler User Manual (PN 40-0094) or A0325 Autosampler User Manual (PN 40025) for detailed installation instructions.
5. Attach the vaporizer switching valve assembly to the vaporizer inlet ports labelled **Purge** and **Sample 2** (Figure 11 and Figure 12).
6. Attach the switching valve wire pair to the connector with the red/white wire pair that is attached to the Vap Valves cable connector.
7. Attach the Zero Air gas line (shown as copper line in Figure 11) to Tee section of the vaporizer switching valve assembly.
8. Sampling tubing for measuring ambient water vapor should be connected to the top of the solenoid valve with the intake line routed outdoors.

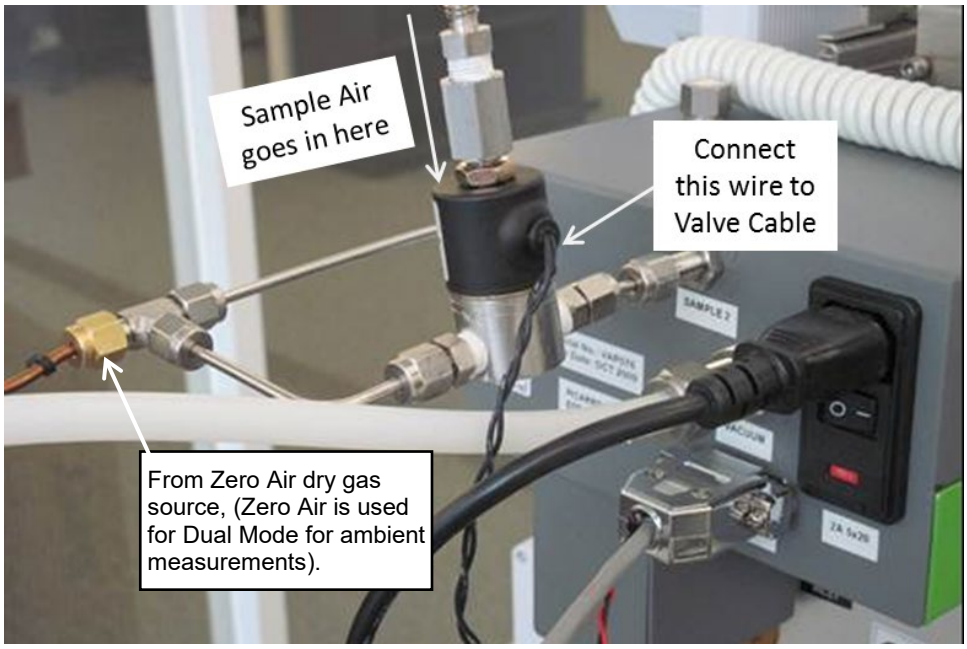


Figure 11: Vaporizer Switching Valve Assembly Connected to Vaporizer

Figure 12: Connections to Back of Vaporizer

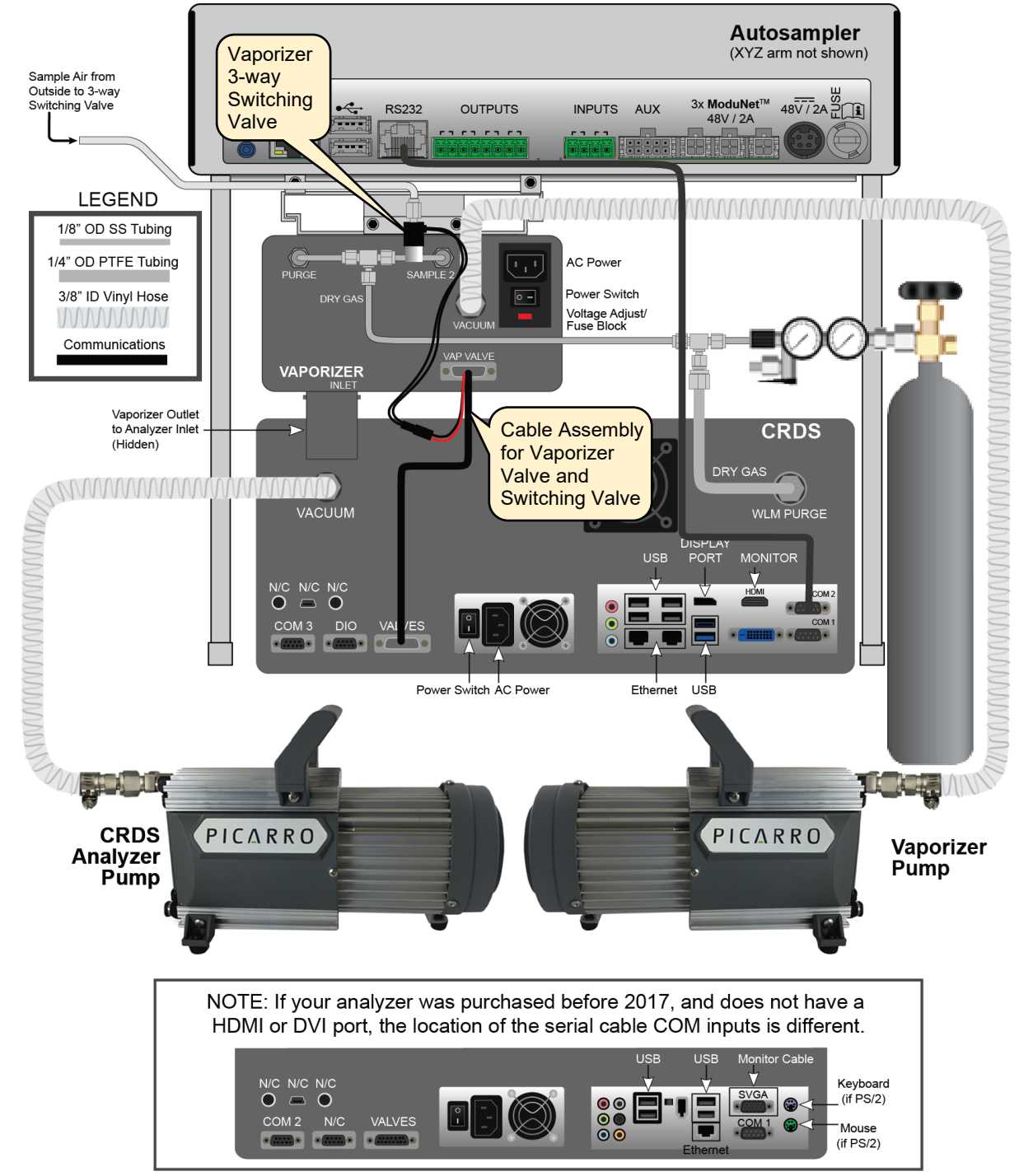


Figure 13: Dual Mode Setup and Connections (Vaporizer Switching Valve Included)

4.7 Manual Mode Setup

Refer to Figure 14 below.

This mode is used for semi-automated measurement of liquid water samples with maximum precision.

The setup requires an **A0211 High Precision Vaporizer**. The user manually injects samples after prompt. The control of the vaporizer and the analysis of liquid samples are automated. Each injection cycle takes 9 minutes.

1. Inspect the boxes of Picarro products before opening. Carefully unpack the boxes and prepare the facility.
2. Please review the important safety notes before continuing on with the installation. See the section, ***Installation Safety***.
3. Install the analyzer and its external vacuum pump per the instructions in sections ***4.1*** through ***4.5***).
4. Place the vaporizer on top of the analyzer using feet of 0.5” (13 mm) thickness to set it to the appropriate height. Align the Inlet port (analyzer) with the delivery port of the vaporizer.
5. Attach a (N_2 or Dry Air) Gas line to the vaporizer and the analyzer (see section ***5, Water Analyzer Dry Gas Supply Setup***).
6. Attach the hose at the vaporizer’s vacuum port and connect it to the second External Vacuum Pump. Attach the power cable to the External Vacuum Pump, but keep the power switch off.
7. Connect the vaporizer and the analyzer using a Valve Cable and the gas delivery port from the vaporizer (see VAPORIZER TO ANALYZER CONNECTIONS).
8. Check the Power Connections to the Machines: Make sure all power cables are attached to the power outlets on the analyzer, Vaporizer, and two External Vacuum pumps. However, keep the power switch off.
9. Carefully slide the complete system into position: Small movement of the components relative to one another is OK. However, do not overly force the system. Check for obstacles if the unit does not slide easily.
10. Plug all the power cables (including the one for the monitor) into a power supply. Switch ON the components in the following order
    a. External Vacuum Pumps (for both the analyzer and the vaporizer).
    b. Everything else.

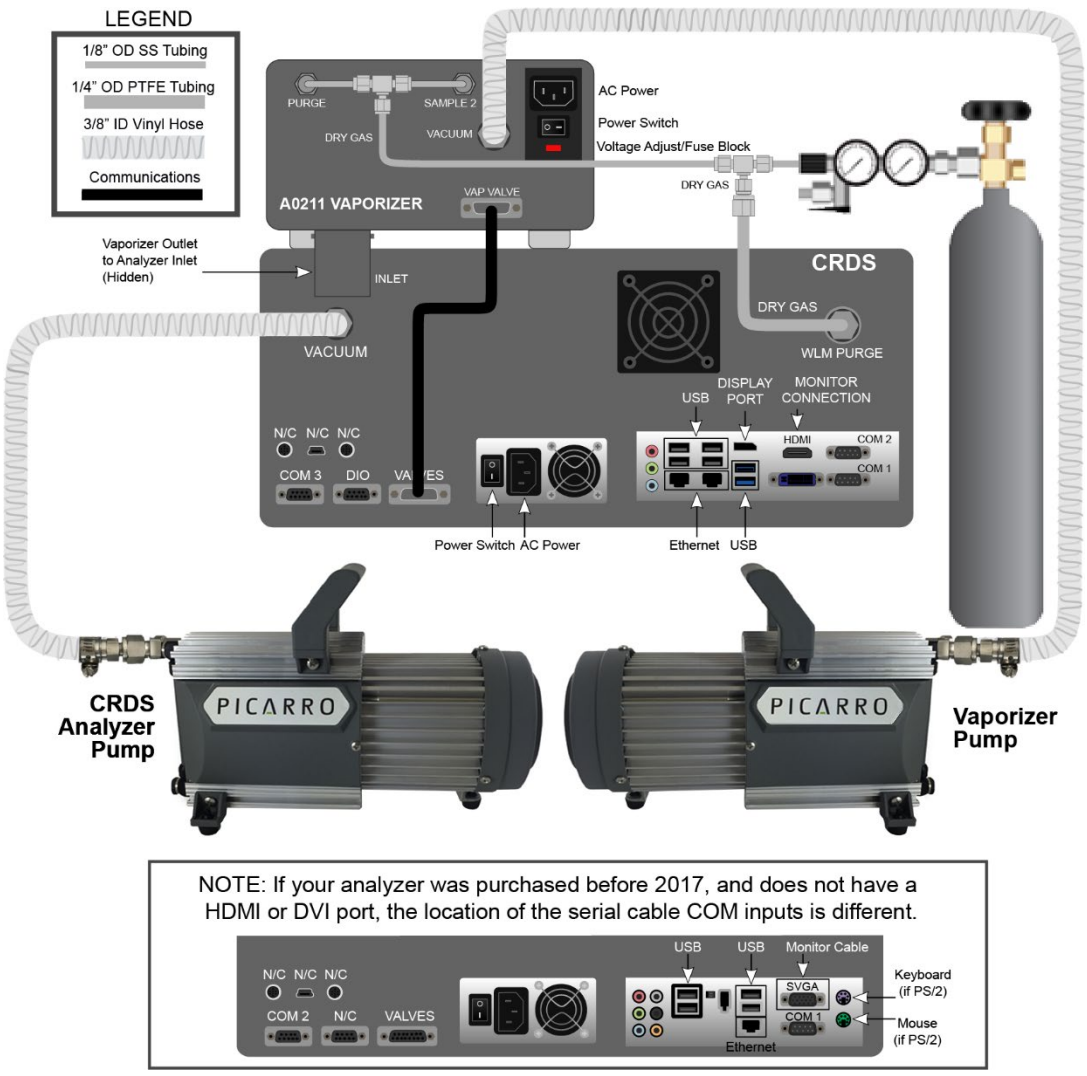


Figure 14: Manual Mode Setup and Connections

4.8 Picarro Autosampler and High Precision Vaporizer (A0211) Setup

This setup is used for automated injection of liquid waters. It consists of two modes that utilize the same hardware: High Precision Mode (same as Standard Mode) and High Throughput Mode.

Refer to Figure 15 below.

1. Inspect the boxes of Picarro products before opening. Carefully unpack the boxes and prepare the facility.
2. Please review the important safety notes before continuing on with the installation. See SAFETY.

3. Install the analyzer and its External Vacuum Pump (see analyzer and Vacuum Setup).
4. Install the Picarro Autosampler (see Installation | Picarro Autosampler chapter in the A0340 Autosampler User Manual (PN 40-0094) or A0325 Autosampler User Manual (PN 40025).
5. Supply dry gas to the analyzer (see WATER ANALYZER DRY GAS SUPPLY SETUP).
6. Carefully slide the complete system into position: Small movement of the components relative to one another is OK, as the units are well locked. However, do not overly force the system: check for obstacles if the unit does not slide easily.
7. Power up the system: Plug in all the power cables (including the one for the monitor) into the appropriate power supply. Switch ON the components in the following order:
    a. External Vacuum Pumps (for both the analyzer and the vaporizer).
    b. Everything else

NOTE

The software to operate the instrument will start automatically after the operating system has loaded. The user interface will appear a few seconds after the instrument software starts. See "Startup Procedure" in section *7 Basic Operation*.

NOTE

As the instrument is starting up, it is normal for there to be a delay in reporting data. This can take several minutes depending on how long it takes for the internal temperature to reach its operating point, and it is normal during this time for some concentration readings to be negative or constant.

Additionally, the data selection pull down menus will not be populated with the appropriate items until data is being reported in the graph. This is typically less than 30 minutes, but depending on ambient temperature, the analyzer can take up to 2 hours to stabilize.

NOTE

Remember that for the SDM operation, the Vaporizer temperature should be set to 140°C. For all the other coordinator modes, the temperature should be set to 110°C.

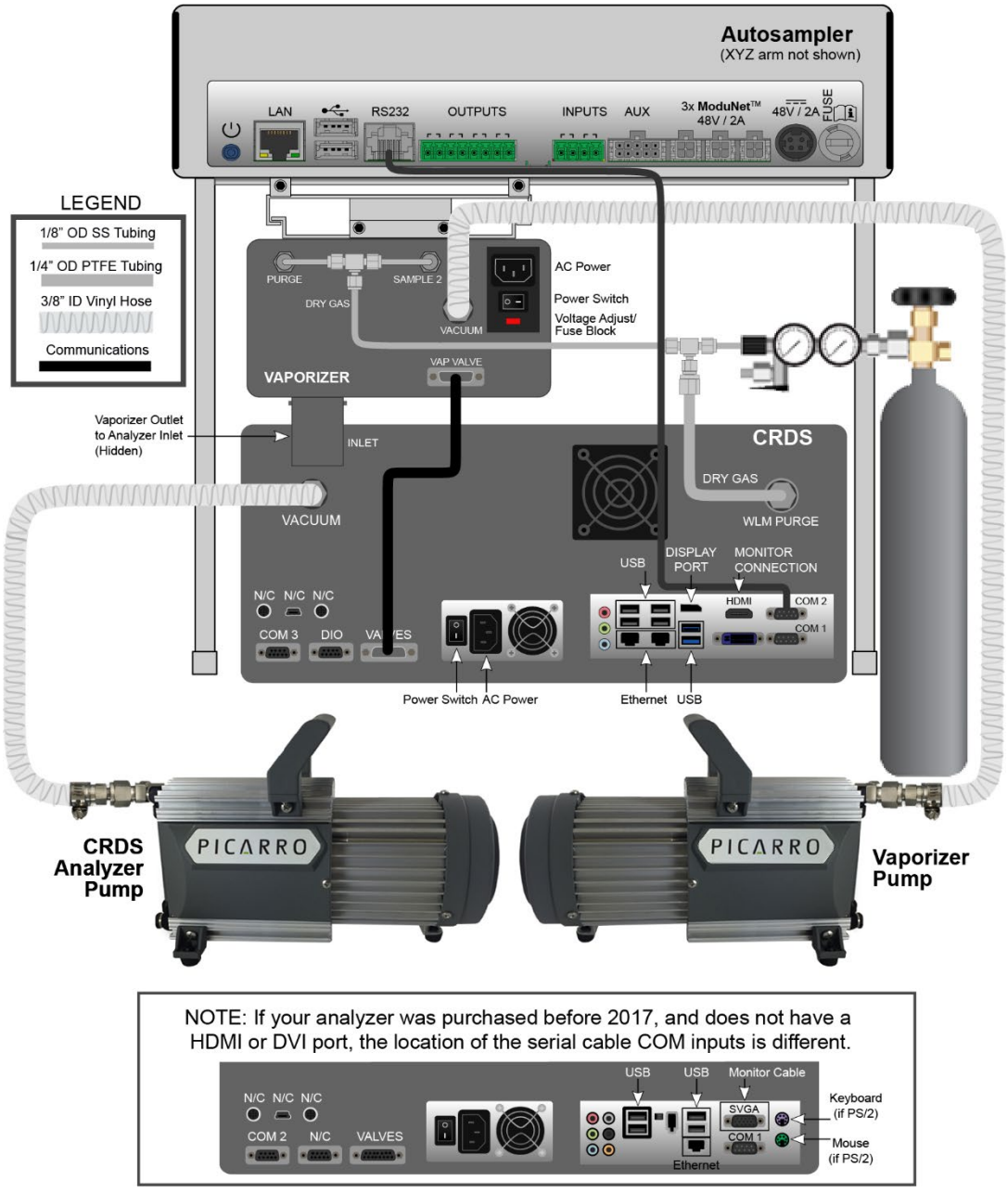


Figure 15: Picarro Autosampler-High Precision Vaporizer Setup and Connections

5. Water Analyzer Dry Gas Supply Setup

The Picarro L2140-*i* and L2130-*i* analyzers each can work in many configurations, allowing a wide application of the analyzer. This section describes how to set up the dry gas supply for all these configurations. Find the section in this chapter that relates to your setup and then complete the dry gas supply installation steps.

- **Manual Mode Setup:** See ***Dry Gas Configuration A***
- **Picarro Autosampler – High Precision Vaporizer (A0211) Setup:** See ***Dry Gas Configuration A***
- **Picarro Autosampler – High Throughput Vaporizer (A0212) Setup:** See ***Dry Gas Configuration B***
- **Basic Water Analyzer Setup:** No dry gas supply necessary
- **Dual Mode Setup:** See ***Dry Gas Configuration C***
- **Induction Module Setup:** See A0213 Induction Module to CRDS Setup User Manual (PN 40039)
- **SDM Setup:** See A0101 Standards Delivery Module CRDS Setup User Manual (PN 40-0005)

5.1 Dry Gas Configuration A

Refer to Figure 16: Dry Gas Configuration A.

You will need a dry gas supply for the analyzer and the vaporizer. You can purchase the pressure regulator kit numbers A0921 or A0923 from Picarro. If you have already purchased a dry gas kit from Picarro, you will need the following additional supply.

- **Dry gas supply of 10-60 psi (4 bar), which is stepped down to 2.5 psi before being connected to the CRDS analyzer.**

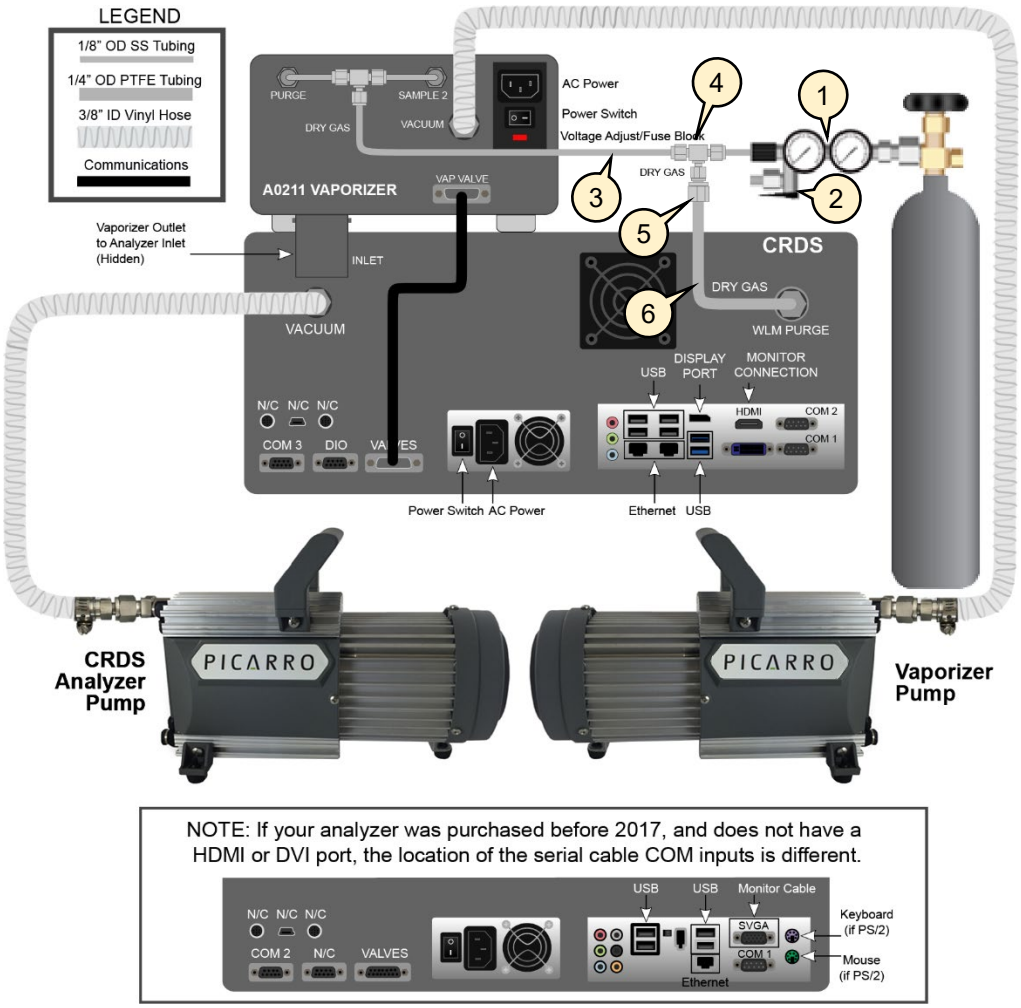
NOTE

The A0921 regulators come with CGA connectors, which may not be compatible with gas tanks used in your region.

Below, you will find a complete part list and diagram on how to connect dry gas to the water analyzer.

1. Attach the (N_2 or Dry Air) Gas Line to the analyzer: Attach a Gas line from the “WLM Purge” Port on the analyzer to the N_2 Regulator, which connects to a (nitrogen or dry air) gas cylinder.
2. To connect 1/4” dry gas tube to the Wavelength Monitor Purge (WLM Purge) Port on the analyzer, use the Push Connector that is attached to the port. The connector is in two pieces: The Outer Flap and the Inner Flap.

3. To connect the tube to the port, simply push the tube into the connector and then pull the tube back. If there is a space between the inner flap and the outer flap, this means that the tube is locked to the port. Do not twist and turn. To take the tube out of the port, push the Outer Flap in against the Inner Flap, and while doing this, pull out the tube. This will cause the gripping mechanism to release from the tube.



1. Q1-14B-580 Air Liquide Scott Regulator
2. SS-OGM2-S2-A Swagelok Toggle Valve
3. SS-T2-S-028-20 Swagelok 1/8" OD stainless steel tubing
4. SS-200-3 Swagelok 1/8" stainless steel Tee union
5. SS-400-R-2 Swagelok 1/8" (adapter fitting) to 1/4" (tube fitting) Reducing Union
6. 5033K31 McMaster-Carr 1/4" OD PTFE tubing

Additional tools and parts are required, some others recommended. For the complete list, click the following link. https://picarro.box.net/shared/static/r19c3z8etk.pdf

Figure 16: Dry Gas Configuration A

4. Attach the Gas (N_2 or Dry Air) Line to the Vaporizer: Using either output from a (nitrogen or dry air) gas cylinder (should be at a pressure of 2.5 ± 0.5 psig (0.17 ± 0.03 bar)) or from the gas supply/regulator, attach the gas line to the open third leg of the gas line that connects the vaporizer purge and the sample ports (that is shipped connected to the vaporizer).

Above is an N_2 Regulator: The semi-transparent tube on the left is routed to the 'WLM Purge" Port on the analyzer. The copper-colored tube on the top left comes from the 'Purge' and the 'Sample' ports on the Vaporizer. The copper-colored tube on the bottom right goes to the (N_2 or Dry Air) Gas Cylinder.

Figure 17: Gas Regulator

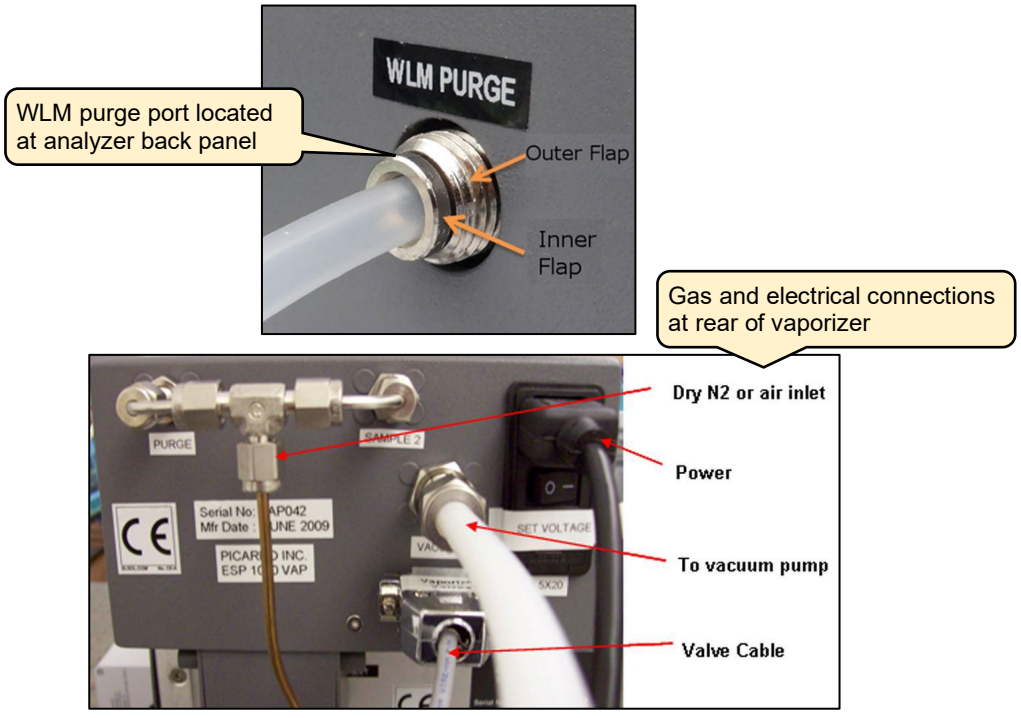


Figure 18: Vaporizer and Analyzer Connections

5.2 Dry Gas Configuration B

The gas connection for the **Dual Mode** setup is similar to the Dry Gas Configuration A except that it also has a Vaporizer Switching Valve. Follow the Dry Gas Configuration A, but also connect the Vaporizer Switching Valve to the back of the Vaporizer according to the schematic and images below.

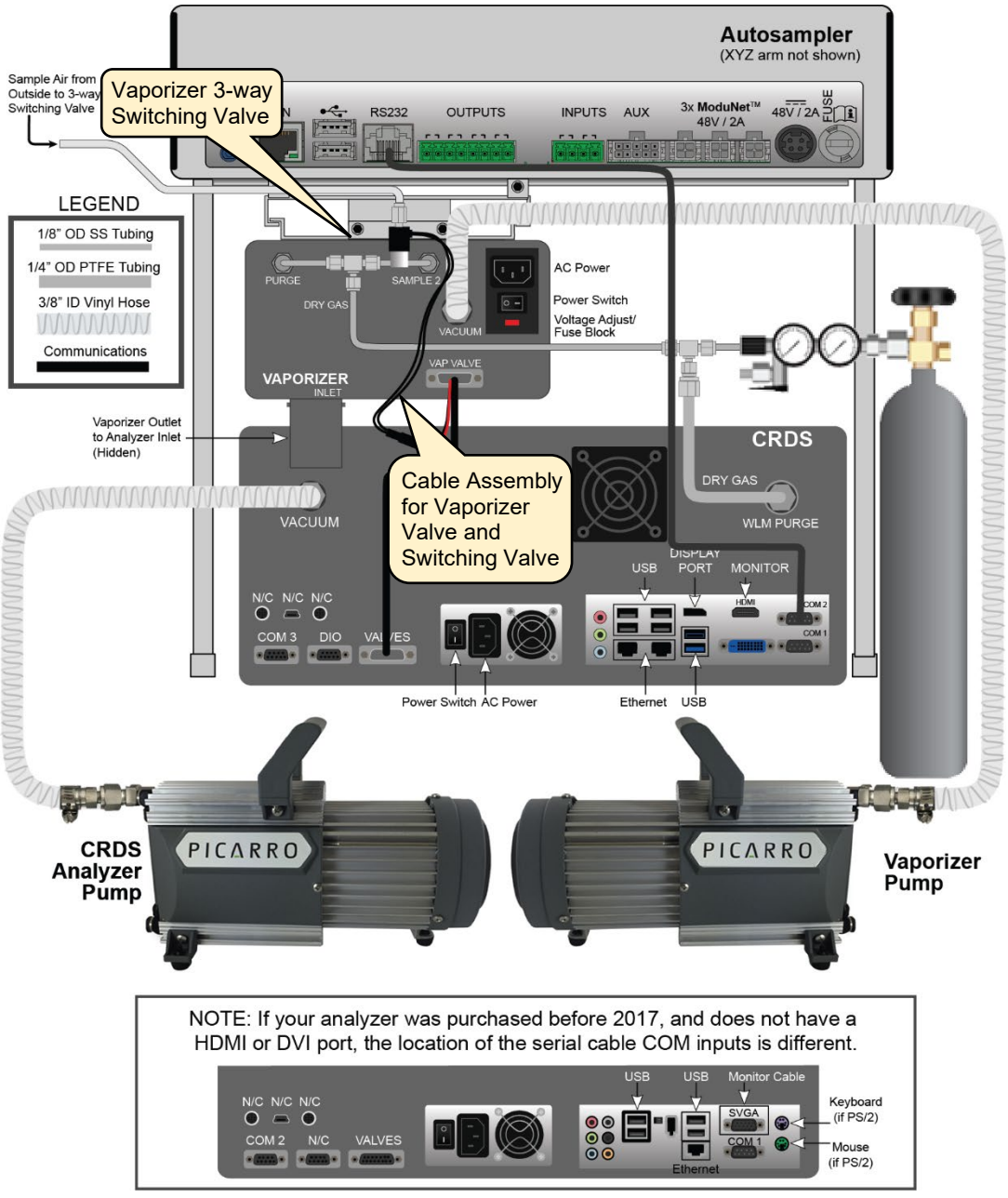


Figure 19: Dry Gas Configuration B

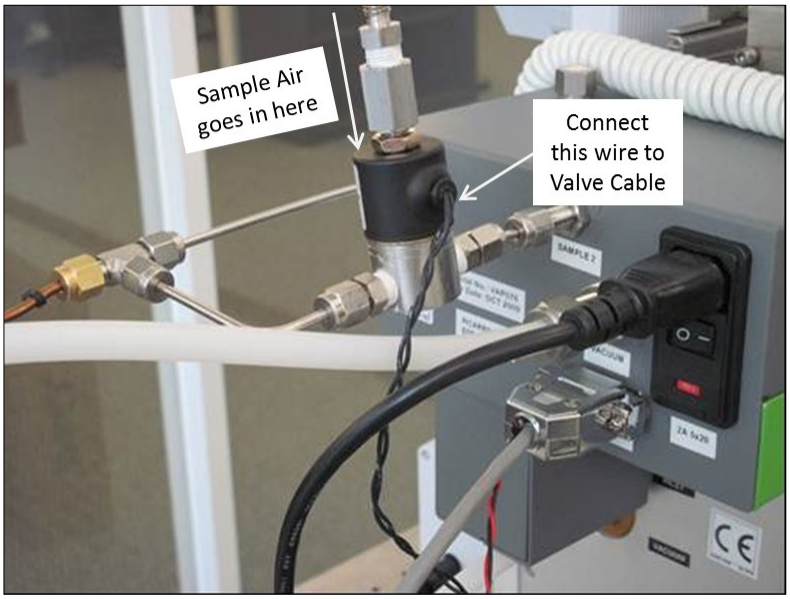


Figure 20: Vaporizer Switching Valve Connected to Vaporizer

5.3 Dry Gas Configuration C

For the SDM setup, you only need to supply dry gas directly to the CRDS analyzer (Figure 21).

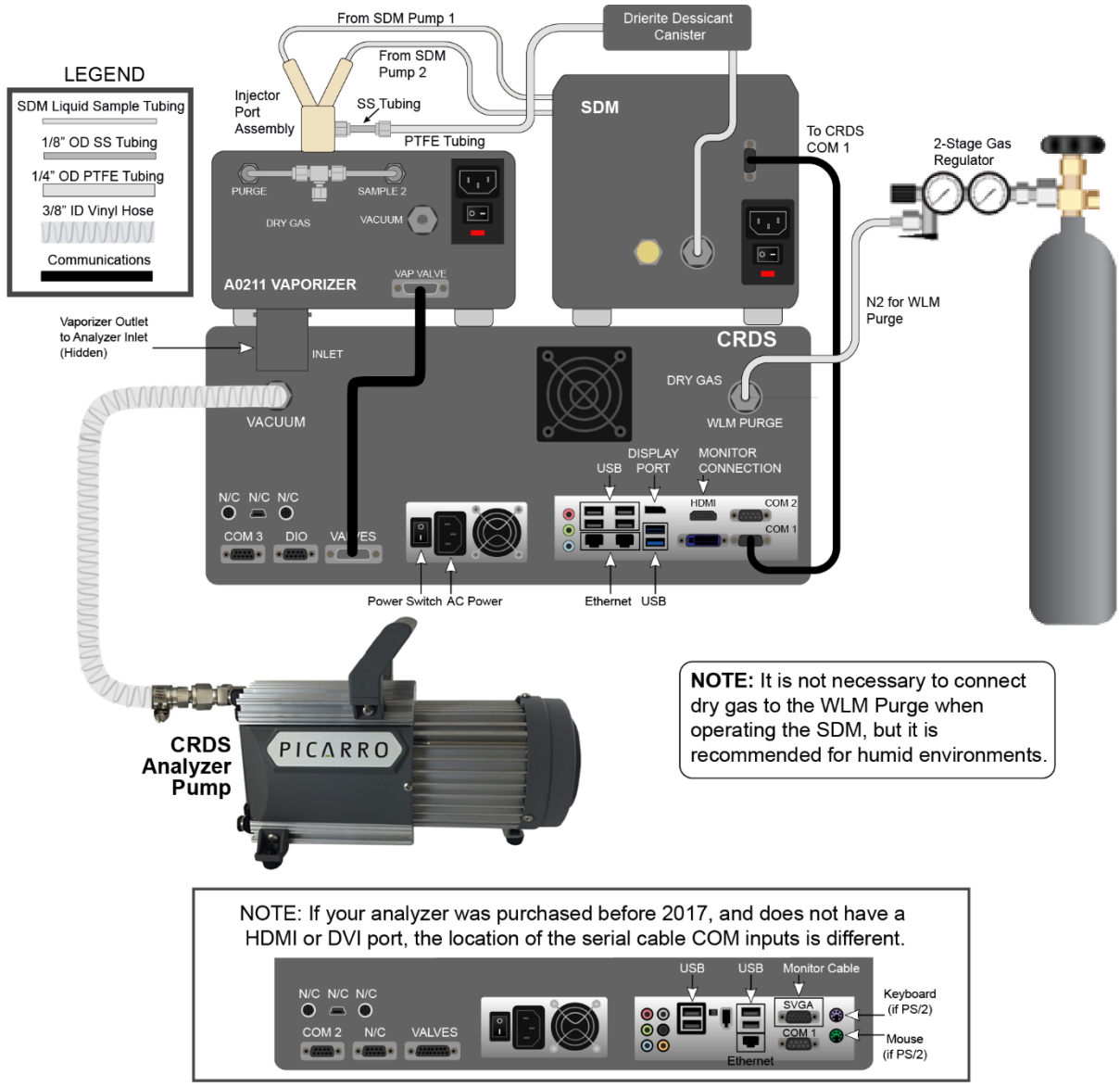


Figure 21: Dry Gas Configuration C

To connect a 1/4" dry gas tube to the Wavelength Monitor Purge (WLM Purge) Port back of the analyzer, use the Push Connector attached to the port.

The connector is in two pieces: The Outer Flap and the Inner Flap. To connect the tube to the port, simply push the tube into the connector and then pull the tube back.

If there is a space between the inner flap and the outer flap, this means that the tube is locked to the port. Do not twist and turn. To take the tube out of the port, push the Outer Flap in against the Inner Flap, and while doing this, pull out the tube. This will cause the gripping mechanism to release from the tube.

Wavelength Monitor Purge Defined

Why do the Picarro isotopic water analyzers (L21x0-*i*) have a wavelength monitor (WLM) purge?

The WLM purge acts to fill the warm box of your analyzer with dry gas. The warm box houses the WLM which is part of the analyzer's laser targeting control loop. The WLM itself enables us to precisely control the wavelength of light being injected into the cavity. Within the warm box there is a distance of about 10 cm which is an open path, i.e., the laser light is seeing the ambient atmosphere at 45°C (the temperature at which the warm box is held). Because water is such a strong absorber, and in the case of our isotopic water systems, the laser is specifically tuned to a frequency of water absorption, this open path segment may result in decay of the light prior to entering the WLM. As a result, the performance of the WLM could vary as ambient conditions change. We elect to dry the gas seen by the laser in the warm box such that any potential decay due to water absorption is limited.

Should I always have dry gas purging the WLM or can I leave it open?

At ambient temperature and pressure, drying the gas that enters the WLM is not essential; however, it is recommended for humid environments and does require a significant amount of gas. If you have access to a zero air or N_2 tank, such as the tank being used as the dry gas source for your vaporizer (High Precision or High Throughput Vaporizer), we recommend adding a T to the line and feeding both your vaporizer and WLM purge with the same dry gas source. You can also purchase a dry gas kit from us with the necessary regulator and fittings to connect a N_2 tank (part # A0921) or zero air tank (part # A0923) to your system. If you are operating your analyzer in a very humid environment, such as above 3% water content (30,000 ppm), we always recommend dry gas be supplied to your WLM purge. Without this dry gas supply, you may experience more drift in the analyzer.

Does the gas used for the WLM purge need to be the same as matrix gas for the cavity?

No, the gas that is used to purge the WLM can differ from the matrix gas seen by the cavity. Picarro isotopic water analyzers have two modes of operation; air and N_2 (use the "Picarro Mode Switcher" to switch between the two). If, for example, you are using the SDM and operating in air mode, you can use N_2 to purge the WLM. The opposite is also fine. If you're running from a tank, you'll typically use the same gas for convenience.

6. Vaporizer to Analyzer Connections

6.1 Valve Controller Cable

Attach the 15 pin end of the grey valve cable to the port labelled Vap Valves on the vaporizer and connect to the port labelled VALVES on the analyzer (third connector from the left at the bottom row of the analyzer).

6.2 Gas Line Connection

1. **(With Autosampler):** If an Autosampler is integrated with your system, carefully align the analyzer and the autosampler relative to each other such that the gas delivery line hanging from the vaporizer is aligned with the inlet port of analyzer. *Do not bend the delivery port in the process*.

   If the delivery port is not horizontally aligned with the analyzer inlet port, gently move the position of the vaporizer on the autosampler by loosening the mounting clamps and retightening them after alignment.

2. **(Without Autosampler):** If an Autosampler is not used with your system, attach the feet to the vaporizer underside or place an object under to level the vaporizer outlet connection to the analyzer inlet.

3. Follow the images below and connect the gas line from the vaporizer to the analyzer as follows.

   a. Remove the insulation box.

   b. Remove the Philips screws of the insulation box visible in Figure 22 (two on each side) and remove the box to allow for easier connection to the analyzer inlet.

   c. Attach the connector to the analyzer inlet and tighten, making sure the 1/16 line goes nice and straight into the aluminum guide (this will become clear to the installation technician with the insulation box removed.)

   d. Move the vaporizer forward, leaving enough space to reinstall the insulation box.

   e. Install the insulation box, then carefully push the autosampler (if used) and/or vaporizer forward so that there is no gap between the insulation around the vaporizer outlet and the analyzer.

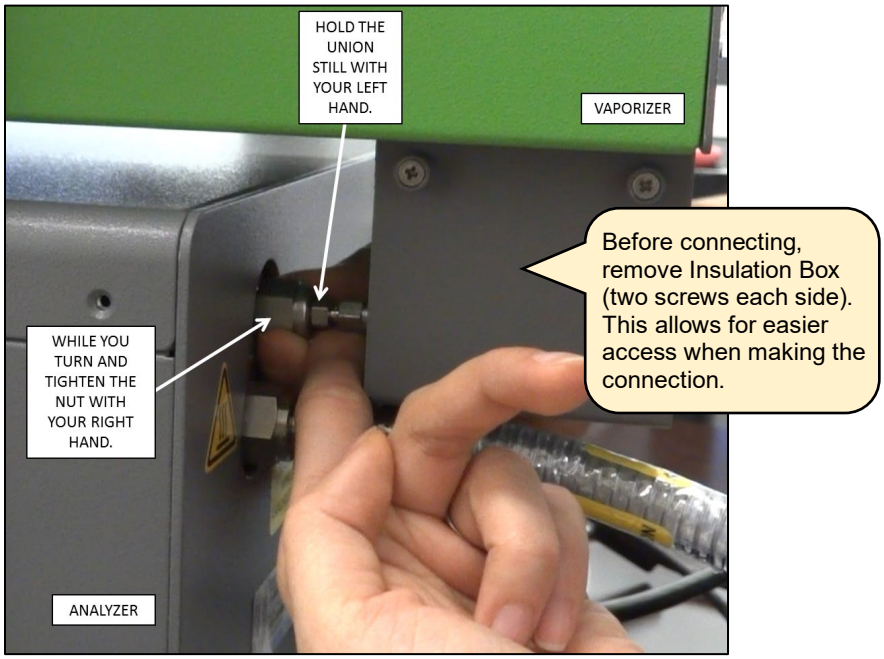


Figure 22: Vaporizer to Analyzer Sample Port Initial Connection

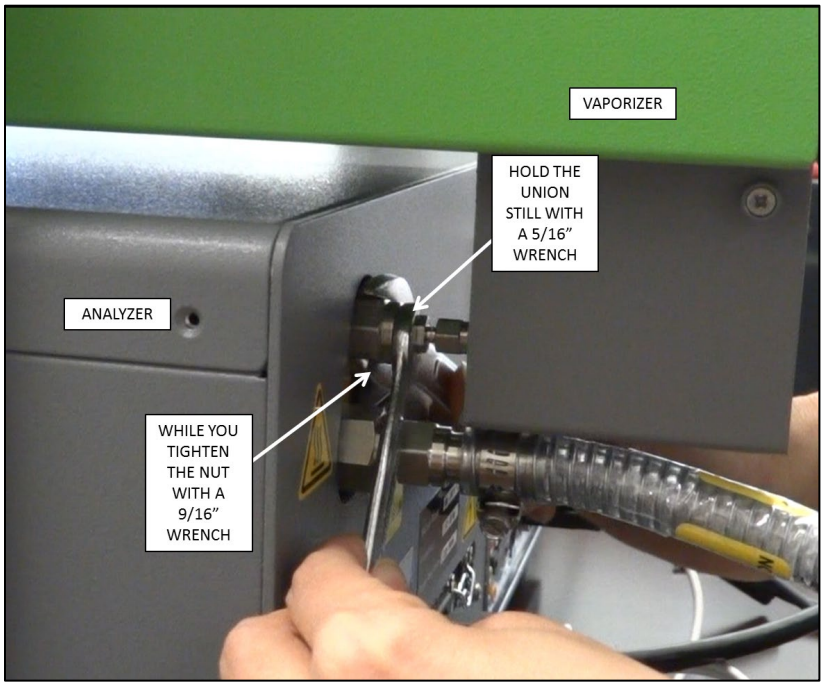


Figure 23: Tightening Vaporizer to Analyzer Connection

7. Basic Operation

This section explains how to operate the analyzer using the GUI. It describes system startup, shutdown, and recovery procedures, desktop features. GUI Functions are detailed in section ***9, CRDS Data Viewer Functions***.

Before continuing, review the important safety notes in the ***Safety*** section.

CAUTION

If one accidentally over-saturates the instrument with water, it is very important to NOT turn the instrument off. Rather, let the instrument pull either room air or dry air/ N_2 through for a few days to dry out the cavity until the instrument can make normal measurements again. If the instrument is turned off right after the accident, water will condense and contaminate the cavity rendering it useless with a very costly cavity repair required for the instrument to operate correctly.

CAUTION

Always turn on the external pump before powering up the analyzer. This ensures a safe start-up sequence. Failure to do so could result in damage to the cavity optics.

7.1 Startup

1. Make sure the pump vacuum hoses are connected between the analyzer and its pump, and the Vaporizer and its pump.

CAUTION

Always turn on the external pump that is attached to the analyzer before powering up the analyzer. This ensures a safe start-up sequence.

2. Verify the power cables to vacuum pumps are plugged in.
3. Switch power on at the pumps.
4. Verify the power cable to the analyzer is plugged in.
5. At the analyzer back panel, press the main power switch to the **ON** (“**I**”) position.
6. If needed, press the round **Soft Power** button on the front panel. The indicator LED will illuminate green.

   The software will start automatically, and the analyzer will display a CRDS Software Loading Status window (Figure 24), then the CRDS Data Viewer window (Figure 25) once loading is complete. Data Viewer features are detailed in section ***9.1***.

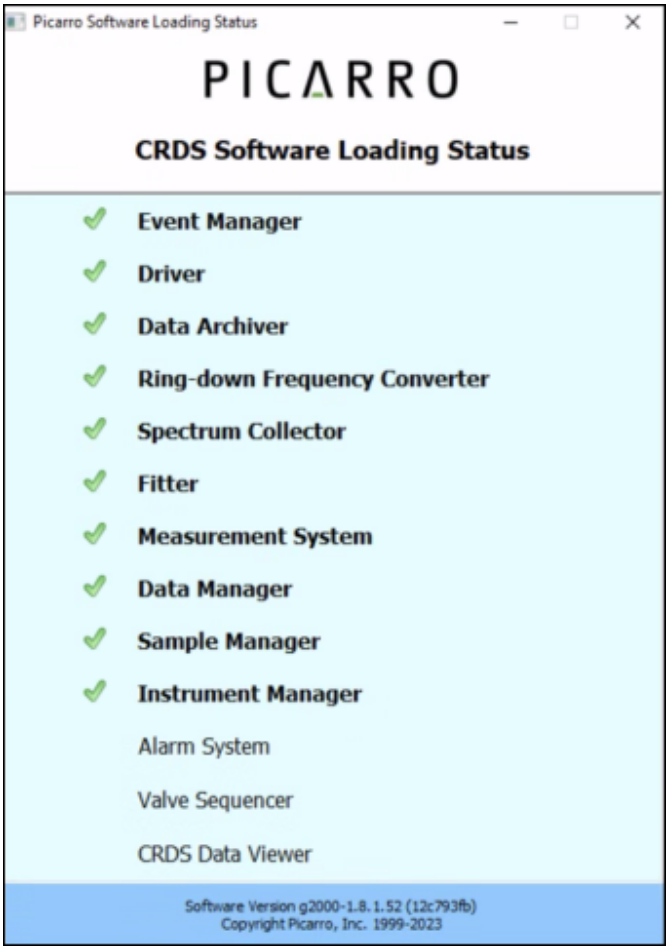


Figure 24: Startup; Software Loading Sequence

The analyzer will not begin producing data until the cavity temperature and pressure have reached their operational set points. A message will be displayed in the Status Log window of the data viewer (see Figure 25, bottom panel) when each set point is reached. An explanation of the most common status log messages can be found in section ***9.10, Analyzer Status Log***.

In the case of the L21x0-*i* analyzer, these are 80°C and 50 Torr. Warm up typically takes about one hour. By design, the cavity pressure will not start to decrease until the cavity temperature is close to its set point. Ideally, the analyzer is open to room air during the warm up, i.e., there is nothing attached to the "Gas Inlet" on the rear of the analyzer. This is desired because ambient water vapor will provide a good signal for the Picarro Wavelength Monitor (WLM) which provides the frequency control for the spectral measurement.

NOTE

The WLM purge is an optional feature and is not required. It is recommended when operating the instrument in a humid environment. For more information, see section *Wavelength Monitor Purge Defined*.

If the analyzer is without a signal for a prolonged period of time (i.e., it is left on dry gas for multiple hours to days), the frequency axis of the analyzer can get lost resulting in incomplete spectra. If you notice an increase in measurement interval or data drop outs after a period of idle time on dry gas, simply disconnect and turn off your dry gas source. The instrument will stabilize after a period of measuring room air.

Data will be saved automatically once the analyzer starts to produce data. The data in the GUI is the continuous real time read out from the analyzer. User data is stored in:

C:\Userdata\DataLog_User \YYYY\MM\DD, where Y=year, M=month, D=day. Further details can be found section ***13 File Management***.

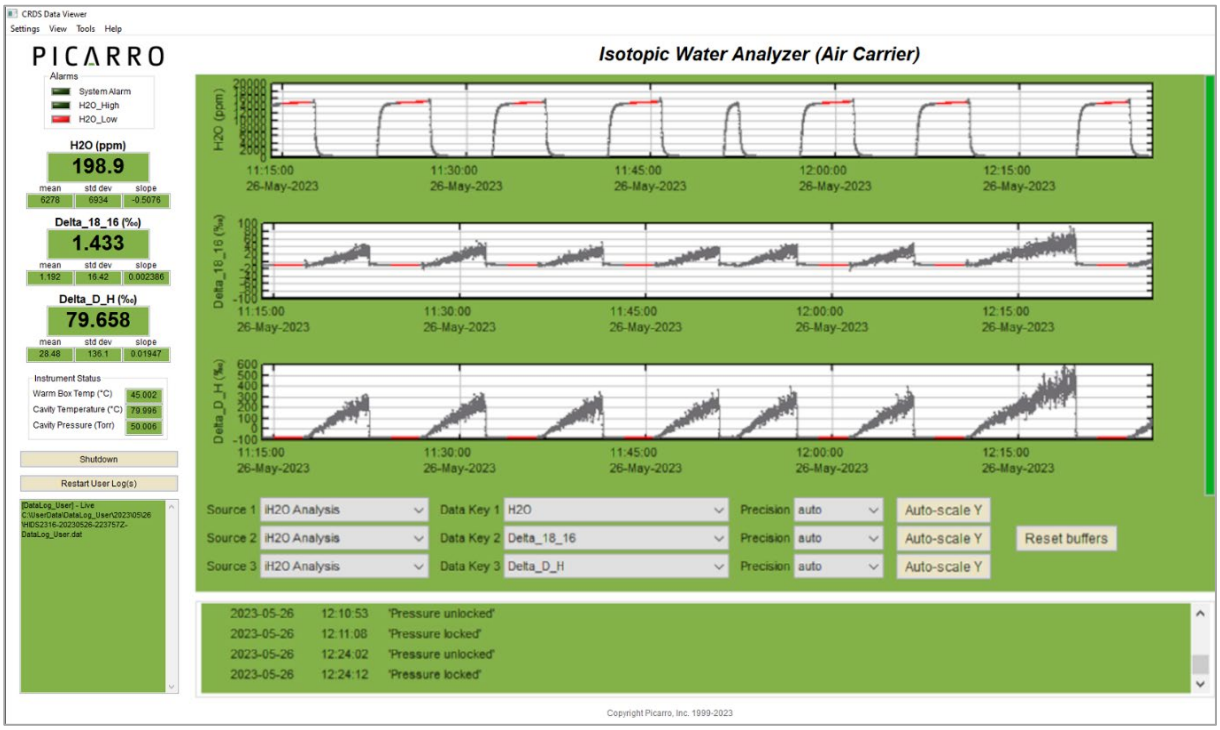


Figure 25: GUI/Data Viewer Screen

7.2 Shutdown

CAUTION

A flow of clean, relatively dry gas should always be directed to the instrument for several minutes prior to shutting down. Trapping a high-moisture content gas sample in the cavity can cause condensation damage to the mirrors as the instrument cools from its operating temperature.

CAUTION

Equipment Damage: If you accidentally over-saturate the instrument with water, it is important that you do not turn the instrument off. Instead, let the instrument pull either room air or dry air/ N_2 through for a few days to dry out the cavity - until the instrument can make measurements normally again. If the instrument is turned off right after the accident, water will condense and contaminate the cavity rendering it useless.

CAUTION

Do not turn off the pump or disconnect the vacuum line while the instrument is operating.

CAUTION

If you have trouble turning off the analyzer software, do not use the Windows Task Manager to kill the process(es). Instead, double-click on the "Stop Instrument" icon in the Diagnostics folder on your desktop and select the default option to stop the software with the drivers running. See Figure 26 below.

Flow Clean, Dry Gas

1. With the pump still running, switch to a source of clean, dry gas at the sample inlet and allow it to run until the water channel reading on the GUI falls below 0.2% (2000 ppm). This will prevent any damage from condensation to the cavity surfaces. This dry gas may be from a tank (target 2-3 PSIG pressure) or from a desiccant column like the Drierite column, C0360, sold on store.picarro.com).

Shutdown

2. Click on the **Shutdown** button located on the left side of the Data Viewer window.
3. A window will pop-up (Figure 26) prompting the user to confirm the shutdown. Once confirmed, the analyzer software and hardware will turn off. (Note: If three options are given on an older instrument, choose the "For **Shipment**" option.)
4. Manually turn off the pump(s) and dry gas (only if system requires it).

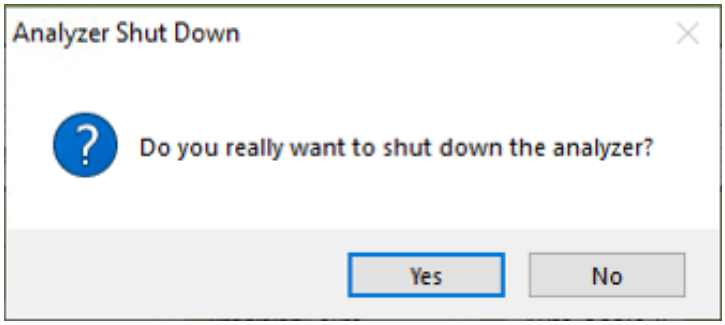


Figure 26: Shutdown Confirmation Pop-Up Dialog

After clicking **Yes** to confirm, the analyzer software, then the computer OS will shut off after a few minutes. *Leave any dry gas or desiccant attached to the inlet during this process*.

5. When the instrument fans audibly turn off, and when the green power button light on the front of the instrument turns off, shut off the pump(s) manually from the rocker switch located on the pump.

7.3 Analyzer Restart after Electrical Power Outage

If power to the analyzer is cut-off for any reason the analyzer will cease operation. However, when the power is reapplied, the analyzer will restart automatically, the Picarro software tools will properly close out previous files and open new files for data collection so that previously collected data, instrument diagnostics and other parameters recorded up to the time of power outage are retained.

If short power outages are common in the user location, Picarro recommends using an uninterrupted power supply (UPS) to protect the data stream and the health of the cavity.

7.4 Desktop Icons and Folders

The following icons and folders related to analyzer operation are populated on the Windows desktop.

Example only: number varies by analyzer model.

Figure 27: Desktop Icons and Folders

Desktop Icons

- **Autosample**r: Launches the Autosampler UI software for managing sample processing tasks.

- **Start Instrument:** If the instrument software is already running, this restarts the software. If the instrument software has been shut down, this starts the software.

- **Coordinator Launcher (not present on all configurations):** Clicking on this icon opens a window that allows you to choose the proper coordinator to operate peripheral modules on certain analyzers.

- **Picarro Mode Switcher (not present on all configurations):** When clicked, a window opens (Figure 28) that allows you to switch between various measurement modes. Most analyzer models are configured for one mode and may not include the Mode Switcher. If the analyzer has multiple modes, this allows the user to switch between them easily.

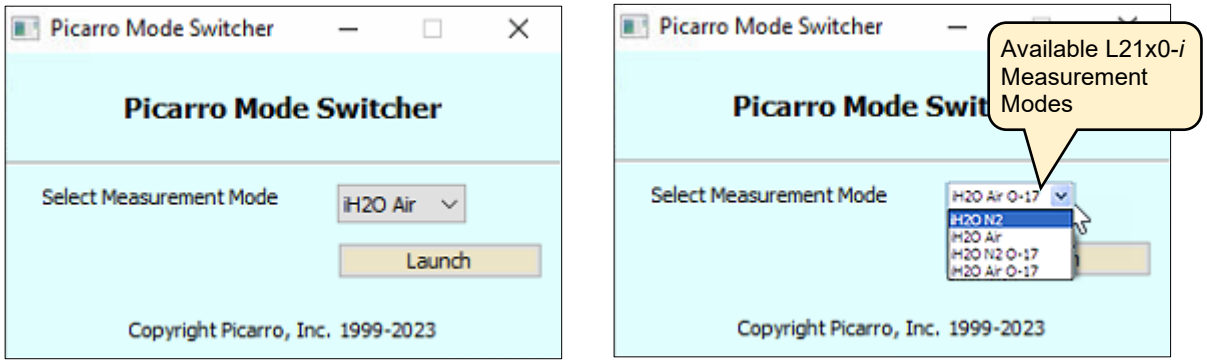


Figure 28: Picarro Mode Switcher

- **Picarro Controller:** When clicked, opens a useful diagnostic panel (Figure 29 below) allowing the user to see the analyzer's internal temperatures, pressure, and spectroscopy in real time. This program has user-accessible functions *but should not be used to change instrument parameters without the direction of Picarro support.*

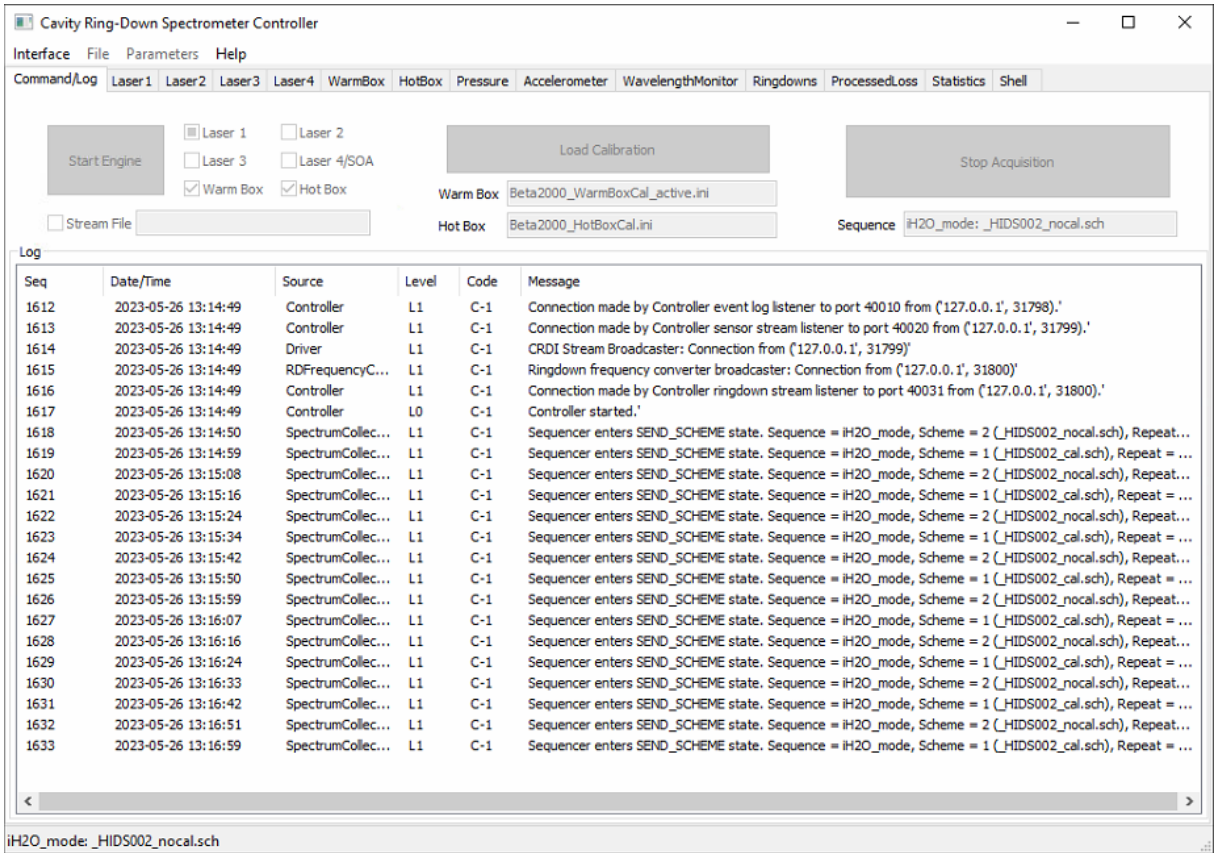


Figure 29: Picarro CRDS Controller Window

- **Picarro Computer Icon:** The Windows Computer Icon is renamed to the analyzer serial number.

- **Data file Viewer**: When clicked, a window opens that allows you to convert between *.dat and H5 data files and to make various graphical representations of your data over time periods longer than what is available in the software buffer. The instructions on using the Data File Viewer software are described in ***APPENDIX B – Data File Viewer***.

Switching Between Measurement Modes

The Picarro Mode Switcher allows users to operate the analyzer in various modes. Switching between measurement modes is accomplished with a few easy steps:

1. Activate the mode switcher interface by double-clicking the Picarro Mode Switcher icon on the desktop (Figure 28).
2. To switch modes, click the drop-down menu, select the desired measurement mode, and then click the launch button.
3. Confirm your selection when prompted by the confirmation dialog box.

4. The analyzer software will then re-start in the new measurement mode. There is no need to turn off the vacuum pump(s) or any other peripherals during this process

Post-Process ChemCorrect

ChemCorrect software is now included in all Picarro water isotope analyzers. The software allows post-acquisition analysis of discrete sample data generated by the coordinator. For more information, see section ***12 ChemCorrect™ Software***.

Picarro Utilities Folder

- **Data Recal:** When clicked, a window opens that allows you to recalibrate your data based on known, certified data.

- **Setup Tool:** When clicked, a window opens that allows you to edit various settings for your analyzer (See ***APPENDIX A – Setup Tool and Communication*** for information.
- **Data file Viewer:** (see above)

Diagnostics Folder

- **Stop Instrument:** When clicked, a window opens that allows you to turn off the analyzer in an emergency event. Upon clicking on this icon, the following window will pop up. Please see section ***7.2, Shutdown*** to shut down the analyzer under normal circumstances.

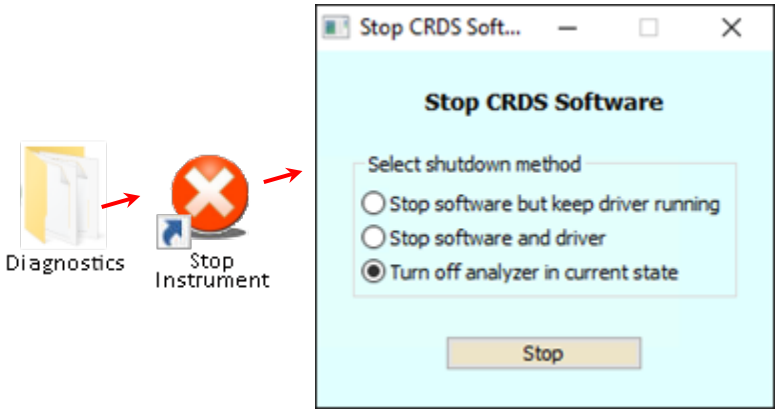


Figure 30: Stop CRDS Software Pop-up

8. Measurement Setup Modes

8.1 Dual Mode Setup

Dual mode is used for measurement of ambient vapor coupled with automated injection of liquid calibration standards. This setup requires A0211 High Precision Vaporizer, A0912 Dual Mode Configuration hardware and software for vapor calibration, and an Autosampler. Each injection cycle takes 9 minutes.

Operation

1. Before continuing, review the important safety notes in the ***Safety*** section.
2. Make sure the hardware setup is complete and the system turned on in the correct sequence.
3. Once turned on, the main CRDS Data Viewer of the analyzer will open automatically on the desktop screen. To understand all the functions of the main CRDS Data Viewer, see the section: ***CRDS Data Viewer Functions***. A sequence of start-up messages will also appear in the Status Log Message window of the main CRDS Data Viewer. For definition, see the section: ***Common Status Log Messages***.
4. Make sure the temperature of the High Precision Vaporizer stabilizes at 110°C by viewing the read out on the front of the vaporizer.


NOTE

Before starting measurements, ensure you are in the correct measurement mode. Select the measurement mode that matches the dry gas supplied to your Vaporizer (either N_2 or zero air). See the section *Switching Between Measurement Modes* for instructions.

5. Make sure the Picarro Autosampler software is running, that the Autosampler has been trained, methods and jobs defined, and samples loaded. For detailed setup instructions, refer to the Picarro A0340 Autosampler User Manual (PN 40-0094) or the Picarro A0325 Autosampler User Manual (PN 40025).
6. Double click on the **Coordinator Launcher** icon on the analyzer's desktop. The coordinator software allows the analyzer to take measurements from multiple samples and is used to control the sample source and match the corresponding real time read out with the sample source. To learn more about the coordinator software (running the software, loading sample description, functions of the coordinator window), see section ***10 Coordinator Software***. Choose and launch an appropriate coordinator mode from the choices in the drop down menu

of the coordinator launcher window. The Dual Mode Setup can operate in one coordinator mode.

7. Once launched, before the Coordinator window opens up, the User Editable Parameters window will pop up (as shown below):

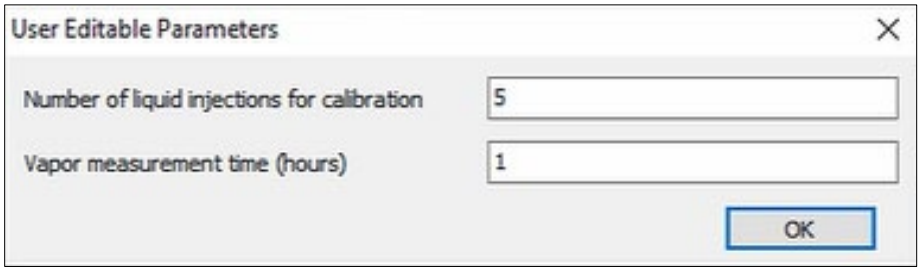


Figure 31: User Editable Parameters Window

This allows measurement of liquid isotopic water standards at fixed time intervals during the measurement of the vapor phase to verify calibration. The analyzer will run the parameters specified in a continuous loop until exiting from the program (i.e., measure 5 liquid injections, 1 hour of vapor, 5 liquid injections, 1 hour of vapor, etc.). Measurement will always start with liquid injections.

- If no liquid samples are to be measured, then enter '0' in the field for liquids. It will then measure the vapor continuously.
- If no vapor samples are to be measured, then enter '0' in the field for vapors. It will then run only the liquid samples specified in the Autosampler job (see later section for details).
- If the analyzer is already running and these parameters need to be changed it will require exiting and restarting the Picarro coordinator software.

NOTE

Analysis of liquid samples requires that both the coordinator software and autosampler job be started. Be sure to start the Autosampler Controller software before launching the Dual Mode Coordinator. Once the Autosampler Controller software is open, you may start the Dual Mode Coordinator. Once open, click "Run" on the Autosampler Controller software.

Picarro highly recommends matching the "Number of liquid injections for calibration" to the injection count set in the Autosampler job. This ensures one sample vial is analyzed completely before returning to vapor measurements. If two or more liquid calibration standards are used, then "number of liquid injections for calibration" can also be an integer multiple of the injection count set in the Autosampler job.

For example, if eight injections each of two liquid standards are to be run every 6 hours during vapor measurements then enter 16 (8 injections * 2 standards) in the first field and 6 in the second field.

Be sure there are sufficient liquid standards available because once all the liquid samples specified in the Autosampler job have been run and the current vapor measurement is complete, the analyzer will wait indefinitely or until a new Autosampler job is started.

NOTE

To calculate the time to complete the autosampler job use the follow formula:

Cycle time = number injections * 9 min + vapor measurement time

Assuming 1 standard per cycle, 8 injections, and 6 hours vapor measurement: the total cycle time is 432 minutes and consumes 1 vial. The Picarro Autosampler has a tray for up to 105 vials. Therefore, one full tray of 105 vials will last 432 * 105 = 45360 minutes or 31.5 days. Thus, plan on one tray lasting for one month of measurements when calibrating every 6 hours.

Once the injection number and vapor measurement duration parameters have been entered, and the 'OK' button is clicked, the coordinator window will pop up on your desktop. The different software element will indicate whether liquid or vapor is being measured.

8. Once launched, the coordinator will automatically start collecting data. The data will also be available in the GUI as pulses. To customize pulse analysis or to adjust the peak of pulse data, please see the section ***Pulse Customization*** located in section ***15 Best Practices and Operational Tips***.

Figure 32: Coordinator Launcher

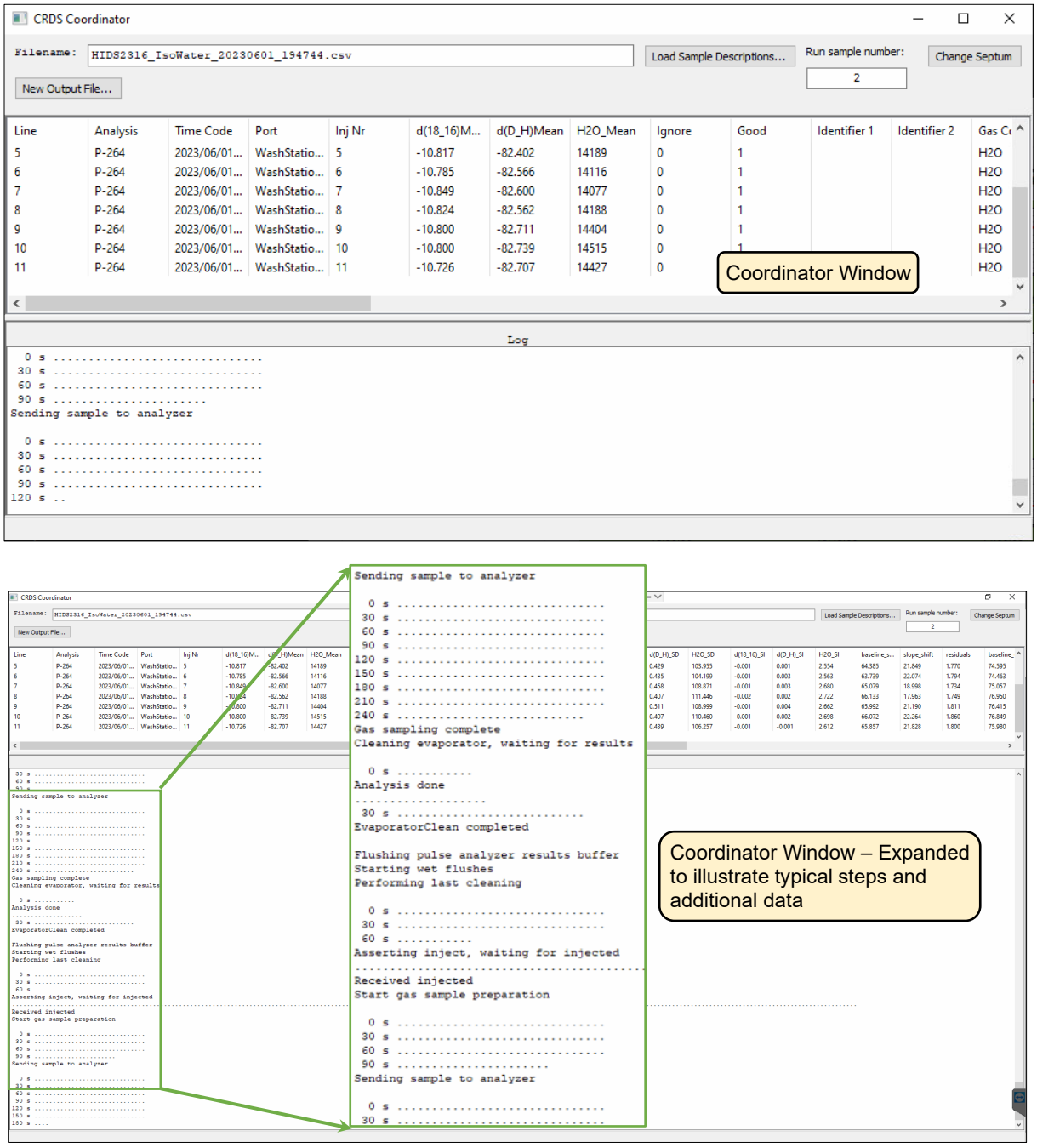


Figure 33: Coordinator Window

Data

To learn where to retrieve the data, and to set the frequency of file archival and automatic deletion of old files, see section ***13 File Management***.

To access one's data remotely, see the section; ***Remote Data Access*** in ***APPENDIX A – Setup Tool and Communication***.

For instruction on configuring data file saving details, including which data elements are written to data files, digital data output (via serial port or TCP/IP), remote data delivery (via email), and general GUI properties, click on the **Setup Tool** icon in the Picarro Utilities folder in the desktop.

The Picarro water analyzers allow users to archive data using a compressed, binary "HDF5" or "h5" format. The Data File Viewer program, which comes installed with the hardware, allows one to open and convert h5 files, as well as viewing the h5 files as graphs. For more information, see ***APPENDIX B – Data File Viewer***.

The Picarro water analyzers come preinstalled with the ChemCorrect software which allows one to screen and quantify contamination in isotopic water samples. To post process data using ChemCorrect Software, see section ***12.2 Analysis of Coordinator Output*** Files located in section***12 ChemCorrect™ Software.***

One may need to adjust the sample injection volume to improve the quality of data. See ***15.2 Adjusting Injection Volume*** in section ***15 Best Practices and Operational Tips***.

8.2 Manual Mode Setup

Operation

1. Before continuing, review the important safety notes in SAFETY.
2. Make sure the hardware setup is complete and the system turned on in the correct sequence.
3. Once turned on, the main CRDS Data Viewer of the analyzer will open automatically on the desktop screen. To understand all the functions of the main CRDS Data Viewer, see CRDS Data Viewer. A sequence of start-up messages will also appear in the Status Log Message window of the main CRDS Data Viewer. For definition, see Common Status Log Messages.
4. Make sure the temperature of the High Precision Vaporizer has stabilized to 110 °C.

NOTE

Before starting measurements, ensure you are in the correct measurement mode. Select the measurement mode that matches the dry gas supplied to your Vaporizer (either N_2 or zero air). See section *Switching Between Measurement Modes* for instructions.

5. Double click on the **Coordinator Launcher** icon on the desktop. The coordinator software allows the analyzer to take measurements from

multiple samples and is used to control the sample source and match the corresponding real time read out with the sample source. To learn more about the coordinator software (running the software, loading sample description, functions of the coordinator window), see section ***10 Coordinator Software***. Choose and launch an appropriate coordinator mode from the choices in the drop down menu. The coordinator window will pop up.

The **Manual Mode** Setup can operate in **one** coordinator mode in the **L2130-*i***.

- **Manual Inject:** Used for semi-automated measurement of liquid water samples with high precision. Requires A0211 High Precision Vaporizer. User manually injects samples after prompt. The vaporizer control and the analysis of liquid samples are automated. Each injection cycle takes 9 minutes.

The **Manual Mode** Setup can operate in **two** coordinator modes for the **L2140-*i***.

- **O^{17} Manual Inject:** Used for semi-automated measurement of liquid water samples for $\delta^{18}O$, $\delta^{17}O$, $\delta^{2}H$ and ^{17}O-excess. Requires A0211 High Precision Vaporizer. User manually injects samples after prompt. The vaporizer control and the analysis of liquid samples are automated. *This coordinator must be run in either the "iH2O N2 O-17" mode or the "iH2O Air O-17" mode*. In this mode the coordinator will output $\delta^{17}O$ and ^{17}O-excess. Each injection cycle takes 9 minutes.
- **Manual Inject:** Used for semi-automated measurement of liquid water samples with high precision on $\delta^{18}O$ and $\delta^{2}H$. Requires A0211 high precision vaporizer. User manually injects samples after prompt. The vaporizer control and the analysis of liquid samples are automated. Each injection cycle takes 9 minutes.

To learn about all the other coordinator modes supported by the Picarro water analyzer (in different setups), see section ***10.5 Coordinator Modes Available On a Picarro Water Isotope Analyzer***.

6. Once launched, the coordinator will direct the user on when to manually inject samples and it will automatically start collecting data. The data will also be available in the GUI as pulses. To customize pulse analysis or to adjust the peak of one's data pulses, see the section ***Pulse Customization*** located in section ***15 Best Practices and Operational Tips***.
7. The status bars at the bottom of the Coordinator window will allow one to know if the analyzer is ready for a manual injection or not. If ready, the sample description (if preloaded) will appear. If not loaded, a description can be added. Manually inject the sample and then press the Injected button in the lower right corner of the Coordinator window. The coordinator software will prepare the sample in the vaporizer in high precision mode (same as Standard Mode). It will take approximately 9 minutes until it is ready for the next injection.

Data

To learn where to retrieve the data, and to set the frequency of file archival and automatic deletion of old files, see section ***13 File Management***.

To access one's data remotely, see the section; ***Remote Data Access*** in ***APPENDIX A – Setup Tool and Communication***.

For instruction on configuring data file saving details, including which data elements are written to data files, digital data output (via serial port or TCP/IP), remote data delivery (via email), and general GUI properties, click on the **Setup Tool** icon in the Picarro Utilities folder in the desktop.

The Picarro water analyzers allow users to archive data using a compressed, binary "HDF5" or "h5" format. The Data File Viewer program, which comes installed with the hardware, allows one to open and convert h5 files, as well as viewing the h5 files as graphs. For more information, see ***APPENDIX B – Data File Viewer***.

The Picarro water analyzers come preinstalled with the ChemCorrect software which allows one to screen and quantify contamination in isotopic water samples. To post process data using ChemCorrect Software, see section ***12.2 Analysis of Coordinator Output*** Files located in section ***12 ChemCorrect™ Software***.

One may need to adjust the sample injection volume to improve the quality of data. See ***15.2 Adjusting Injection Volume*** in section ***15 Best Practices and Operational Tips***.

8.3 Picarro Autosampler and High Precision Vaporizer Setup

This setup is used for automated injection of liquid waters. It consists of two modes that utilize the same hardware: High Precision Mode (same as Standard Mode) and High Throughput Mode.

Operation

1. Before continuing, review the important safety notes in SAFETY.
2. Make sure the hardware setup is complete and the system is turned on in the correct sequence.
3. Once turned on, the main CRDS Data Viewer of the analyzer will open automatically on the desktop screen. To understand all the functions of the main CRDS Data Viewer, see CRDS Data Viewer. A sequence of start-up messages will also appear in the Status Log Message window of the main CRDS Data Viewer. For definition, see Common Status Log Messages.

4. Make sure the temperature of the High Precision Vaporizer has stabilized at 110°C by viewing the read out on the front of the vaporizer.

NOTE

Before starting measurements, ensure you are in the correct measurement mode. Select the measurement mode that matches the dry gas supplied to your Vaporizer (either N_2 or zero air). See the section *Switching Between Measurement Modes* for instructions.

5. Make sure the Picarro Autosampler software is running, that the Autosampler has been trained, methods and jobs defined, and samples loaded. For detailed setup instructions, refer to the Picarro A0340 Autosampler User Manual (PN 40-0094) or the Picarro A0325 Autosampler User Manual (PN 40025).
6. Double click on the Coordinator Launcher icon on the analyzer's desktop. The coordinator software allows the analyzer to take measurements from multiple samples and is used to control the sample source and match the corresponding real time read out with the sample source. To learn more about the coordinator software (running the software, loading sample description, functions of the coordinator window), see section ***10 Coordinator Software***. Choose and launch an appropriate coordinator mode from the choices in the drop down menu of the coordinator launcher window. The coordinator window will pop up.

The Picarro Autosampler – High Precision Vaporizer Setup can operate in following coordinator modes:

For the L2140-*i*:

- **High Precision (same as Standard Mode):** For interfacing with an autosampler for highest precision measurements of $\delta^{18}O$ and $\delta^{2}H$. This coordinator must be run in either the iH2O N2 mode or the iH2O Air mode. In this mode the coordinator will not output $\delta^{17}O$ and ^{17}O-excess. Each injection cycle takes 9 minutes.
- **High Throughput:** For interfacing with an autosampler for faster measurements of $\delta^{18}O$ and $\delta^{2}H$ with good precision. This coordinator must be run in either the iH2O N2 mode or the iH2O Air mode. In this mode the coordinator will not output $\delta^{17}O$ and ^{17}O-excess. Each injection cycle takes 4 minutes.
- **O^{17} High Precision:** For interfacing with an autosampler for highest precision measurements of $\delta^{18}O$, $\delta^{17}O$, $\delta^{2}H$ and ^{17}O-excess. This coordinator must be run in either the "iH2O N2 O-17" mode or the "iH2O Air O-17" mode. In this mode the coordinator will output $\delta^{17}O$ and ^{17}O-excess.
- **Express*:** Used for faster measurement of liquid water samples with good precision. This coordinator must be run in either the "iH2O N2" mode or the "iH2O Air" mode. Automatically injects and analyzes liquid water

samples. When using the Express coordinator, we recommend 10 injections, the first 6 injections take 1.5 minutes each, while the last 4 injections take 5 minutes each. The first 7 injections will be discarded to achieve optimal memory reduction.

- **Standard* (same as High Precision Mode):** Used to measure liquid water samples with maximum precision. This coordinator must be run in either the “iH2O N2” mode or the “iH2O Air” mode. Automatically injects and analyzes liquid samples. Each injection cycle takes 9 minutes.
- **Survey*:** Used for super-fast measurements of large sample batches at moderate precision and enables efficient sample sorting. Automatically injects and measures liquid samples. This coordinator must be run in either the “iH2O N2” mode or the “iH2O Air” mode.

Only available with Coordinator software upgrade

Survey mode has two use cases:

- Sample Sorting and Rearrangement: Survey large sample batches and use the output values to manually rearrange samples. This will result in reducing the memory effect of the followed measurements (either by Express mode or by Standard mode). In this use case we recommend doing 1 injection per sample, with sample volume of 2.5 µl. Using these parameters, measurement time is 95 seconds per sample.
- Sample Measurement with Moderate Precision: Use the survey mode to quickly measure samples with moderate precision. Here we recommend 6 injections with sample volume of 2.5 µl. The first 3 injections should be discarded to achieve acceptable levels of memory. Using these parameters, measurement time is reduced to 9.5 minutes per sample.

For the L2130-*i*:

- **High Precision (same as Standard Mode):** Used to measure liquid water samples with maximum precision. This coordinator must be run in either the “iH2O N2” mode or the “iH2O Air” mode. Automatically injects and analyzes liquid samples. Each injection cycle takes 9 minutes.
- **High Throughput:** Used for faster measurement of liquid water samples with good precision. This coordinator must be run in either the “iH2O N2” mode or the “iH2O Air” mode. Automatically injects and analyzes liquid water samples. Each injection cycle takes 4 minutes.
- **Express*:** Used for faster measurement of liquid water samples with good precision. This coordinator must be run in either the “iH2O N2” mode or the “iH2O Air” mode. Automatically injects and analyzes liquid water samples. When using the Express coordinator, we recommend 10 injections, the first 6 injections take 1.5 minutes each, while the last 4 injections take 5 minutes each. The first 7 injections will be discarded to achieve optimal memory reduction.

- **Standard* (same as High Precision Mode):** Used to measure liquid water samples with maximum precision. This coordinator must be run in either the “iH2O N2” mode or the “iH2O Air” mode. Automatically injects and analyzes liquid samples. Each injection cycle takes 9 minutes.
- **Survey*:** Used for super-fast measurements of large sample batches at moderate precision and enables efficient sample sorting. Automatically injects and measures liquid samples. This coordinator must be run in either the “iH2O N2” mode or the “iH2O Air” mode.

Only available with Coordinator software upgrade

Survey mode has two use cases:

- Sample Sorting and Rearrangement: Survey large sample batches and use the output values to manually rearrange samples. This will result in reducing the memory effect of the followed measurements (either by Express mode or by Standard mode). In this use case we recommend doing 1 injection per sample, with sample volume of 2.5 µl. Using these parameters, measurement time is 95 seconds per sample.
- Sample Measurement with Moderate Precision: Use the survey mode to quickly measure samples with moderate precision. Here we recommend 6 injections with sample volume of 2.5 µl. The first 3 injections should be discarded to achieve acceptable levels of memory. Using these parameters, measurement time is reduced to 9.5 minutes per sample.

NOTE

Analysis of liquid samples requires that both the coordinator software and autosampler job be started. Be sure to start the Autosampler Controller software before launching the Dual Mode Coordinator. Once the Autosampler Controller software is open, you may start the Coordinator. Once open, click “Run” on the Autosampler Controller software.

7. Once launched, the coordinator will automatically start collecting data, assuming the Autosampler job has been started. The data will also be available in the GUI as pulses. To customize pulse analysis or to adjust the peak of pulse data, please see the section ***Pulse Customization*** located in section ***15 Best Practices and Operational Tips***.

Figure 34: Coordinator Launcher

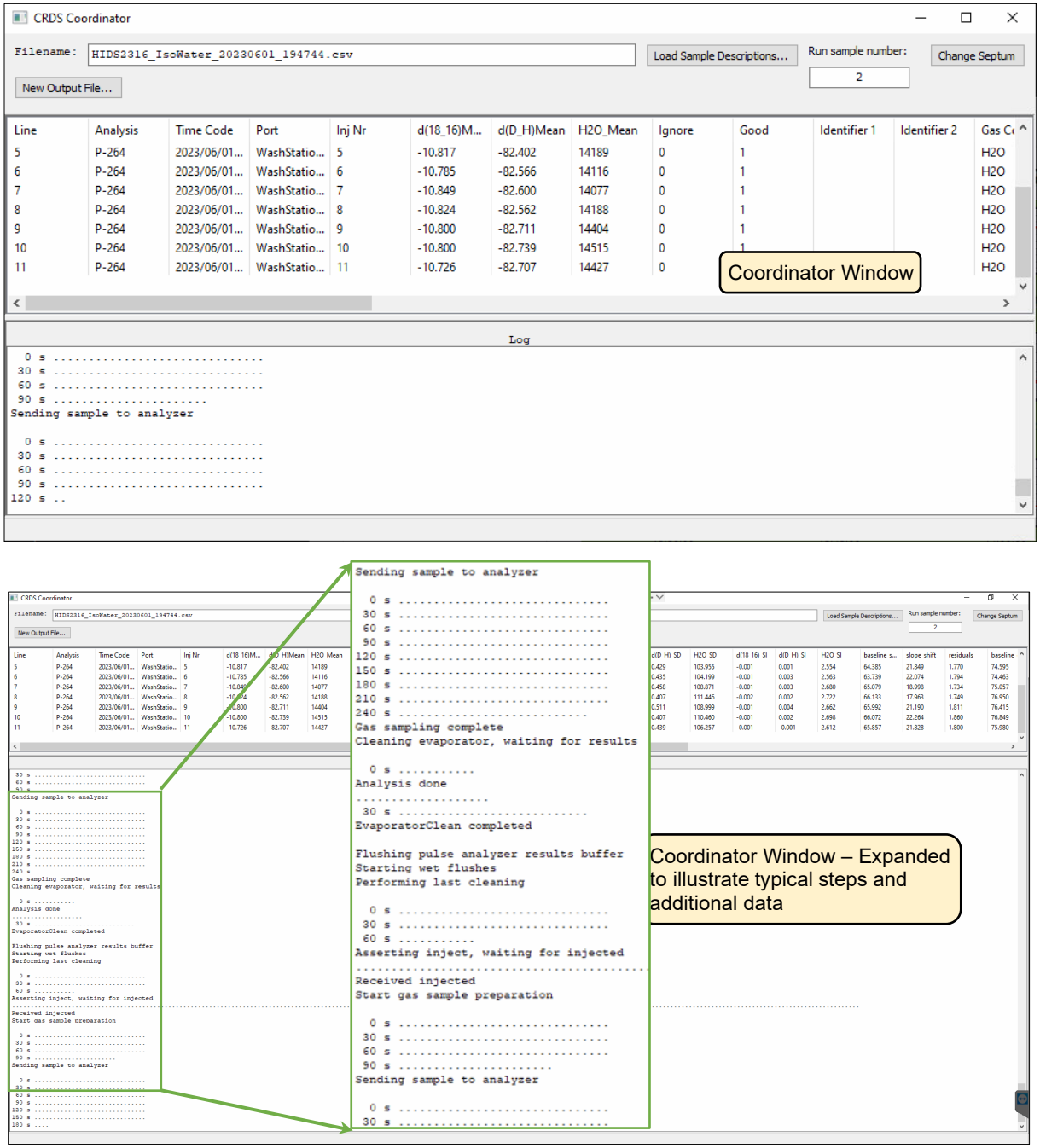


Figure 35: Coordinator Window

Data

To learn where to retrieve the data, and to set the frequency of file archival and automatic deletion of old files, see section ***13 File Management***.

To access one's data remotely, see the section; ***Remote Data Access*** in ***APPENDIX A – Setup Tool and Communication***.

For instruction on configuring data file saving details, including which data elements are written to data files, digital data output (via serial port or TCP/IP), remote data delivery (via email), and general GUI properties, click on the **Setup Tool** icon in the Picarro Utilities folder in the desktop.

The Picarro water analyzers allow users to archive data using a compressed, binary "HDF5" or "h5" format. The Data File Viewer program, which comes installed with the hardware, allows one to open and convert h5 files, as well as viewing the h5 files as graphs. For more information, see ***APPENDIX B – Data File Viewer***.

The Picarro water analyzers come preinstalled with the ChemCorrect software which allows one to screen and quantify contamination in isotopic water samples. To post process data using ChemCorrect Software, see section ***12.2 Analysis of Coordinator Output*** Files located in section ***12 ChemCorrect™ Software***.

One may need to adjust the sample injection volume to improve the quality of data. See ***15.2 Adjusting Injection Volume*** in section ***15 Best Practices and Operational Tips***.

8.4 Picarro Autosampler and High Throughput Vaporizer Setup

Picarro removed the High Throughput Vaporizer (part number A0212) from the price list in December 2013. Since that time, we have not shipped new High Throughput Vaporizers; however, we do continue to support High Throughput Vaporizers that are in the field. If you own a High Throughput Vaporizer, please contact support@picarro.com for operational instructions. They will refer you to an earlier version of this manual.

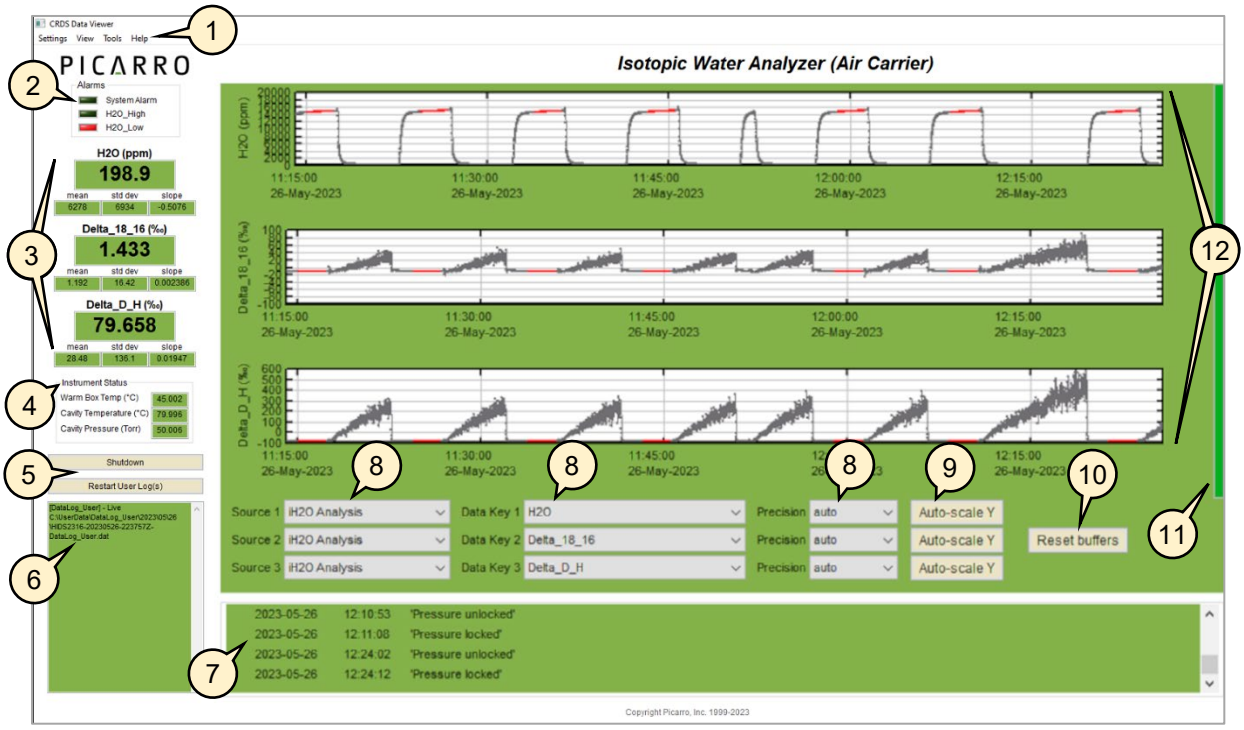
9. CRDS Data Viewer Functions

NOTE

The illustrations shown in this chapter are for example only. What is shown on your instrument is dependent on the analyzer model and its configuration which may differ from these examples.

9.1 CRDS Data Viewer Overview

The features of the Data Viewer shown in Figure 36 are described in the following sections.



1. Settings, View, Tools, and Help menus
2. Alarm Panel
3. Digital Readouts and Statistics
4. Instrument Status
5. Shutdown and Restart Log Buttons
6. Data Log; Filename, and Path
7. Status Log Window
8. Data Source, Data Key, and Precision pull-down menus for data window content
9. Axis Auto Scaling
10. Reset Data Buffer
11. Data Buffer Level Meter
12. Data Windows

Figure 36: Layout of Analyzer Data Viewer

9.2 Settings, View, Tools, and Help Menus

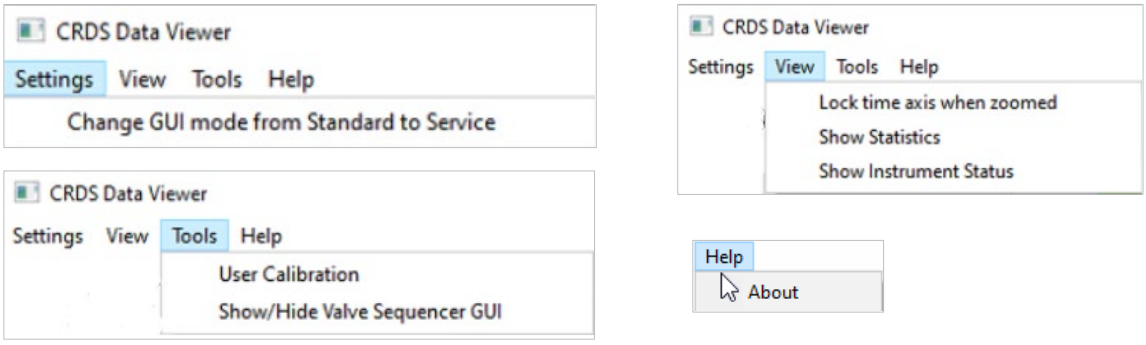


Figure 37: Menu Toolbar Options

Settings Menu

Left clicking on the **Settings** menu pulls down a menu that has one entry: **Change GUI Mode from Standard to Service (or Change GUI mode from Service to Standard if it is already in service mode)**.

This is the access point to a password protected service mode (default password is **picarro**) where additional operational and measurement parameters are available in the data keys. Selecting and clicking on this entry opens the Cavity Ring-Down Spectrometer Controller.

View Menu

This menu item has three entries:

1. **Lock time axis when zoomed/Unlock time axis:** When locked, forces the two graphs to display the same time scale during zoom.
1. Show/Hide Statistics: Toggles the measurement statistics display, see the section ***Digital Readouts*** below.
2. Show/Hide Instrument Status: Toggles the instruments status display. See the section ***Instrument Status***, below.

Tools Menu

This menu item has two entries:

1. **User Calibration:** Opens the password protected user calibration window (default password is **picarro**).

   Calibration slope and intercept can be entered, and their effects are immediately seen in the data. See section ***11, Calibration*** for more information.

2. **Show/Hide Sequencer GUI:** Toggles the display of the external valve sequencer window (user may need to hit **alt-tab** to bring it to the front).

Help Menu

About: Displays the version number of the instrument.

9.3 Alarms Panel

This panel is used to monitor the status of the internal instrument alarms. These indicators are gas concentration alarms, such as “H2O Too High/Low” depending on instrument configuration. The gas concentration alarm icons are off (grayed) when the respective concentrations are below a certain value, and they are illuminated red when the respective concentrations are above/below a certain value.

CAUTION

High/low alarm settings are not intended as a safety measure as configured at the factory, either with respect to human health or the health of the analyzer. It is up to the customer to determine the meaning and level of a “high” or “low” value based on their application.

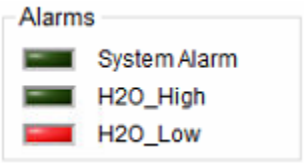


Figure 38: Alarm Panel

To view the alarm set point, click on the **Alarm Icon** and a dialog box will appear indicating the alarm setting and allow the user to enable it or change the setpoint.

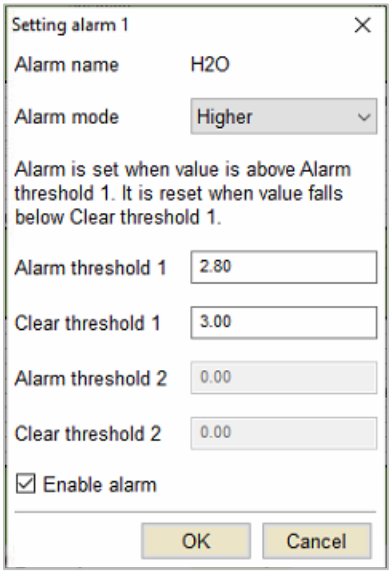


Figure 39: Alarm Settings Dialog Box Example

Type the value you wish to set the alarm to and click the **OK** button or **Cancel** if you do not wish to change the alarm value. If you do nothing, the dialog box will disappear, and the alarm value will remain unchanged. The units are those that appear in the GUI graph.

9.4 Digital Readouts

Displays the latest value recorded for the selected Data Key for each Data Window. Changing the Data Key changes the Digital Readout as well as the Data Window view. If the **Show Statistics** entry is enabled in the **View** menu, the mean, standard deviation, and slope of the data in the graph is dynamically calculated and indicated below the digital concentration readout. These numbers change to reflect statistics of whatever data is in the data window. **Zooming** into a section of existing data will show the statistics statically for that time period, while the digital readout above the statistics continues to update with the latest value. See ***9.12, Reset Buffers*** Button

Click this button to clear the internal data buffer of the GUI (this clears the current data traces from the graphs). This has the effect of clearing all data in the data window. *Pressing this button has no effect on any of the data log files stored by the instrument.*

Graph Zooming for more information.

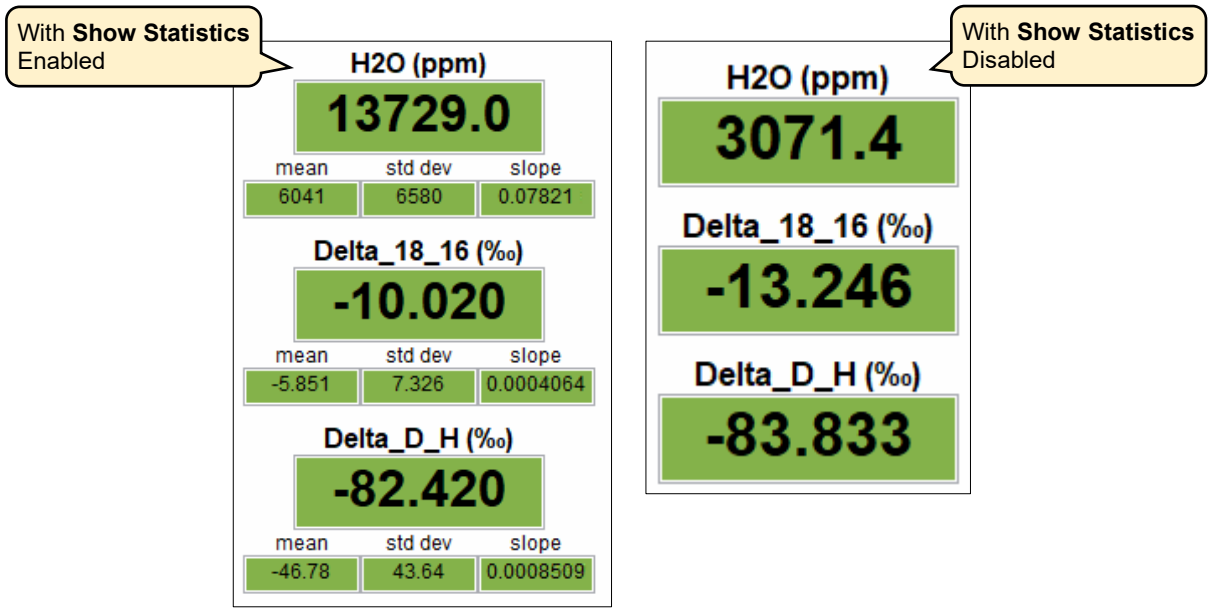


Figure 40: Digital Readouts Panel

9.5 Instrument Status

If these parameters are enabled through the **Show Instrument Status** entry in the **View** menu on the main toolbar, digital readouts for Warm Box temperature, Cavity Temperature and Cavity Pressure are displayed to the left of the main trend graphs.

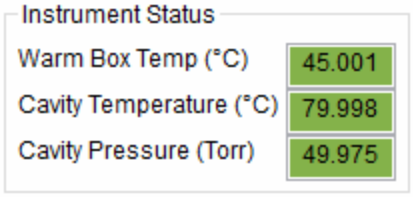


Figure 41: Instrument Status Panel

9.6 Shutdown and Stop User Log(s) Buttons

Figure 42: Shutdown/Stop User Log

Shutdown Button:

Shuts down the analyzer. See section ***7.2, Shutdown*** for more information.

Restart User Log(s) Button

The analyzer automatically records all data collected on the instrument as .dat files. These are described further in 13 File Management.

To start a new data file (time-coded to the current second), click the **Restart User Log(s)** button. The new file name should be visible beneath the button in a few seconds.

Data Log Filename and Path

The filename and path of the active data log is displayed in this pane. The indicator is grayed-out when there is no active data log before gas measurement reporting begins. A new file is generated when the instrument starts reading gas concentrations, (e.g., “201301Z”) and subsequently at 1 hour increments (e.g., “211301Z”, “221301Z”). A new day folder (e.g., “2023\06\01”) will be generated at midnight, as will month and year folders at the appropriate times.

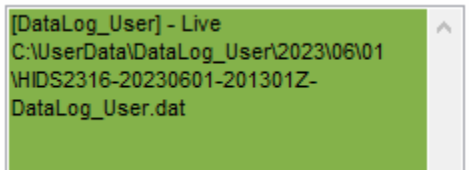


Figure 43: Data Log Filename and Path Panel

9.7 Data Window

The data window displays a graph of any stream of data vs. system time, with a format of hh:mm:ss. The user can select which data streams are displayed using combinations from the **Data Source** and **Data Key** pull down menus. The precision displayed can be adjusted using the **Precision** menu. Auto-Scaling of the **Y-axis** is also available. Clicking any Autoscale button autoscales its Y-axis if the plot hasn't done this automatically.

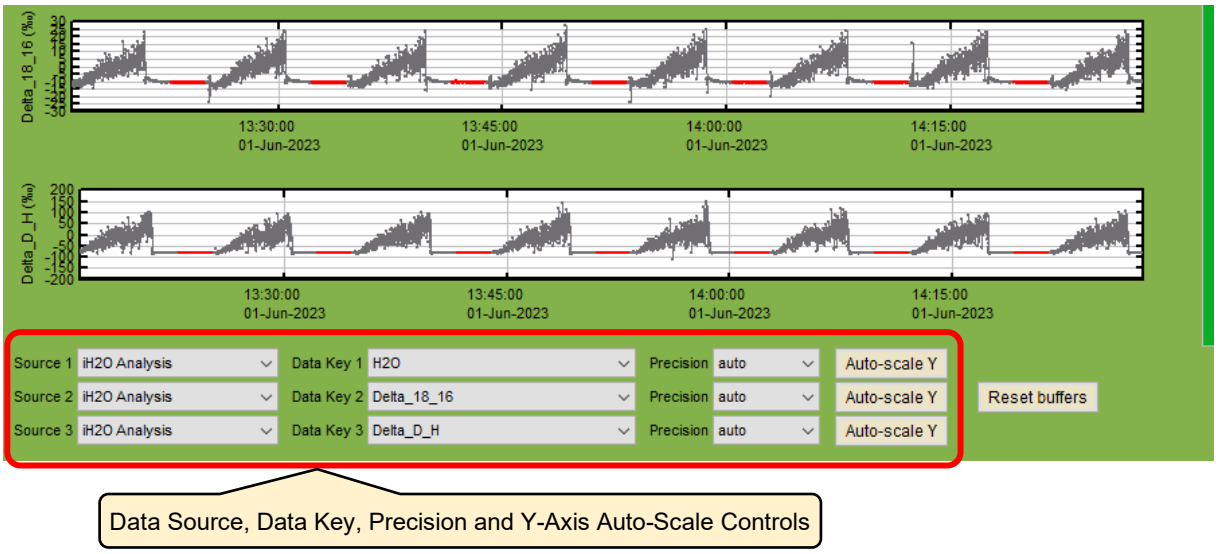


Figure 44: Data Window Panel

9.8 Data Source and Data Key Pull Down Menus

Data Source and Data Key menus (Figure 45) enable selection of the data stream that is viewed in the data window.

- Gas concentrations if 'instrument Analysis' (where instrument represents the system installed) is selected.
- Sensor Readings: If "Sensors" is selected, the analyzer's optical cavity pressure or temperature can be viewed, as well as the temperature of the electronics of the analyzer ("DASTemp," not directly controlled), and the

temperature of the analyzer's wavelength monitor, indicated as "WarmBoxTemp."

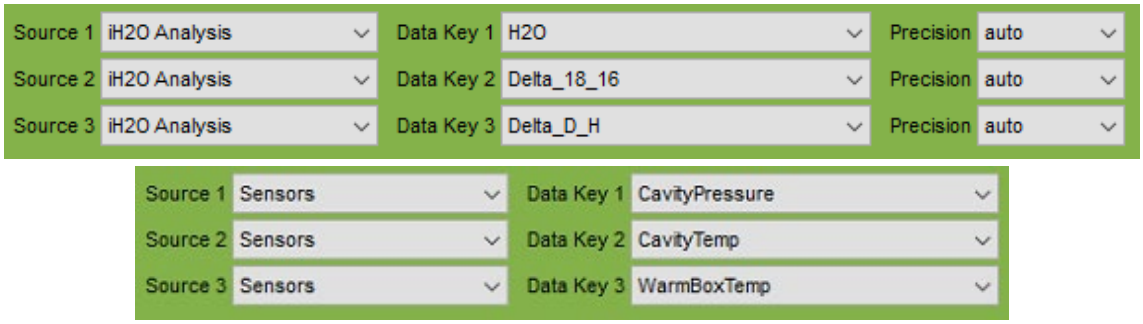


Figure 45: Data Source and Data Key Pull Down Menus

9.9 Precision Pulldown Menu

Precision default selection is "auto" Click on the pull-down to select the precision displayed on the y-axis; between **0** and **4** digits of precision or **auto**. The currently selected precision is displayed during operation. This does not affect the precision of the saved data in the data log files or results files. Auto precision is sufficient for nearly all applications.

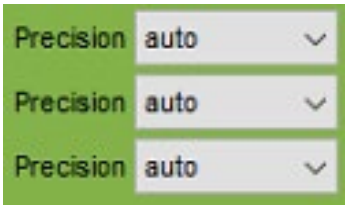


Figure 46: Precision Pull-down Pane

9.10 Analyzer Status Log

This window displays instrument status messages, in the following form: **YYYY-MM-DD HH:mm:ss** then '**Generic message text.'**

Common Status Log Messages

Following are the most common messages that appear:

- **Pressure Stabilizing/Locked: Displayed when** the valve control system begins to allow flow through the analyzer and stabilizes the pressure inside the cavity.
- **Temperature Locked: WB (HB): When the temperatures of the warmbox (wavelength monitor) and hotbox (cavity) have stabilized.**

This is typically the longest step in the startup sequence. **Startup:** Depending on ambient temperature, the analyzer and its hotbox temperature set point, this step may take as little as 20, or as much as 60 minutes. **Restart:** If the instrument is only stopped briefly, this may take a few seconds to a few minutes.

- **Preparing to Measure:** Spectral scanning has started. Concentration measurements will be available in approximately 30 seconds. The instrument will continue to scan and report concentration measurements until the instrument is shut down.
- **Measuring:** This is the normal mode of operation after startup has completed.

2023-05-26	12:42:47	'Pressure unlocked'
2023-05-26	12:43:02	'Pressure locked'
2023-05-26	12:52:14	'Pressure unlocked'
2023-05-26	12:52:24	'Pressure locked'

Figure 47: Analyzer Status Log

9.11 Data Buffer Level Meter

The meter to the right of the Data Window (Figure 48) indicates how much of the internal memory of the GUI is used to retain historical data collected with the instrument. There is an internal limit of a finite number of points. Once that number of data points is collected, the buffer is full, and old data is removed from the buffer as new data is collected. *This buffer affects only the data displayed in the data window, not the data stored in any files.* This buffer is empty upon instrument startup and can also be emptied by pressing the **Reset buffers** button in the lower-right-hand corner of the GUI.

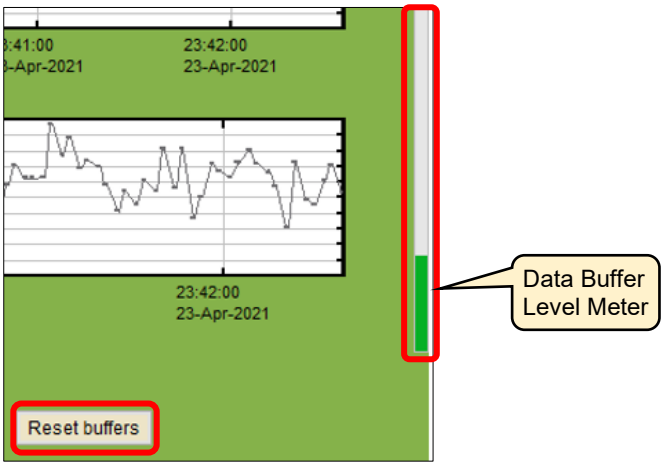


Figure 48: Data Buffer Level Meter and Reset Buffers Button

9.12 Reset Buffers Button

Click this button to clear the internal data buffer of the GUI (this clears the current data traces from the graphs). This has the effect of clearing all data in the data window. *Pressing this button has no effect on any of the data log files stored by the instrument.*

9.13 Graph Zooming and Panning

Zooming In/Out

To zoom in on a specific region of the graph, move the cursor to the area of interest, **click/hold** the left mouse button, **then drag** as desired to create a box that covers the region of interest (see Figure 49). When the box is drawn, release the left button and the boxed area will automatically scale to fill the data window.

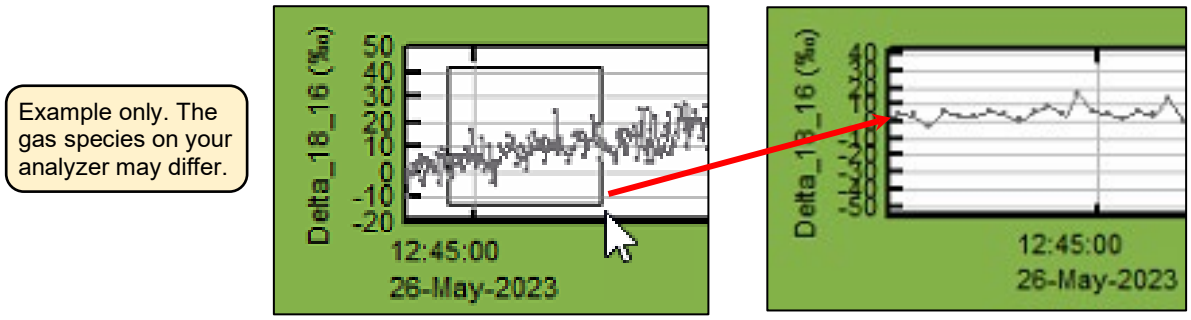


Figure 49: Data Graph Zoom Function

To zoom back out to see all data in the buffer, **double-click the left button** within the graph display. **To zoom out indefinitely**, right click. Right clicking multiple times zooms out further. **To auto scale** the y-axis of either graph, use the auto-scale buttons below the graph.

To Zoom the X and Y axes: hold down the control button and move the cursor up/down or left/right using the right mouse button.

Lock/Unlock Time Axis

Zoom and pan features are often useful when time axes are locked, and the user wishes to align the Y axis in multiple plots. To lock or unlock the time axis of each graph during zooming, from the **View** menu, select **Lock time axis when zoomed** or **Unlock time axis**.

Panning

To pan the data in the X or Y axis: hold down the control button and drag the cursor using the left mouse button.

10. Coordinator Software

10.1 Introduction

To measure discrete samples or to control external peripherals and accessories a separate software tool (Coordinator) is used to control the sample source and match the corresponding real time read out with the sample source. The Coordinator programs that are accessible to a user are dependent on the system configuration.

NOTE

Although this section will provide an overview to the concept of Coordinators, it does not necessarily provide the detail on all Coordinators available on a Picarro water isotope system. Instead, refer to the separate User Manual provided with each of your Picarro accessories:

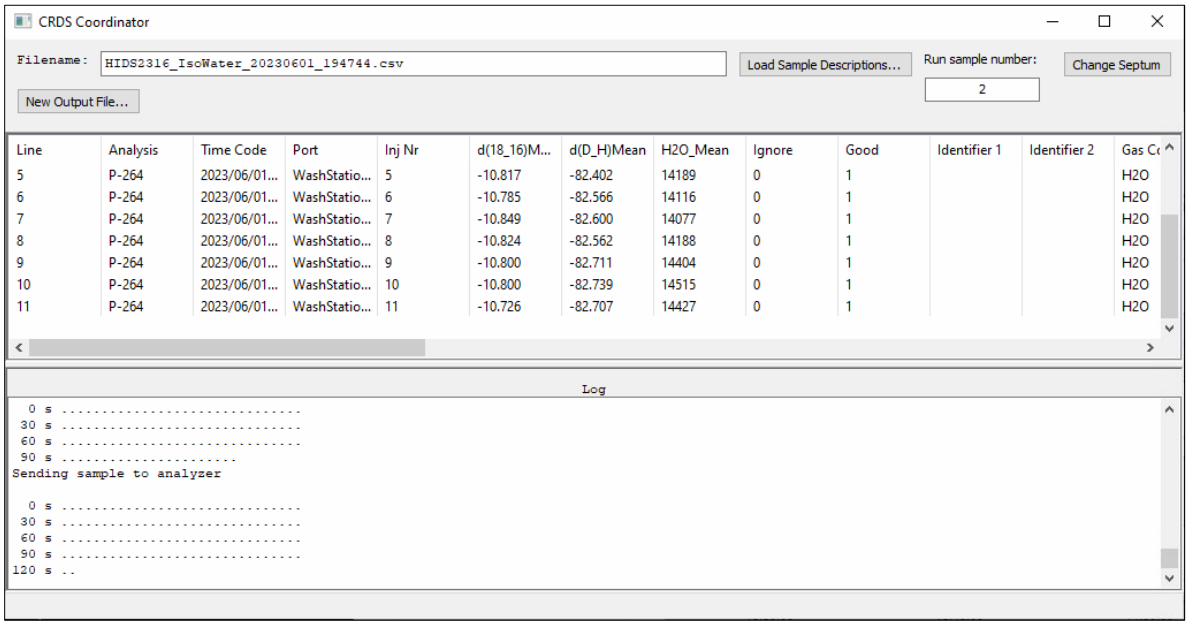
- A0101 SDM (Standards Delivery Module) User Manual (PN 40-0005)
- A0213 IM (Induction Module) User Manual (PN 40039)
- A0214 MCM (Micro Combustion Module) User Manual (PN 40022)
- A0217 CWS (Continuous Water Sampler) User Manual (PN 40003)

10.2 How to Run Coordinator Software:

1. First, make the required hardware connections for your system of interest. Afterwards, turn on the analyzer and wait for the CRDS Data Viewer of the analyzer's software to open up automatically on your desktop screen.

2. Next, launch the coordinator software by double clicking on the **Coordinator Launcher** icon on your desktop.
3. After double clicking on the Coordinator Launcher icon, a window will appear. Choose the appropriate coordinator from the drop down menu, and then click the **Launch** button. *Make sure that the chosen coordinator is supported by your hardware connections and that samples are ready to be analyzed*.

Figure 50: Coordinator Launcher Window



The look of the window may vary depending on the configuration of your analyzer.

Figure 51: CRDS Coordinator Window

4. After clicking on the **Launch** button, the coordinator window (Figure 51) will pop up. (Depending on the coordinator mode chosen, you may or may not be asked to set parameters for your analysis). From the Coordinator window, you will be able see results from sample analysis,

Coordinator Window Descriptions

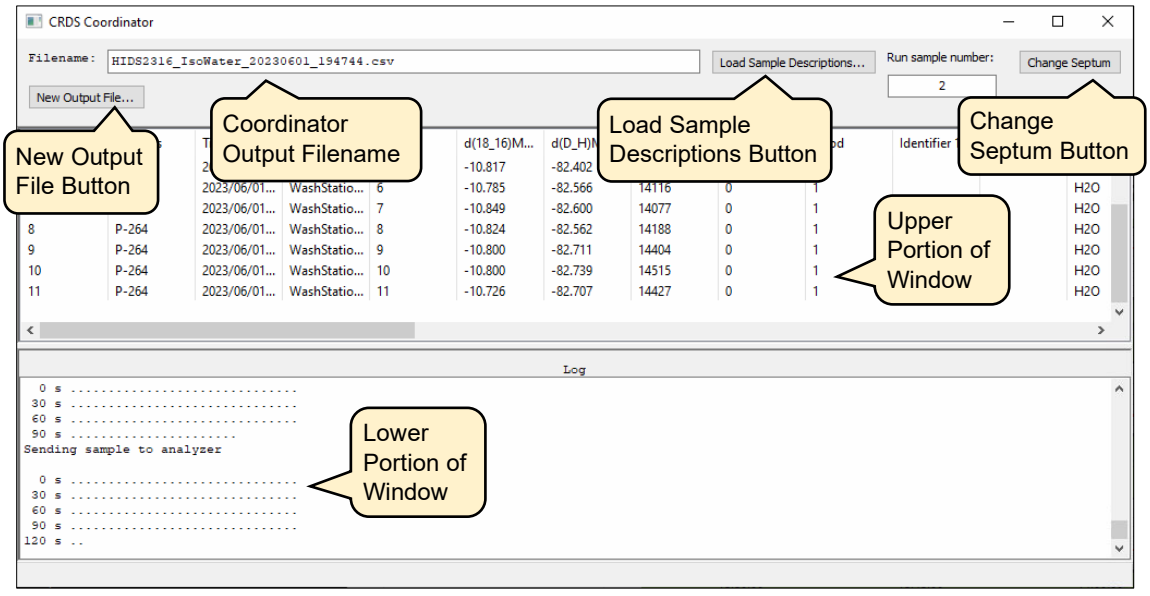


Figure 52: Coordinator Window Descriptions

1. **Coordinator Output Filename:** Can be seen in the upper left of the Coordinator window. It follows an automated convention of:

   model, serial number, mode, year, month, date, and time. For example:

   HIDS2316_IsoWater_20230601_194744.csv

   This means the coordinator file output was taken using analyzer HIDS2316 in high throughput isotopic water analysis starting on 1 June 2023 at 7:47:44 pm.

2. **New Output File Button:** Clicking on this button will save the data that you see on the coordinator window into a file, and then clear the data from the Coordinator Window.

3. **Load Sample Descriptions Button**: Located around the upper right corner of the Coordinator Window. The button allows the user to include a description for each vial in the data file output on the coordinator window.

4. **Change Septum Button:** Used to pause the Autosampler and the vaporizer in the middle of an analysis to physically change the septum on the vaporizer.

   In order to load the sample description file, press the button labeled **Load Sample Descriptions**. A dialog box will appear. Select the sample description file, and then click **Open**. If a certain tray (front or rear) is not being used, use the 'Cancel' button to dismiss the dialog.

5. **Upper Portion of The Window:** Each row represents the analysis results from a single injection. The types of columns are pre-selected by Picarro to include the most useful values for isotopic water analysis and for diagnostic indications.

   The values for the columns, unless otherwise noted, are the average value for time period of the injection, which was marked in red on the CRDS Data Viewer. Values of the form *_SD are standard deviations for that same time period. The time period is selected by trigger thresholds based on the water vapor concentration. The analyzer is characterized and specified based on the factory default trigger thresholds—changing these values is not recommended, please contact Picarro if you feel this is necessary.

6. **Lower Portion Of The Window (labeled "Log"):** This window displays the action that is currently taking place. For those actions that take some time to complete, a period is displayed each second and a new line is started every thirty seconds to show progress.

10.3 How to Make the Sample Description File

The sample description file should be in CSV (comma separated value) format. Use the supplied NotePad++ software. Write the sample descriptions in the format as shown below.

Tray,Vial,Identifier 1,Identifier 2

1,1,Picarro 00,standard

1,2,Picarro 11, standard

1,3,Picarro 22, standard

1,4,WA 1,first sample from Washington

1,5,WA 2,second sample from Washington

1,6,CA 1, first sample from California

1,7,CA 2, second sample from California

1,8,Picarro 00, standard

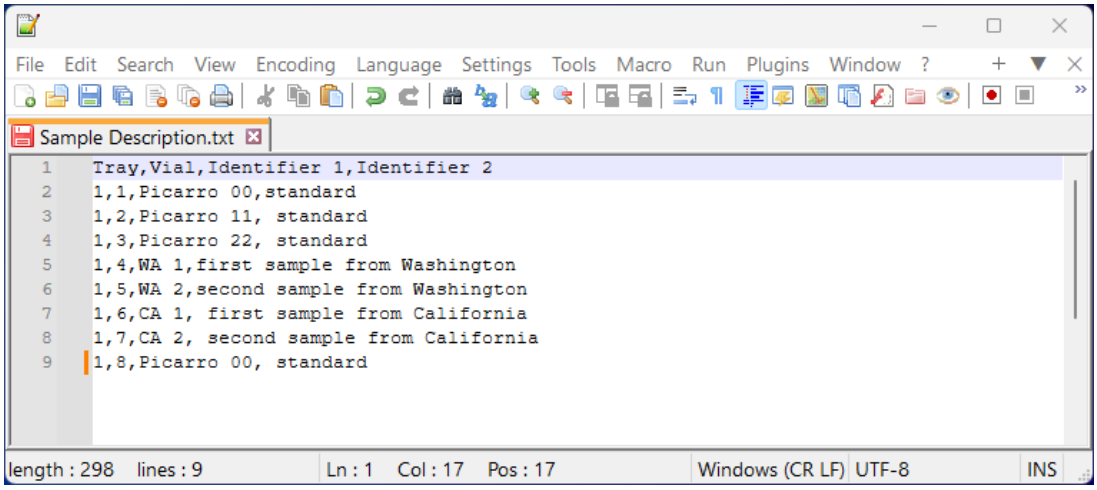


Figure 53: Sample Description Example

After the first line (which should contain the column heading), each line should represent a sample description for the analysis results from a single injection. The lines in the file may be arranged in any order. The capitalization and spacing of the first line must exactly match the provided example. MS Excel can be used if the file is saved in CSV format. It is recommended to generate the file using Windows operating systems (as on the analyzer) as there are differences in CSV format between different operating systems. It is permissible to load the sample description files at any time during the data collection. The output file is rewritten to use the new sample descriptions, so that the most recently loaded descriptions are always used.

10.4 Parameters Recommended for Standard, Express, and Survey Modes

The widely accepted standard protocol for water isotope analysis is to run 6 injections of the sample, and average only the last 3 data points to obtain the isotopic values of the sample.

Using the **Express** mode, Picarro recommends running 10 injections per sample, and in similarity to the standard mode, averaging only the last 3 data points to obtain the isotopic values of the sample stage.

Before launching the Express coordinator, please set number of injections to 10, and volume of sample to 1.8 µl, in the Autosampler user interface.

Using the **Survey** mode requires only one injection.

Before launching the Survey coordinator, please set number of injections to 1, and volume of sample to 2.5 µl, in the Autosampler user interface.

The following table summarizes Picarro's recommendations for processing samples.

Table 6: Picarro Recommendations for Processing Samples.

Coordinator	Number of Injections*	Sample Volume* (µl)	Number of Injections to Discard**
Standard	6	1.8	3
Express	10	1.8	7
Survey	1	2.5	0

*Edits are done to the autosampler software method tab.

**Edits are done to the ChemCorrect post processing parameters.

When using samples with large isotopic range, more injections can be added to help reduce the memory effect.

10.5 Coordinator Modes Available On a Picarro Water Isotope Analyzer

The CRDS analyzer needs to be equipped with the appropriate hardware to support a coordinator mode.

Hardware	Associated Coordinator(s)
High Precision Vaporizer (A0211) CRDS Analyzer (L21x0-*i*)	Manual Injection
High Precision Vaporizer (A0211) Autosampler (A0340 or A0325) CRDS Analyzer (L21x0-*i*)	**L2130-*i*:** • High Precision* (same as Standard Mode) • High Throughput* • Standard** (same as High Precision Mode) • Express** • Survey** **L2140-*i*** • High Precision* • High Throughput* • High Precision ^{17}O* • Express** • Survey** *Only available without Coordinator software upgrade ** only available with coordinator upgrade
High Precision Vaporizer (A0211) Autosampler (A0340 or A0325) CRDS Analyzer (L21x0-*i*) Vaporizer Switching Valve (A0912)	Dual Mode Dual Mode ^{17}O (if L2140-*i*)
High Precision Vaporizer (A0211) Micro Combustion Module (A0214) CRDS Analyzer (L21x0-*i*)	MCM Manual Mode
High Precision Vaporizer (A0211) Standards Delivery Module (A0101) CRDS Analyzer (L21x0-*i*)	Standards Delivery Module (SDM)
High Precision Vaporizer (A0211) Micro Combustion Module (A0214) Autosampler (A0340 or A0325) CRDS Analyzer (L21x0-*i*)	MCM High Precision MCM High Throughput

Induction Module (A0213) CRDS Analyzer (L21x0-*i*)	Induction Module
Continuous Water Sampler CRDS Analyzer (L2130-*i* or L2140-*i*)	Continuous Water Sampler

Description of Different Coordinator Modes

1. **High Precision (same as Standard Mode):** Used to measure liquid water samples with maximum precision. Automatically injects and measures liquid samples. Each injection cycle takes 9 minutes. High Precision and High Throughput Coordinator Modes operate in the exact same fashion except that the steps of sample preparation and analysis are faster in the high throughput coordinator.
2. **High Throughput:** Used for faster measurement of liquid water samples with good precision. Automatically injects and measures liquid samples. Each injection cycle takes 4 minutes. High Precision and High Throughput Coordinator Modes operate in the exact same fashion except that the steps of sample preparation and analysis are faster in the high throughput coordinator.
3. **Standard* (same as High Precision Mode):** Used to measure liquid water samples with maximum precision. Automatically injects and measures liquid samples. Each injection cycle takes 9 minutes.
4. **Express*:** Used for faster measurement of liquid water samples while retaining high precision. Automatically injects and measures liquid samples. Here we recommend 10 injection the first 6 injections take 1.5 minutes while the last 4 injections take 5 minutes. The first 7 injections will be discarded to achieve the optimal memory reduction.
5. **Survey*:** Used for super-fast measurements of large sample batches at moderate precision and enables an efficient sample sorting. By rearranging samples accordingly, we can reduce the memory effect between adjacent sample. Automatically injects and measures liquid samples. Each injection cycle takes 95 seconds. For best practice, we recommend 1 injection per sample followed by manual sorting of samples according to survey results.

   Only available with Coordinator software upgrade.
6. **Manual Inject:** Used for semi-automated measurement of liquid water samples with maximum precision. Requires A0211 High Precision Vaporizer. User manually injects samples after prompt. The vaporizer control and the analysis of liquid samples are automated. Each injection cycle takes 9 minutes.
7. **Dual Liquid/Vapor:** Used for measurement of ambient vapor coupled with automated injection of liquid calibration standards. Requires A0211 high precision vaporizer, A0912 Dual Mode Configuration hardware and

software for vapor calibration and Autosampler. Alternates between analyzing ambient vapor and liquid standards based on user defined sequence. Uses high precision method for liquid calibration. Each injection cycle takes 9 minutes.

8. **Standards Delivery Module (SDM):** Used for measurement of ambient vapor coupled with automated injection of liquid calibration standards. Requires A0211 High Precision Vaporizer and A0101 standards delivery module. Alternates between analyzing ambient vapor from multiple points and a continuous stream of vaporized standard. The alternation is based on user defined sequence. A calibration measurement takes approximately 20 minutes per concentration/standard. Before operating in SDM mode, set the vaporizer temperature to 140°C.
9. **IM CRDS (Induction Module):** Requires the IM. Used for isotopic analysis of extracted water from samples such as soil, plants, or tissues and allows the isotopic analysis of the extracted water. This requires the Induction Module.
10. **Micro Combustion Module (MCM):** Used to measure liquid water samples while destructively removing potential contaminants with maximum precision. Requires A0211 High Precision Vaporizer, A0214 Micro Combustion Module and Autosampler. Automatically injects and measures liquid samples. Each injection cycle takes 9 minutes. In addition to controlling the valve sequence for injection liquid water samples, the MCM coordinator also control the heating of the MCM to ensure removal of interfering organics.
11. **Continuous Water Sampler (CWS):** Used for continuous, real-time measurements of water. Requires A0217 Continuous Water Sampler. No discrete sampling is required. Automatically switches between calibration standards and samples using four inlet ports.


NOTE

IMPORTANT: The L2140-*i* can operate in four instrument modes (iH2O N2, iH2O Air, iH2O N2 O-17 and iH2O air O-17). Due to the high precision demands of ^{17}O - excess science, only the 'High Precision', 'Dual Mode' and 'Manual Inject' coordinator modes will work for the two O-17 instrument modes

Description of Column Headers Used in Coordinators:

The following table provides information regarding the column headers presented in the Coordinator output files available on a Picarro water isotope analyzer. The table below lists the possible fields in the coordinator results file header:

Coordinators vary by analyzer product number, therefore not all columns will be visible on an individual analyzer.

Table 7: Column Headers Used in Coordinators

Item	Description
Line	Line counter. Each line represents a single injection or data point (for vapor measurements in the dual mode).
Analysis	Sequential number of the sample run over the history of the analyzer.
Time Code	Time the line was recorded in "Year/Month/Day Hours:Minutes:Seconds." This time stamp is linked to the local time of your computer's clock.
Port	Reports the vial position on the tray where the autosampler is sampling from.
Inj Nr	Sequential injection number from the port (vial).
d(17_16)Mean	The average $\delta^{17}O$ value, in per mil (‰), measured at that interval (Line). The typical raw data acquisition rate on a L2140-*i* is ~ 1 Hz, therefore this represents the average of 1 Hz data points across the water pulse. The averaging window is shown in red on the CRDS Data Viewer. The reported delta values are not calibrated. Post-processing is required for calibration. Only available on a L2140-*i*.
d(18_16)Mean	The average $\delta^{18}O$ value, in per mil (‰), measured for that injection (Line). The typical raw data acquisition rate on a L21x0-*i* is ~ 1 Hz, therefore this represents the average of 1 Hz data points across the water pulse. The averaging window is shown in red on the CRDS Data Viewer. The reported delta values are not calibrated. Post-processing is required for calibration.
d(D_H)Mean	The average $\delta^{2}H$ value, in per mil (‰), measured for that injection (Line). The typical raw data acquisition rate on a L21x0-*i* is ~ 1 Hz, therefore this represents the average of 1 Hz data points across the water pulse. The averaging window is shown in red on the CRDS Data Viewer. The reported delta values are not calibrated. Post-processing is required for calibration.

Item	Description
E17_Mean	The average ^{17}O-excess value, in per mil (‰), measured for that injection (Line). ^{17}O-excess is the deviation the expected relationship between $^{17}O/^{16}O$ and $^{18}O/^{16}O$ ratios and is defined by: E17_Mean = ln[d(17_16)Mean + 1] – 0.528ln[d(18_16)Mean + 1] The typical raw data acquisition rate on a L2140-*i* is ~ 1 Hz, therefore this represents the average of 1 Hz data points across the water pulse. The averaging window is shown in red on the CRDS Data Viewer. The reported delta values are not calibrated. Post-processing is required for calibration. Only available on an L2140-*i*.
H2O_Mean	The average water concentration, in ppm, is measured for that injection (Line). The typical raw data acquisition rate on a L21x0-*i* is ~ 1 Hz, therefore this represents the average of 1 Hz data points across the water pulse. The averaging window is shown in red on the CRDS Data Viewer. The reported delta values are not calibrated.
Ignore	-1 or 0: -1 indicates the measurement should be ignored and is based on the first three injections from each sample vial being ignored due to sample-to-sample isotopic memory.
Good	0 or 1: 1 indicates that the mean H_2O concentration is within the required range. 0 indicates that the mean H_2O concentration is outside the required range.
Vapor d(17_16)	Only reported when operating in Dual Mode. Populated when the Dual Mode is measuring ambient vapor. Raw $\delta^{17}O$ output from the analyzer with no averaging. The typical raw data acquisition rate on a L2140-*i* is ~ 1 Hz, therefore during the vapor measurement phase a line will be created every ~ 1 second. Only available on a L2140-*i*.
Vapor d(18_16)	Only reported when operating in Dual Mode. Populated when the Dual Mode is measuring ambient vapor. Raw $\delta^{18}O$ output from the analyzer with no averaging. The typical raw data acquisition rate on a L21x0-*i* is ~ 1 Hz, therefore during the vapor measurement phase a line will be created every ~ 1 second.

Item	Description
Vapor d(D_H)	Only reported when operating in Dual Mode. Populated when the Dual Mode is measuring ambient vapor. Raw δ^2H output from the analyzer with no average. The typical raw data acquisition rate on a L21x0-*i* is ~ 1 Hz, therefore during the vapor measurement phase a line will be created every ~ 1 second.
Vapor E17	Only reported when operating in Dual Mode. Populated when the Dual Mode is measurement ambient vapor. Raw ^{17}O -excess output from the analyzer with no averaging. The typical raw data acquisition rate on a L21x0-*i* is ~ 1 Hz, therefore during the vapor measurement phase a line will be created every ~ 1 second. Only available on a L2140-*i*.
Vapor H2O	Only reported when operating in Dual Mode. Populated when the Dual Mode is measurement ambient vapor. Raw H_2O concentration output from the analyzer with no averaging. The typical raw data acquisition rate on a L21x0-*i* is ~ 1 Hz, therefore during the vapor measurement phase a line will be created every ~ 1 second.
Identifier 1	First identifier of the sample. Only populated if a sample description file is loaded when the coordinator is open.
Identifier 2	Second identifier of the sample. Only populated if a sample description file is loaded when the coordinator is open.
Gas Configuration	Indicates the type of gas being measured. Water isotope analyzers measure water vapor sample.
Timestamp Mean	Unix timestamp.
d(17_16)_SD	Standard deviation of the measured $\delta^{17}O$ across an injection's averaging window. The averaging window is shown in red on the CRDS Data Viewer. Only available on a L2140-*i*.
d(18_16)_SD	Standard deviation of the measured $\delta^{18}O$ across an injection's averaging window. The averaging window is shown in red on the CRDS Data Viewer.
d(D_H)_SD	Standard deviation of the measured δ^2H across an injection's averaging window. The averaging window is show in red on the CRDS Data Viewer.

Item	Description
H2O_SD	Standard deviation of the measured H_2O concentration across an injection's averaging window. The averaging window is show in red on the CRDS Data Viewer.
E17_SD	Standard deviation of the measured ^{17}O-excess across an injection's averaging window. The averaging window is show in red on the CRDS Data Viewer. Only available on a L2140-*i*.
d(18_16)_SI	The slope of the measured $\delta^{18}O$ across an injection's averaging window. The averaging window is show in red on the CRDS Data Viewer.
d(D_H)_SI	The slope of the measured $\delta^{2}H$ across an injection's averaging window. The averaging window is show in red on the CRDS Data Viewer.
H2O_SI	Slope of the measured H_2O concentration across an injection's averaging window. The averaging window is show in red on the CRDS Data Viewer.
baseline_shift	The average value for baseline shift, in ppb/cm, measured for that injection (Line). Baseline_shift is a spectral term that is measured on the L2130-*i* and L2140-*i*. It is the change in the constant term of the fitted baseline, relative to an empty cavity baseline which is measured at the Picarro factory. This column can be used to track potential spectral interference and data integrity. See ChemCorrect section.
slope_shift	The average value for slope shift, in ppb/cm, measured for that injection (Line). Slope_shift is a spectral term that is measured on the L2130-*i* and L2140-*i*. It is the change in the linear term of the fitted baseline, relative to an empty cavity baseline which is measured at the Picarro factory. This column can be used to track potential spectral interference and data integrity. See ChemCorrect section.
residuals	The average value for residuals, in ppb/cm, measured for that injection (Line). Residuals is a spectral term that is measured on the L2130-*i* and L2140-*i*. This term represents the root mean squared residual of the least-squares fit of the measured spectra versus the expected spectra. This column can be used to track potential spectral interference and data integrity. See ChemCorrect section.

Item	Description
baseline_curvature	The average value for baseline curvature, in ppm*cm, measured for that injection (Line). Baseline_curvature is a spectral term that is measured on the L2130-*i* and L2140-*i*. This term represents the quadratic term in the fitted baseline. This column can be used to track potential spectral interference and data integrity. See ChemCorrect section.
interval	Average of the elapsed time between each fitted spectrum for an injection's averaging window.
ch4_ppm	The average methane concentration, in ppm, is measured for that injection (Line). This column can be used to track potential spectral interference and data integrity. Methane concentration is not calibrated and should not be used directly to determine the methane concentration in the water source.
h16od_adjust	This term represents an adjustment applied to WLMh16od_offset, a filtered and scaled frequency error derived from least-squares fit. h16od_adjust is only reported on the L2130-*i* and L2140-*i*. This column may be used to the Picarro Technical Support team in diagnosing wavelength locking.
h16od_shift	This term represents an adjustment applied to WLMh16od_offset, a frequency error derived from least-squares fit. h16od_shift is only reported on the L2130-*i* and L2140-*i*. This column may be used to the Picarro Technical Support team in diagnosing wavelength locking.
n2_flag	Flag for reported the measurement mode at the time of measurement. n2_flag will equal 1 for operation in the N2 mode, and equal to 0 for operation in the Zero Air mode.
DAS Temp	Temperature measured at the DAS board in the Picarro analyzer.
Tray	Tray name (a number for the older versions of the Autosampler)
Sample	Vial sample number.
Job	Line in the autosampler job queue.
Method	Autosampler method that is associated with the autosampler sequence.
Error Code	Error code associated with Autosampler operation.

11. Calibration

11.1 Introduction

Calibrating your Picarro water isotope analyzer involves three steps:

- Measuring the isotopic composition of known standards
- Determining the relationship between the measured value and the known value
- Adjusting the settings on the analyzer to account for any difference between the measured and known values, so that the on-screen readings are accurate.

Picarro recommends calibrating your Picarro L21x0-*i* analyzer using liquid water samples. All water isotope standards should have accepted values for $\delta^{18}O$ and $\delta^{2}H$. If applicable, the standards should also be calibrated for ^{17}O-excess. *Picarro recommends referencing all isotope data back to the internationally-recognized VSMOW-SLAP scale*.

NOTE

Upon manufacturing, Picarro guarantees the performance of your analyzer with respect to precision. The system is also calibrated using isotope standards, however Picarro does not certify the analyzer for accuracy. It is the responsibility of the instrument user to verify the factory-calibration and to calibrate the instrument for accuracy.

11.2 Primary and Secondary Standards

The isotopic composition of a water sample is typically determined relative to the known value in a standard using the delta notation and expressed as per mil (‰):

$$\delta\,^{2}H = \left(\frac{\left({}^{2}H/{}^{1}H \right)_{sample}}{\left({}^{2}H/{}^{1}H \right)_{standard}} - 1 \right) \times 1000$$

$$\delta^{18}O = \left(\frac{\left({}^{18}O/{}^{16}O \right)_{sample}}{\left({}^{18}O/{}^{16}O \right)_{standard}} - 1 \right) \times 1000$$

$$\delta^{17}O = \left(\frac{\left({}^{17}O/{}^{16}O \right)_{sample}}{\left({}^{17}O/{}^{16}O \right)_{standard}} - 1 \right) \times 1000$$

These delta values can be used to construct secondary parameters:

Deuterium-excess (expressed as per mil (‰)):

$$d - excess = \delta\,^{2}H - 8 \times \delta^{18}O$$

^{17}O-excess (expressed as per mil (‰)):

$$^{17}O - excess = 1000 \times ln\left(\frac{\delta^{17}O}{1000} + 1\right) - 0.528 \times 1000 \times ln\left(\frac{\delta^{18}O}{1000} + 1\right)$$

There are three international "primary" standards:

- **VSMOW2 –** Vienna Standard Mean Ocean Water 2
- **SLAP2 –** Standard Light Antarctic Precipitation 2
- **GISP –** Greenland Ice Sheet Precipitation

The GRESP standard is replacing the GISP standard that was available until 2012. The table below shows the isotopic compositions of each standard:

Table 8: Isotopic Compositions of VSMOW2, SLAP2 and GRESP Standards

	$\delta^{18}O$ (‰)	**$\delta^{2}H$ (‰)**	**^{17}O-excess (‰)**	**$\delta^{17}O$ (‰)**
VSMOW2	0 ± 0.02 [1]	0 ± 0.3 [1]	0 [2]	0 [2]
SLAP2	-55.50 ± 0.02 [1]	-427.5 ± 0.3 [1]	0 [2] −0.015±0.005 [3]	-29.6968 [2] −29.741±0.100 [3]
GRESP	-33.40 ± 0.04 [1] -33.45 ± 0.034 [4] -33.426 ± 0.028 [5]	-258.0 ± 0.4 [1] -257.87 ± 0.52 [4] -258.20 ± 0.08 [5]	0.025 ± 0.005 [4] 0.038 ± 0.008 [5]	-17.7784 ± 0.02 [4]

[1] IAEA, [2] Schoenemann et al. (2013), [3] Wostbrock et al. (2020), [4] Vallet-Coulomb et al. (2021), [5] Keinan and Goldsmith (2023)

The $\delta^{18}O$ and $\delta^{2}H$ values are defined based on publications by the International Atomic Energy Agency (IAEA):

VSMOW2 and SLAP2:

https://nucleus.iaea.org/sites/AnalyticalReferenceMaterials/Shared%20Documents/ReferenceMaterials/StableIsotopes/VSMOW2/VSMOW2_SLAP2.pdf

GRESP:

https://nucleus.iaea.org/sites/AnalyticalReferenceMaterials/Shared%20Documents/ReferenceMaterials/StableIsotopes/Gresp/RS_GRESP-2021.pdf

There is no consensus on the $\delta^{17}O$ reference values for SMOW2, SLAP2 and GRESP. The table above provides an overview of the commonly assigned values as suggested by Schoenemann et al. (2013), Wostbrock et al. (2020), Vallet-Coulomb et al. (2021), and Keinan and Goldsmith (2023).

Picarro provides a Secondary Water Isotopes Standard Kit (part number C0356) that is based on standards provided by the United States Geological Survey [USGS]:

Table 9: USGS Standards

Standard	$\delta^{18}O$ (‰)	$\delta^{2}H$ (‰)
USGS46	–29.80 ± 0.03	–235.8 ± 0.7
USGS47	–19.80 ± 0.02	–150.2 ± 0.5
USGS48	–2.224 ± 0.012	–2.0 ± 0.4

Since the IAEA and USGS primary and secondary standards are expensive and sample limited, each laboratory should develop their own working standards. Example sources of working standards include:

- **Local precipitation (variable isotopic composition)**
- **Local tap water (variable, related to local precipitation)**
- **Kona Deep, Destiny Deep Sea Water (~ 0 ‰)**
- **Snow or ice from your favorite alpine region (depleted)**
- **Tap water from your colleagues across the globe (variable)**

The isotopic composition of a secondary standard should first be measured against a primary standard. Once calibrated with respect to the VSMOW-SLAP isotope scale, it can be used for routine, daily calibration. About 1.2 L of secondary standard would be enough for a year's supply. This assumes each standard is measured 2x per day using a standard 2 mL autosampler vial, and that the analyzer is operated 300 days per year (2 mL / vial x 2 standard vials / day x 300 days = 1.2 L).

References

- Schoenemann, S. W., Schauer, A. J., & Steig, E. J. (2013). Measurement of SLAP2 and GISP $\delta^{17}O$ and proposed VSMOW-SLAP normalization for $\delta^{17}O$ and ^{17}Oexcess. *Rapid Communications in Mass Spectrometry*, 27(5), 582–590.
- Wostbrock, J. A. G., Cano, E. J., & Sharp, Z. D. (2020). An internally consistent triple oxygen isotope calibration of standards for silicates, carbonates, and air relative to VSMOW2 and SLAP2. *Chemical Geology*, 533, 119432.
- Vallet-Coulomb, C., Couapel, M., & Sonzogni, C. (2021). Improving memory effect correction to achieve high-precision analysis of $\delta^{17}O$, $\delta^{18}O$, $\delta^{2}H$, ^{17}O-excess and d-excess in water using cavity ring-down laser spectroscopy. *Rapid Communications in Mass Spectrometry*, 35(14), e9108.

- Keinan, J., & Goldsmith, Y. (2023). A simple method for rapid removal of the memory effect in cavity ring-down spectroscopy water isotope measurements. *Rapid Communications in Mass Spectrometry*, 37(19), e9600

11.3 Tools, Equipment and Samples Required

1. Waters with known isotope signatures, i.e., a verified $\delta^{18}O$, $\delta^{2}H$ and ^{17}O-excess (if applicable) value.
   - **Picarro recommends all labs purchase one supply of primary isotope standards from IAEA or USGS. These primary standards should not be used on a daily basis. Instead, they can be used to calibrate secondary or in-house standards.**
   - **Secondary or in-house standards that bracket the isotope space of your sample set. A set of three working water isotope standards is also available from Picarro (part number C0350). These standards have been calibrated for $\delta^{18}O$ and $\delta^{2}H$ against the VSMOW-SLAP scale.**
2. 2 mL sample vials with caps. Picarro sells water isotope kits for 500 or 1,000 samples (part number C0328 and C0329, respectively). These kits include 10 µL syringes, 2 mL glass vials with caps and injection port septa. Quantities vary based on the kit selected; visit the Picarro Store for more information: https://picarroinc.force.com/picarrosupport
3. Pipette for transferring water from primary storage (e.g., pressurized stainless steel barrels) to secondary storage (e.g., sealed amber vials) and eventually into sample vials (2 mL sample vials with caps and septa).
4. Permanent marker or label maker for labeling sample vials.
5. Refrigerator (or freezer) for storing water standards. If storing waters in the freezer, ensure the water is either stored in an expandable container or that the container has ample room for water expansion upon freezing. Also ensure the water is completely defrosted before conducting any analysis or sub-sampling from the water. For additional information on storing water isotope standards, please see *section **15.5 Sample and Standard Handling***.

11.4 Calibration Methodology

You should calibrate your samples using water standards that are introduced to the analyzer using an identical (or as close to identical) methodology as the samples.

- **For clean liquid water samples, analyze your standards using the same method, i.e., with the High Precision Vaporizer and Autosampler.**
- **When using the Micro Combustion Module (MCM) to analyze plant waters and other contaminated waters, also analyze your standards using the MCM.**
- **For ambient atmospheric monitoring, calibrate your system using liquid water standards of known isotopic composition using a Standards Delivery Module or dual mode kit. You can also design your own lab-built nebulizer or bubbler. For ambient atmospheric studies, calibrate for both accuracy in delta space and the dependence of delta value on water vapor concentration.**
- **For matrix bound water analyzed using the Induction Module (IM), measure your liquid water standards using the sample introduction methodology and heating recipe.**
- **For the Continuous Water Sampler, produce large volumes of tertiary water standards that can be analyzed on the CWS. Calibrate these standards using the High Precision Vaporizer and Autosampler.**

NOTE

Picarro isotopic water analyzers are not calibrated for water vapor concentration. If high accuracy water vapor concentration is desired, calibrate your system with a dew point generator that can introduce vapor streams of known concentration.

11.5 Performing Calibration Measurements

Since the Picarro analyzer is extremely linear, it is only necessary to use three calibration standards to calibrate each isotopic species (two points define the calibration line and a third intermediate point is used for verification). The exact value of each calibration standard is not of particular importance, as long as they span a representative range of values over which the analyzer will typically be operated. Although it is not necessary to use more than three standards, additional standards can be used to further constrain the linear calibration coefficients.

Each calibration standard should be introduced into the analyzer for an interval long enough for the analyzer to yield a stable measurement of that sample. In the case of water isotopes, it is important to ensure sample-to-sample isotopic memory is overcome prior to using injection pulses for calibration. For example, if there is a significant difference in the isotopic composition of two adjacent standards, it is important to increase the number of injections per vial for the purpose of calibration. For example, if the system is calibrated directly with VSMOW and SLAP, which represent the largest natural variability in oxygen and

hydrogen isotopes, Picarro recommends at least 10 injections are made per vial prior to averaging 3-5 injections for the purpose of calibration. Such a high number of injections is not required for samples that are more closely spaced in isotopic composition.

For routine daily calibration, secondary standards can be interspersed with samples during a given run. The order in which you run the standards can provide information about parameters, such as drift and sample-to-sample isotopic memory, which are helpful in assessing data quality. Picarro recommends the following daily calibration procedure:

- **Measure three standards that bracket the expected composition of samples at the beginning of the autosampler run.**
- **Measure one of those standards again in the middle of the autosampler run.**
- **Measure the three same standards again at the end of the autosampler run.**

At the completion of the autosampler sequence, the standards can be used to construct a bracketed calibration. Plot the measured values of the standards on the x-axis, and the known values (versus VSMOW-SLAP) of those standards on the y-axis. A linear regression can then be used to correct your sample data to the VSMOW-SLAP scale. If necessary, the standard that was run at the beginning, middle and end of the autosampler sequence can be used to correct drift. Finally, remember that standard operating procedure is to discard the first three injections for any sample vial and then average the remaining injections to get the value of that water. The total number of injections made, and the number discarded can be optimized based on performance requirements and the sample-to-sample jumps in isotope space. It is possible to correct sample data to the VSMOW-SLAP scale by post-processing the Coordinator output data. Alternatively, Coordinator data can be analyzed using ChemCorrect™. Finally, if there is a desire to update the on-screen readings, the Picarro software can be updated by following the instructions given in the next section.

11.6 Updating the Instrument Calibration for Accurate On-Screen Readings

Once you have measured your standards, you can use either of the two methods described below to calibrate the analyzer. **Method 1** requires you to make a graph (known standards versus measured standards) to calibrate the analyzer. **Method 2** does not require you to make a graph; *however, the effect of this calibration is harder to reverse than Method 1*.

Method 1: Using the CRDS Data Viewer to Update the On-Screen Readings

For isotope standard measurements, plot the analyzer's reported isotope value on the horizontal (x) axis and the standards' known isotopic composition on the vertical (y) axis. This graph will help you to determine the linear relationship between the known calibration values and the analyzer's reported values.

Calculate a linear best-fit equation from the data. The slope and intercept of the best-fit line through these points are the two values that are used to calibrate the analyzer. Determining the linear relationship between the known values and the analyzer's reported values enables the calculation of a calibration offset (slope and intercept). This adds a correction term to the analyzer's factory or previous calibration.

The analyzer's calibration is intended to be altered infrequently. Instead of recalibrating frequently to increase the accuracy of the data, users often verify the calibration by measuring three or more water standards and using the same regression procedure described here to calculate an offset by which to correct their data offline (see previous section). In the calibration example data below, fitting the three standards yields the linear equation y = 0.9866x + 5.2658 with the slope m = 0.9866 and the intercept b = 5.2658. This equation would be used with x = raw data measured by the analyzer (labelled "CRDS Reported") to give y = corrected data (labelled "Certified" value).

Table 10: Calibration Example Data

	CRDS Reported Value	Certified Value
Calibration Point #1	200.1	202.7
Calibration Point #2	600.3	597.6
Calibration Point #3	400.0	400.0

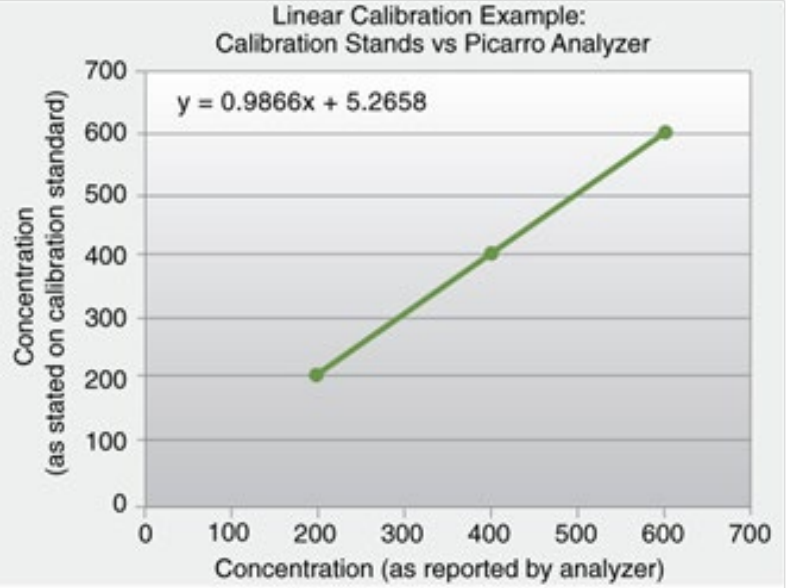


Figure 54: Linear Calibration Example

Enter these calibration values into the software by selecting **User Calibration** from the **Tools** menu on the CRDS Data Viewer. Enter the slope and intercept for each species. This is a password-protected function, with the default password “picarro."

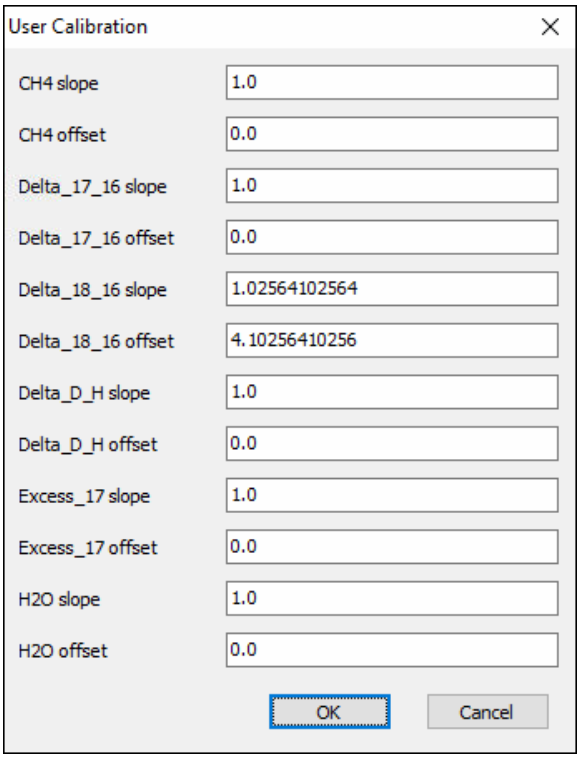


Figure 55: User Calibration Dialog

After the calibration is entered, it will take effect immediately after clicking **OK**.

To return to the factory calibration, simply set the slope to “1” and the intercept to “0” for each species.

This calibration approach and functionality is available across all Picarro analyzers. In the example data given above the species measured were CO_2, CH_4 and H_2O concentration. The same method applies for isotope data, including $\delta^{18}O$, $\delta^{17}O$, $\delta^{2}H$.

Method 2: Using the “Picarro Data Recalibration Tool” to Calibrate the Analyzer

This tool can be used after you have performed the calibration measurements of standards with your Picarro analyzer.

The **Picarro Data Recalibration** (“Data Recal” icon) software can be found in the **Picarro Utilities** folder in the desktop, and it can be used to recalibrate the data analyzed by Picarro analyzers.

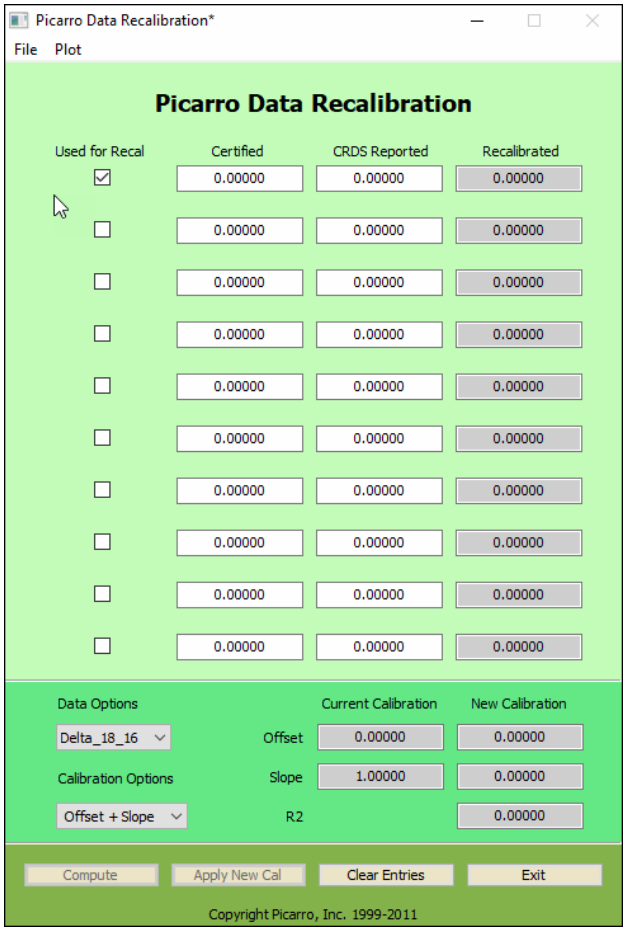


Figure 56: Data Recalibration Tool

1. Double-click the **Data Recal** icon to pull up the window to the left.
2. Click on **Clear Entries** to reset the values in the “Picarro Data Recalibration” window.
3. Enter data values into the **Certified** (expected delta values) column.
4. Enter data values into the **CRDS Reported** (delta reported by Picarro analyzer) column.
5. Check the boxes in the **Used for Recal** column that you want the software to base the calibration on.
6. Click the **Compute** button located at the bottom of the window.

   The recalibrated values will appear in the rightmost column called **Recalibrated**.
7. Click **Apply New Cal** if you want to apply the calibration to your future measurements.
8. The default User Calibration Password is “picarro.” Click **OK** to continue. **NOTE: This action cannot be undone from the “Picarro Data Recalibration Window,” but it CAN be undone in Method 1 in the “User Calibration” window.**

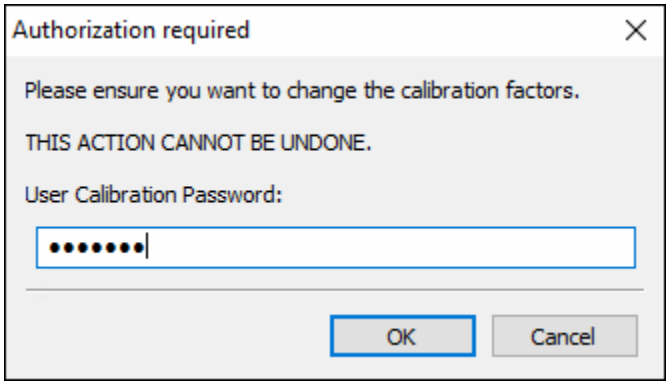


Figure 57: Password Window

9. Review the values in the window (Figure 58), and click **YES** to confirm, then **OK** to continue.

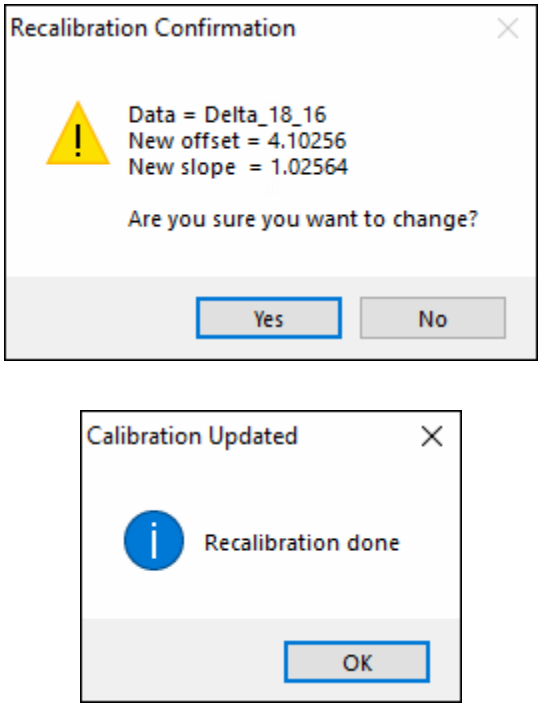


Figure 58: Confirmation Windows

10. A Save Calibration Dialog window appears giving the option to save your calibration settings. Click **Cancel** if you don't want to save your new calibration setting.

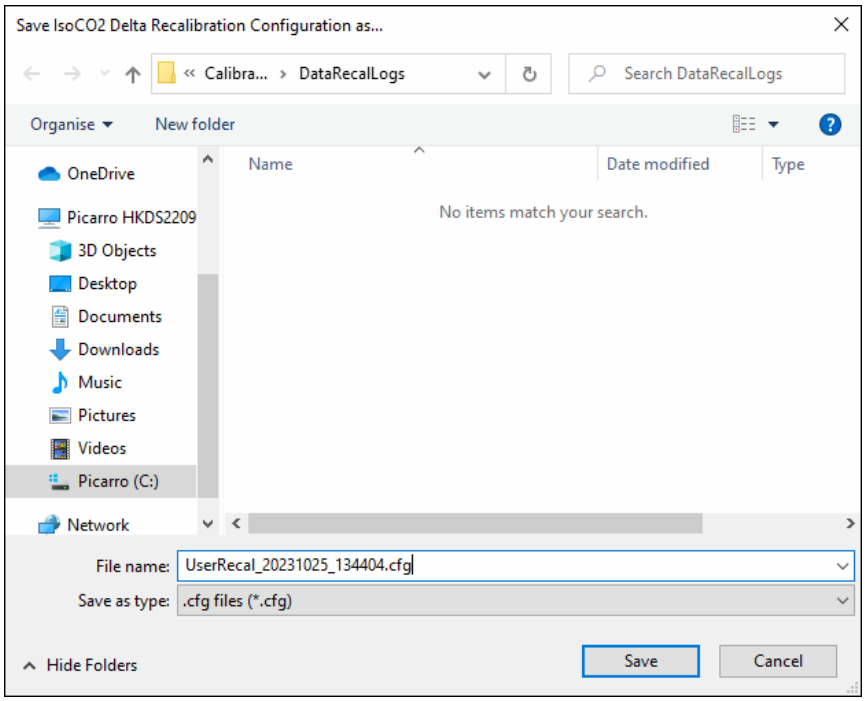


Figure 59: Save Calibration Dialog

11. You have now calibrated your analyzer. The next time you do any sample measurements, the on-screen measurement readings will be based on the new calibration setting.

11.7 Literature and Other Useful Resources

There are many useful resources regarding calibrating systems for accurate water isotope measurements. A non-exhaustive list is below:

- Gröning, M. (2018). *TEL Technical Note No. 03. Stable isotope internal laboratory water standards: Preparation, calibration, and storage*.

  https://nucleus.iaea.org/sites/AnalyticalReferenceMaterials/SharedDocuments/Publications/TechnicalNotes/TELTechNote03_WaterInternalLaboratoryStandards.pdf

- Hachgenei, N., Vaury, V., Nord, G., Spadini, L., & Duwig, C. (2022). Faster and more precise isotopic water analysis of discrete samples by predicting the repetitions' asymptote instead of averaging last values. *MethodsX, 9*, 101656.

- Keinan, J., & Goldsmith, Y. (2023). A simple method for rapid removal of the memory effect in cavity ring-down spectroscopy water isotope measurements. *Rapid Communications in Mass Spectrometry, 37*(19), e9600.

- Terzer-Wassmuth, S., Wassenaar, L. I., Araguás-Araguás, L. J., Stumpp, C., & Terzer, S. (2023). Balancing precision and throughput of $d^{17}O$ and $\Delta'^{17}O$ analysis of natural waters by Cavity Ringdown Spectroscopy. *L.I. Wassenaar, L.J. Araguás-Araguás et Al. MethodsX, 10*, 102150.

- Vallet-Coulomb, C., Couapel, M., & Sonzogni, C. (2021). Improving memory effect correction to achieve high-precision analysis of $\delta^{17}O$, $\delta^{18}O$, $\delta^{2}H$, ^{17}O-excess and d-excess in water using cavity ring-down laser spectroscopy. *Rapid Communications in Mass Spectrometry, 35*(14), e9108.

12. ChemCorrect™ Software

12.1 Principle of Operation

Picarro CRDS has become a *de facto* standard for many water sample research areas, such as ice core, watershed, and aquifer studies. For various reasons, samples can contain a variety of chemical contaminants, which in some cases can lead to spectral interference that can degrade the accuracy of results. It is difficult to eliminate these contaminants from water samples without fractionating the isotope ratios and diminishing sample fidelity.

Proprietary software, called ChemCorrect, comes pre-loaded on your Picarro water isotope analyzer. This program solves the problem of data degradation and fidelity resulting from water samples contaminated with trace hydrocarbons. The software makes the *a priori* assumption that your standards are clean waters that do not contain any contamination. Then the program compares a number of features in the spectra from the samples and the standards, applies a statistical test to see if the samples are different from the standards, and assigns flags based on the statistical differences. These flags alert you to artifacts, potentially from contamination, which may affect the accuracy of your results. Finally, the software uses a linear regression to correct your samples to an isotope reference scale by comparing the measured values of your standards to their accepted values. For more information on organic interferences, see the Picarro application note: ***Plant Water: Accurate Water Stable Isotope Analysis of Organic Contaminated Water***.

How Contaminants Impact The Optical Spectrum

Contaminants fall into one of the following three categories, based on the nature of the distortion to the optical spectrum:

1. Compounds that do not affect the spectrum (at concentrations up to 10-20% of the water sample). Most compounds fall into this category. In the presence of these contaminants, Picarro analyzers will report accurate and precise isotope values without bias or increase in noise.
2. Large compounds (with more than about 6-8 atoms) contribute a broad, spectrally unresolved absorption baseline beneath the target molecules. To first order, this baseline will cause no systematic bias to the reported values. Because optical absorption is a linear, additive process, the water vapor spectrum will ‘float’ on top of the contaminant baseline. The linearity and wide dynamic range of CRDS makes the technique particularly insensitive to these baseline offsets.
3. In some cases, however, this baseline offset is accompanied by a tilt of the spectrum with wavelength. This larger offset, if uncorrected, can

cause bias in the measurements and degrade the precision of the instrument.

4. Small compounds (with fewer than 6-8 atoms) have spectrally resolved absorption lines that can interfere with the lines from the observed water vapor. This can lead to systematic errors in the reported isotope ratios. One example of such a molecule is methanol, which has a particularly complex absorption spectrum in this spectral region.

   ChemCorrect software uses known spectral interferences or general spectral patterns to identify trends due to contamination.

ChemCorrect on the L2130-*i* and L2140-*i*:

The L2130-*i* and L2140-*i*, when operating in 'normal' measurement mode ($\delta^{18}O$ and $\delta^{2}H$), also measure spectral indicators that can be used to determine the integrity of the spectra and resulting data.

Using the spectral indicators listed below, the ChemCorrect software performs statistical tests to determine how those spectral features differ between the samples and the standards.

- **RESIDUAL:** The root mean squared residual of the least-squares fit to a spectra, in units of ppb/cm, is used to screen for potential small molecule contaminants, e.g., methanol.
- **BASELINE SHIFT:** The spectral baseline is a good early indicator of a potential issue with a sample. The baseline shift term is a change in the constant term of a fitted baseline, in units of ppb/cm.
- **BASELINE CURVATURE**: The spectral baseline is a good early indicator of a potential issue with a sample. The baseline curvature team is a change in the quadratic term of a fitted baseline, in units of ppb*cm.
- **SLOPE SHIFT:** The slope of the spectral baseline or change in the linear term of the fitted baseline, in units of ppb/cm, although not unique is also a useful indicator for moderately-sized molecules, e.g., ethanol that can interfere with nearby spectral features.

The software flags these indicators if they deviate from the thresholds set in ChemCorrect.

For example, a red flag can be triggered by any of the following:

- **The sample residual being 1.5 σ away from the mean of the standards residual**
- **The sample baseline shift being 18 σ away from the mean of the standards baseline shift**
- **The sample baseline curvature being 3 σ away from the mean of the standards baseline curvature**

Sometimes the software generates false positives by flagging features that do not arise from contamination. To reduce the number of false positives, the notification thresholds can be changed to be less stringent. This can be done by editing the ChemCorrect Instruction Set. If a user edits the Instruction Sets, we recommend changing the name of the Instruction Set so that it is possible to revert to the original set supplied by Picarro.

If a flag is raised, a number of things can be done. First, try some offline sample treatment methods, such as the use of activated charcoal. Second, if you suspect alcohols may be present in your samples, you can utilize Picarro's Micro Combustion Module (MCM) to remove those artifacts. Third, and as a last resort, you can analyze your samples using an alternative technique, such as Isotope Ratio Mass Spectrometry (IRMS). IRMS is not susceptible to spectral interference from alcohols; it can, however, introduce other analytical artifacts and have other interferences, such as mass interference, which can affect accuracy.

12.2 Analysis of Coordinator Output Files

The following Coordinator output files can be post-processed using ChemCorrect:

- High Precision
- High Throughput
- Manual Injection
- Standard
- Express
- Micro Combustion Module

ChemCorrect cannot be applied to data $\delta^{17}O$ and ^{17}O-excess data. Nor can it be applied to Coordinators generated during SDM, IM, Dual Mode, or Continuous Water Sampler Setups.

12.3 Preparing the Run Sequence

1. Each run needs at least 2 standards (3 is recommended but more is better) with known $\delta^{18}O$ and $\delta^{2}H$ values. These values create a linear fit, which is used in calibration of the samples.
2. The standards must be run one after another at the beginning of each sequence to be analyzed. The post processing software works sequentially and therefore requires the linearity of the known standards before it can correct the unknown values of the samples. It is recommended to include standards in the middle and end of the sample set as controls. An example is shown (Figure 60), vials with the CYAN stars indicate the standards:

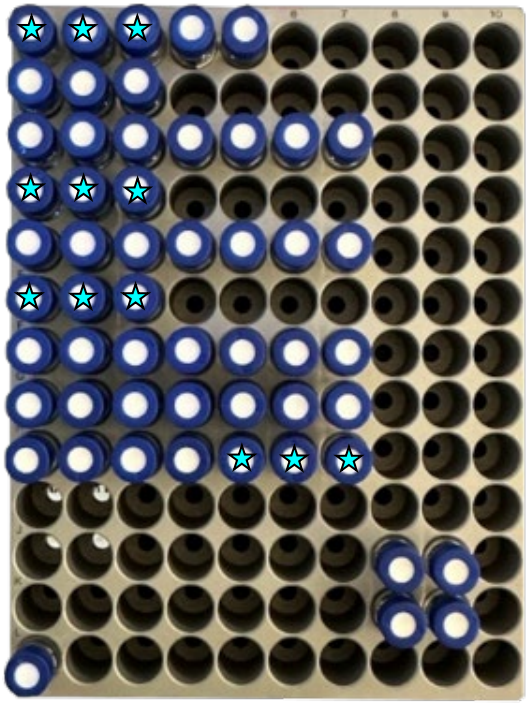


Figure 60: Run Sequence with Standards

3. Due to memory, the first two to three injections of each vial should be ignored. Because of this, a minimum of six injections should be run per vial. The number of injections is set using the Autosampler Controller software (A0340 or A0325).

12.4 Files Required to Run ChemCorrect

ChemCorrect requires a standards file, an instruction set, and a source file (data output from the coordinator software that is in C:\IsotopeData). Each of these files are provided in .csv formats. To ensure the standards file format is preserved, Picarro recommends editing the file using Notepad++ which is provided with the analyzer.

A sample data file along with the standards and instruction files can all be found in the ChemCorrect main folder C:\Picarro\ChemCorrectExe.

Standards File

The standards.csv file must contain the name and known $\delta^{18}O$ and $\delta^{2}H$ values of each standard (relative to an isotope reference scale, typically VSMOW-SLAP for water isotopes). The names in the standards.csv file must match (case-sensitive)

the names in the source file under “Identifier 1”. If they do not match, standards will be treated as samples.

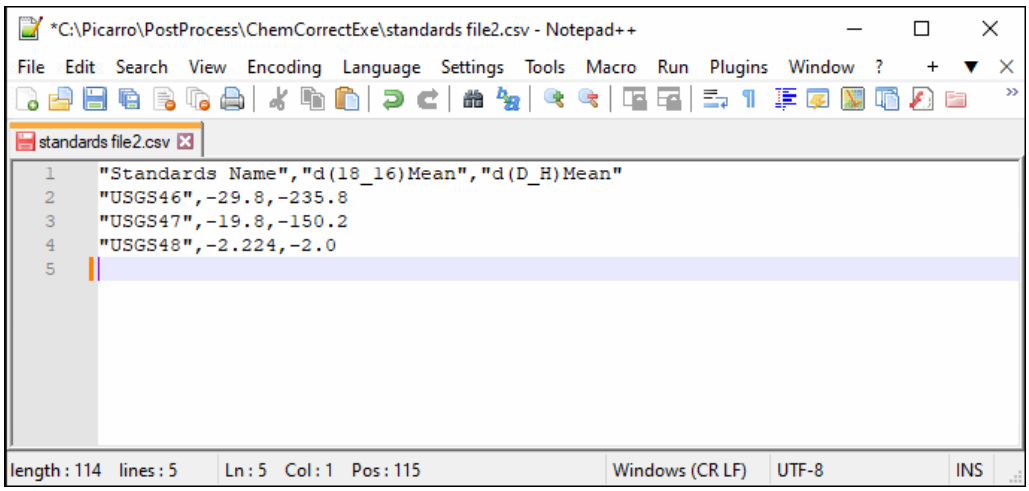


Figure 61: Standards CSV File Example

Instruction Set

The instruction set is provided by Picarro.

- **L2130-*i* / L2140-*i* Instruction Set:** chemcorrect_inst avg_orgeval_10.csv

Source File

This is the output file from the Coordinator (stored in C:\IsotopeData). Before closing the Coordinator at the end of an Autosampler Sequence, it is advised to load the sample description file. Below is an example of a sample description file. Ensure that the “Identifier 1” for standards is identical to the “Standards Name” list in the standards file.

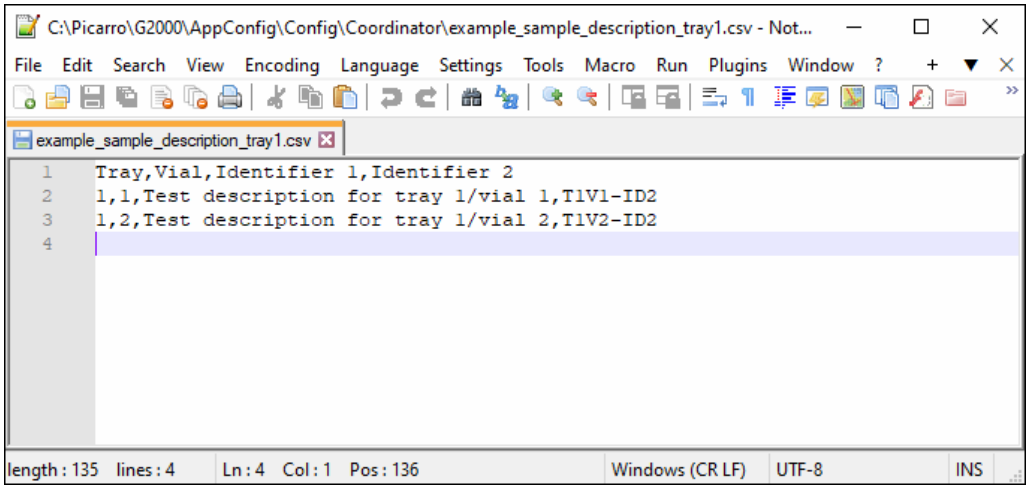


Figure 62: Sample Description File

12.5 Running ChemCorrect

1. Double-click the ChemCorrect icon on the analyzer desktop. The ChemCorrect program will now open.
2. The top four boxes are the required fields: the most recent **Source** file name (sometimes empty), ***Instruction Set*** name, ***Standards File*** and the number of ***Injections to Ignore***. You also have an option to plot additional graphs for other parameters.
3. To choose a different source file to be analyzed, click the **Source** button located on the bottom of the window. Then use the finder window to locate the desired raw data file and click **Open**.
4. To select a different instruction file than the one displayed, click the **Instruction Set** button located on the bottom of the window. Then use the finder window to locate the desired instruction file and click **Open**.
5. To change the number of injections to be ignored, highlight the existing number and type in the preferred one (required 2 but 3 is recommended). ***Do not leave this field blank***.
6. When the correct source and instruction files are shown, click the **OK** button at the bottom of the window to start the ChemCorrect analysis.

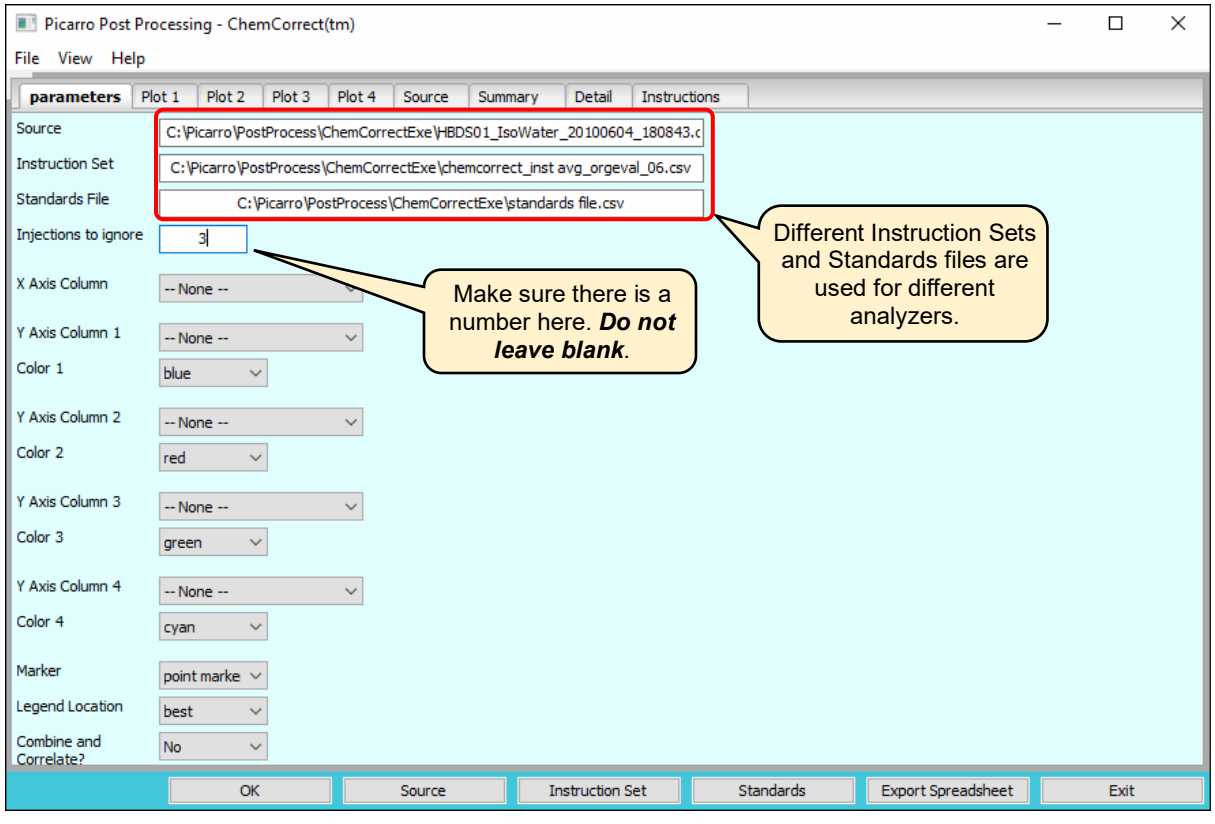


Figure 63: ChemCorrect Window

12.6 Example Analysis

See the Figure 64 below.

1. Select **HBDS01_IsoWater_20100604_180843.csv** (which Picarro has provided in C:\Picarro\PostProcess\ChemCorrectExe\) as the source, and chemcorrect_inst avg_orgeval_10.csv as the instruction file. Then click **OK**.
2. The first display is called the **Summary**. Contained here are: the calibrated isotope values and visual indicators as to the severity of contamination by sample.
3. The CYAN rows are standards.
4. The GREEN rows are samples that have been determined to have little to no contamination.
5. The YELLOW rows are samples that contain trace values of contamination that may slightly shift the isotope values.
6. The RED rows are samples with severe contamination leading to inaccurate δ^2H and $\delta^{18}O$ readings.
7. A star next to a sample indicates a problem, e.g. missing rows in the source file resulting in an inaccurate calculation.
8. Red/yellow rows display relative contamination due to methane, methanol, or “other” hydrocarbons in the respective columns on the right.

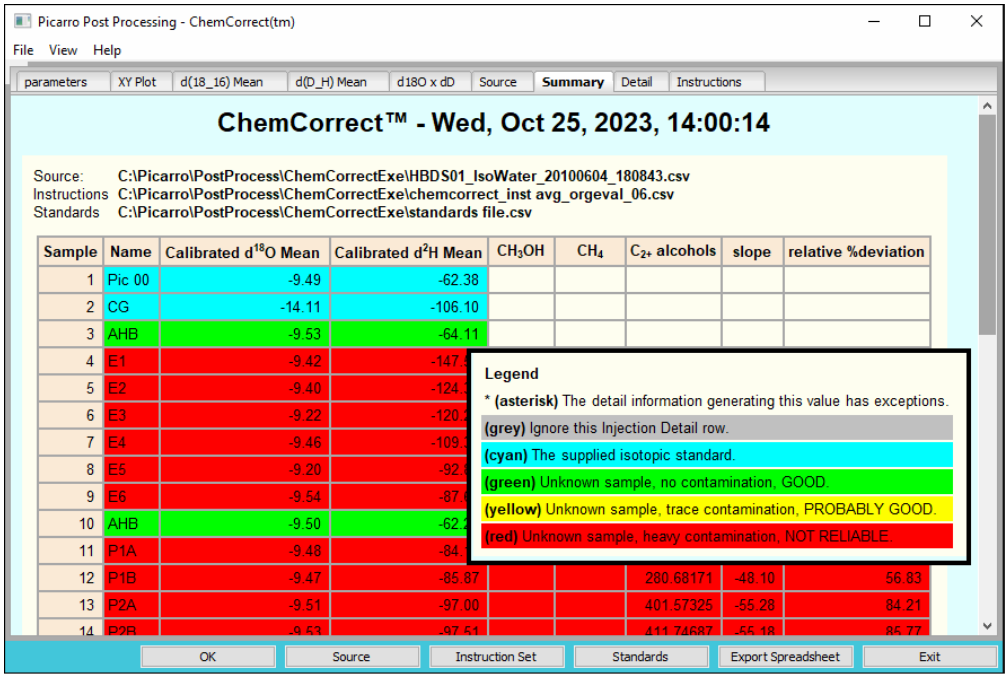


Figure 64: ChemCorrect Analysis

9. There are other tabs that can be accessed by clicking on them in the top left corner of the window:
10. **Detail:** Summons a list of summarized charts by injection and sample chronologically. The un-calibrated and calibrated values, as well as the measurements taken to calibrate the values are included per injection. Below each chart is a summary.
11. **Source:** Displays the original raw data file without any changes or calibration.
12. **Instructions:** Displays the raw instruction file used by ChemCorrect as well as comments on the far right of each instruction.
13. **Additional plots** for visualizing your data.
14. At the bottom of the ChemCorrect window are additional buttons **OK**, **Export Spreadsheet**, and **Exit** buttons.
15. **OK:** Each time you reload the source and instruction sets, you can click OK again to process more data without closing and re-opening ChemCorrect. Once you make your edits, export the result to save your processed data.
16. **Export Spreadsheet:** Creates an excel spreadsheet complete with all the information contained in the four tabs in the ChemCorrect main window as well as all the data sets and formulas used to calibrate the isotope values.
17. **Exit:** Quits ChemCorrect.
18. The standards.csv file can be amended if needed, but the format must remain the same. To edit, simply open the file, make the desired changes, and click save. For the changes to be reflected in ChemCorrect, click the **OK** button at the bottom of the ChemCorrect.
19. For more advanced users, *Instruction Sets* can be edited to perform your required calculations. ***NOTE:*** *If editing the Instruction Set, we recommend changing the name of the Instruction Set so that it is possible to revert to the original set supplied by Picarro.*

NOTE

Picarro recommends running the post processing within 7 days of initially acquiring the data. If a sample is flagged as contaminated, the post processing software will automatically set aside the associated spectral files. These files can be sent to Picarro for further analysis and spectral library development. Once set aside, these files will not be affected by the automatic file management software which is running on the analyzer.

Due to the large amount of data generated by the analyzer a buffer of approximately 10 GB of spectral files are kept, after which point, they are erased. This corresponds to approximately 2 weeks of operation. Running the post processing ensures that any spectra associated with contamination are not erased.

13. File Management

The Picarro analyzer generates ASCII-format text output files that are updated after each batch of concentration measurements is complete. The data files are stored primarily in UserData folders and are also mirrored in folders which retain more situational data. Some analyzers also produce discrete measurements stored in separate isotope data folders. All user data is archived, compressed, and retained, either shortly after the measurements or at a later point, to optimize space on the hard drive.

13.1 User Data Folder

The User Data folder is located at:

C:\UserData\DataLog_User - with files arranged by year\month\day\hour.

The User Data files are in a simple text format (white-space delimited) with a DAT file extension. By default, each file stores one hour of data.

Using the **Setup Tool**, the user can select and customize the data columns, file length, total storage size and folder structure for the user data logs. Setup Tool is described in more depth in ***APPENDIX A – Setup Tool and Communication*.**

Certain instruments may contain additional sub-folders under C:\UserData\ relating to time synced file formats, soil flux, or GPS data, among others. If the user has any questions about this file structure, they can contact Picarro Support.

13.2 Data File Name

The file name is generated from the analyzer serial number, the date, and the time when the file was started. The specific time stamp will depend upon the time the instrument was started and began measuring sample gas, so files seldom begin exactly at the top of the hour. For example:

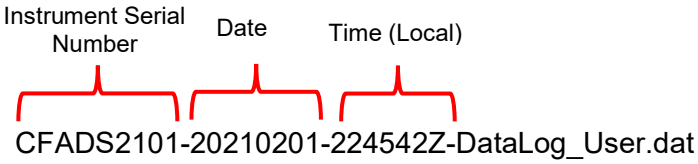


Figure 65: Example Data File Name

- **CFADS2101** is the analyzer serial number
- **20210201** is the date, in format *yyyymmdd* (to allow chronological sorting of data files).

- **224542** is the time the file was started in the computer's Local Time as displayed in the lower right hand side of the Windows OS screen, 22:45:42, formatted as *hhmmss* using a 24-hour clock. Note that the time stamp of samples within the file is usually recorded in UTC (GMT) relative to the local time. For example, an analyzer in California will usually have a time stamp (UTC) within the file that is 8 hours ahead of the time stamp in the file name itself (UTC - 8).

13.3 Data Archive

The archive directory is:

C:\Picarro\G2000\Log\Archive

and has subdirectories:

DataLog_Private, **DataLog_EventLogs**, and **DataLog_Mailbox.**

DataLog_Private

These data files contain a comprehensive list of system parameters such as instrument temperatures and pressure, set points and spectroscopy. This additional information is not broadly relevant to the user for day-to-day operation but can be useful for diagnostic purposes. Files are stored by the convention:

C:\Picarro\G2000\Log\Archive\DataLog_Private \[year]\[month]\[day]\[hour]

The archive files are in a more efficient HDF5 format, with extension .h5.

DataLog_EventLogs

Event logs contain records of the operation of the instrument, the performance of the wavelength monitor and lasers, and record exceptional events like pressure or temperature instability. This is also a critical resource for Support to diagnose or troubleshoot an issue with an analyzer. Files are stored by the convention:

C:\Picarro\G2000\Log\Archive\DataLog_EventLogs
\[year]\[month]\[day]\[hour]

DataLog_Mailbox

The Mailbox folder contains individually zipped files which have been compressed to allow automated transfer via email. Unlike the folders above, this folder is not subdivided by year, month, and day. Email synching is described in greater detail in ***APPENDIX A – Setup Tool and Communication***.

13.4 User Data Folder

The User Data folder *C:\UserData* contains one or more subfolders associated with real-time instrument data.

DataLog_User (all instruments)

Raw user data is contained in the DataLog_User folder, with format:
C:\UserData\DataLog_User\[year]\[month]\[day]\hour

This is the most relevant folder for users of non-isotopic instruments, as this provides the real time data output in its most digestible form. These data files reflect the native time interval of the instrument, typically between 0.1Hz and 10 Hz.

DataLog_Sync

Some instruments will also contain a *(C:\UserData\DataLog_Sync\...) directory,* which includes data that is evenly spaced in time as specified by the user in the Setup Tool, covered in ***APPENDIX A – Setup Tool and Communication.*** This format is preferred by some users who need e.g., 1Hz data exactly, or who prefer to record smaller data files with data spaced, e.g., every 60 seconds.

DataLog_GPS

Instruments may come with the ability to log GPS data, which can be found in this subdirectory.

DataLog_SFP

Instruments may come with the soil flux processor software. Associated data files may be found in this subdirectory.

13.5 Isotopic Data

Isotopic instruments use Coordinator programs to produce discrete isotopic values for individual samples or injections. Each time a Coordinator is opened, a data file will be produced in one of two places, depending on the peripheral used, either:

C:\IsotopeData (sometimes called ***C:\IsotopicData***)

or

C:\Picarro\IsotopicData (sometimes called ***C:\Picarro\IsotopeData***)

While the coordinator program is running, individual sample value outputs will be populated as a new line into the coordinator window, and the respective data file.

13.6 File Archiving

Picarro instruments will not delete data. Some instruments will, however, compress and archive older data to conserve hard drive space. Raw data file archiving frequency and details can be modified in the file:

C:\Picarro\G2000\AppConfig\Config\Archiver\Archiver.ini.

CAUTION

To avoid losing data, discuss with Picarro support before attempting any changes to the Archiver.ini file.

For each file type, there are various items along with some recommended default settings which may vary by file type:

- **Directory = *C:/UserData/DataLog_Sync***

  Optionally specifies which directory to find files to archive.

- **MaxCount = -1**

  Specifies how many files to keep. A setting of -1 indicates that there is no maximum number of files. Generally, -1 is used in conjunction with a maximum size limit, below.

- **MaxSize_MB = 1500**

  Specifies that a maximum of 1.5 GB of data is to be kept before the system begins to archive old data.

- **Compress = True/False**

  Specifies if archived files are to be zipped – recommended setting is true to save hard drive space. True means files are zipped, false means files are not zipped.

- **AggregationCount = 0**

  If compression is set to TRUE, specifies how many files to be included in each zip archive.

- **StorageMode = FIFO**

  First in first out. Specifies that old data is archived first.

- **Quantum = 4**

  Generally, should not be changed. Specifies the files be sorted by year\month\day\hour in the archived directory structure.

13.7 Measuring Time in Picarro Data Files

Since measurements performed by Picarro analyzers are asynchronous (they require a variable and unpredictable amount of time to complete) data reported by the analyzer is time stamped. Each independent measurement is given a time derived from the Windows™ computer's system clock (reference http://en.wikipedia.org/wiki/System_time). This time can be reported by one or many of the following variables.

Table 11: Time Measuring Variables

Variable Name	Description	Units
DATE	The calendar date formatted as YYYY-MM-DD **Example:** August 24, 2023 is formatted as 2023-08-24	-NA-
TIME	The time of day formatted as HH:MM:SS.SS on a 24-hour clock **Example:** 4:18:53.12 PM is formatted as 16:18:53.12	-NA-
FRAC_DAYS_SINCE_JAN1	The number of days since midnight January 1 of the current year **Example:** at 3:00:00 PM on January 12 the value is 11.625	days
FRAC_HRS_SINCE_JAN1	The number of hours since midnight January 1 of the current year **Example:** at 3:00:00 PM on January 12 the value is 279.0 (=FRAC_DAYS_SINCE_JAN1*24)	hours
JULIAN_DAYS	The number of the day of the current year **Example:** at 3:00:00 PM on January 12 the value is 12.625 (=FRAC_DAYS_SINCE_JAN1+1)	days
EPOCH_TIME	The number of milliseconds since midnight January 1, 1970 **Example:** at 3:00:00 PM on January 12 the value is 1421074800000 (= time)	ms
timestamp	The number of milliseconds since midnight January 1, 1 if the current Gregorian calendar was extended back to that time **Example:** at 3:00:00 PM on January 12 the value is 63556671600000	ms

Variable Name	Description	Units
time	The number of milliseconds since midnight January 1, 1970 **Example:** at 3:00:00 PM on January 12 the value is 1421074800000 (= EPOCH_TIME)	ms
ymd	The calendar date formatted as YYYYMMDD **Example:** August 24, 2023 is formatted as 20230824	-NA-

In the table above, all times are reported in GMT (also known as Zulu time and very closely related to UTC – reference: http://en.wikipedia.org/wiki/Greenwich_Mean_Time). We express these timestamps in GMT to avoid complications during Daylight Saving Time or when instruments are moved across time zones. The accuracy of the times are, of course, only as good as the accuracy of the Windows™ clock. To learn how to automatically synchronize the computer's clock to a time standard, see section ***A.2 Remote Data Access*** located in ***APPENDIX A – Setup Tool and Communication*** There are many online calculators (for example, http://www.epochconverter.com) that convert Epoch Time to local time at any time zone, as well as many functions in commonly used data analysis programs that perform the same calculations.

14. Performance Verification

14.1 Drift and Precision Testing

Precision and drift tests for $\delta^{18}O$ and $\delta^{2}H$ ($\delta^{2}H$) are recommended every 6 to 12 months throughout an analyzer's lifetime. This will allow you to verify a new installation, track performance as the instrument ages, determine if it is time for a Factory Refresh, and perhaps identify a small problem before it becomes a major setback. These tests can also be performed when data quality suddenly and inexplicably deteriorates.

The drift and precision test for a L2130-*i* and L2140-*i* is conducted by measuring water from the wash station, instead of vials. These analyzers are precise enough to detect small variability in the composition of water from individual vials, even if it was sourced from the same supply. By running the drift and precision test from the wash station, vial to vial noise is avoided.

The following instructions contain sections specific for each of the Picarro Autosamplers (model number A0340 or A0325), covering small setup and software settings differences.

1. Fill a wash station jar with water and screw on the cap. The water should be pure deionized water, with no organics or salts, although tap water, bottled water, or one of your secondary standards can be used. Because of the large volume required, we do not recommend using primary standards for this test. The sample should be filtered if it contains particulate matter.
2. **Autosampler (A0340)** – Users place the wash station jar in either one of the two wash station jar positions. (Picarro_DIW_Analysis_Station in the software) The software is instructed to pull from the correct jar.

   Note: In Autosampler (A0340) the was station are designated 1 and 2 from front to back. Contrary in older models this designation is reversed.

   Autosampler (A0325) – Users place the wash station jar in the rear wash station jar position (Wash Station 1).
3. Double-click on the desktop icon **Autosampler Control**. This opens the program that controls the Autosampler.
4. **Autosampler (A0340)** – Create a job with 210 injections from the position of the Picarro_DIW_Analysis_Station that you want to measure.

   Autosampler (A0325) – In the top row of the sample list, check the box to the right of the **Clear button**. Then use the keyboard command '**Ctrl** + **i**' to switch to the wash station test mode.

Note: This is a run sequence that will only draw water out of wash station 1. Select the method **Picarro** from the drop down list and enter 210 into the box underneath the column '#Inj.'. This will set up a run of 210 injections from the wash station.

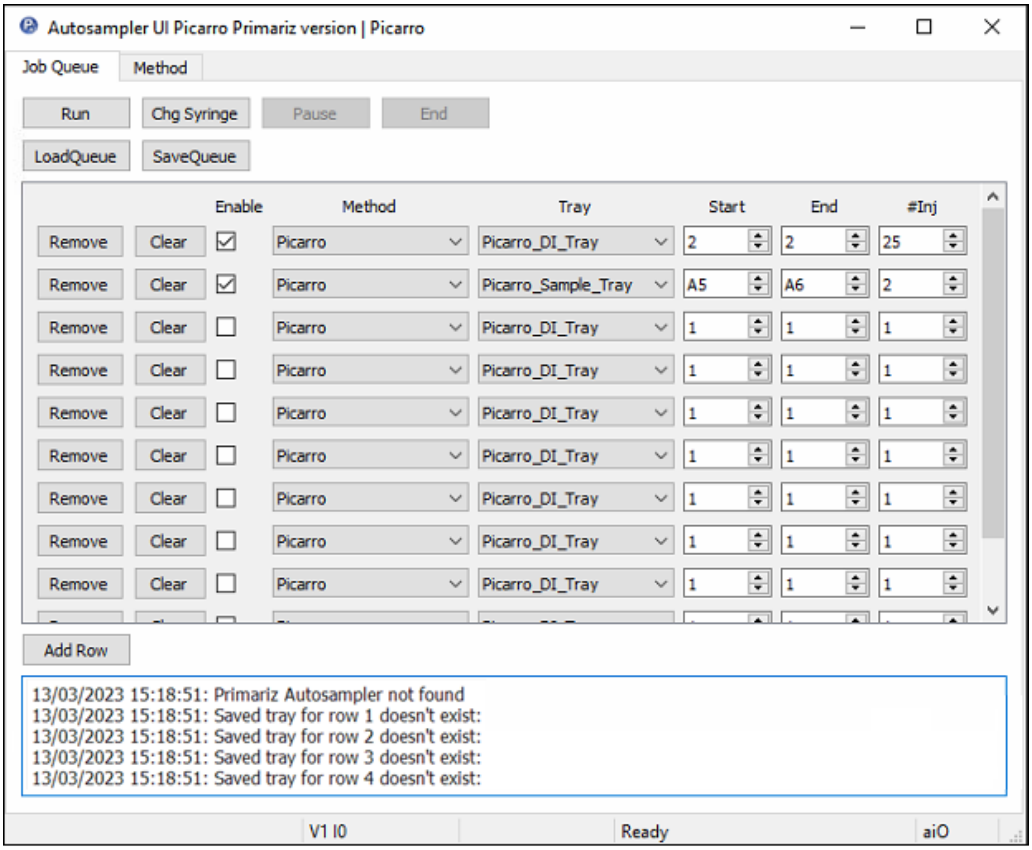


Figure 66: Autosampler Control Window

5. Click **Run**.
6. Minimize the Autosampler window and double-click on the desktop icon **Coordinator Launcher**.

   This will open the window 'Picarro Coordinator Launcher' with a dropdown menu 'Select Coordinator.'
7. Select **High Precision** and click **Launch**.

   Once the 'CRDS Coordinator' window is open, it will start to run through a series of checks, which include cleaning the vaporizer by opening and closing valves.
8. Once the vaporizer cleaning has finished, the Coordinator will initiate the first injection from the Autosampler. Then it will run through the entire Autosampler queue that was set up in step 5. The complete Autosampler queue will include 210 injections and it will take approximately 24 hours.

You can monitor the progress of the run in the **CRDS Coordinator** window. Please check to ensure that H_2O concentrations of the first few injections fall within about 15,000 to 20,000 ppm, and that the injection concentrations are within about ± 1,000 ppm of each other. You can now leave the system to run for 24 hours, during which time it will collect the necessary data to test the precision and drift of the instrument.

9. When the run is complete, navigate to the file C:\IsotopeData and identify the Coordinator output file. The correct file name can be found in the CRDS Coordinator window in the **Filename** box, and the file will have the format .csv (comma-separated values). Move this file to another computer with Microsoft Excel or similar spreadsheet program.

10. Open the .csv Coordinator output file. Then copy and paste data from the columns labeled **d(18_16)Mean** and **d(D_H)Mean** into a drift and precision test analysis spreadsheet that can be downloaded here:

    https://picarro.box.com/s/f660al39eiacqvmss40bt57tuq47dbfy

    The spreadsheet is set up to calculate precision and drift and record the values in table provided. Within the spreadsheet, you will find a table labeled **Report**. Review this table and check the cells underneath the column **State**. If these cells read **pass**, the instrument passed the standard drift and precision test. If any boxes are labeled **fail**, you should contact Picarro's Technical Support team at support@picarro.com. Please be prepared to provide the serial number of your analyzer.

14.2 Leak-Free Operation with a High Precision Vaporizer (A0211)

Following an injection of liquid into the water isotope analyzer, the shape of the square "pulse" in the water concentration versus time graph provides information about the quality of the injection and any potential problems that can lead to poor data.

One potential problem is a leak between the vaporizer and the analyzer. These leaks can be detected by plotting the water concentration along with the "outlet proportional valve" setting during the analysis. The outlet valve performance provides a way to identify unexpected pressure changes in the system, and it is a useful indicator of vaporizer performance. Here's why: The vaporizer converts a liquid sample into gas. At the beginning of sample analysis, one of the vaporizer valves is opened to the analyzer to allow gas to pass from the vaporizer into the analyzer cavity. During analysis, the pressure in the cavity steadily decreases because the gas is leaving the fixed volume of the vaporizer. To keep the cavity pressure constant, the outlet proportional valve slowly adjusts to compensate for the pressure change at the inlet.

For additional background on the operation of the High Precision Vaporizer, you can review the following Picarro Community post online:

http://www.picarro.com/community/picarro_community/vaporizer_a0211_operation_schematic (Access requires user login; If you do not yet have an account, please send an email to: support@picarro.com to request access to documents and manuals.)

14.3 Viewing the Outlet Valve Position

To access the outlet valve position plot within the CRDS Data Viewer GUI, go to **Settings** > **Change GUI Mode**. When asked for a password, use the default Picarro password ("picarro"), and press **OK**. Now you can select the Outlet Proportional Valve plot.

The outlet valve position is also recorded in the Private Data Log files (see section ***13 File Management*** for details on how to access these files). If you would like the data stored in the User Data, you can refer to ***Setup Tool*** to include the outlet valve in your user data files.

14.4 Typical Appearance of Water Concentration and Outlet Proportional Valve Graphs

For all of the following plots, the water concentration is the top graph and outlet proportional valve position is on the bottom. Ideally, the water pulse should be square, and the outlet proportional valve position should gradually decrease at the flat top of the water pulse, as shown below. These features correspond to the outlet valve gradually closing during the analysis of the pulse.

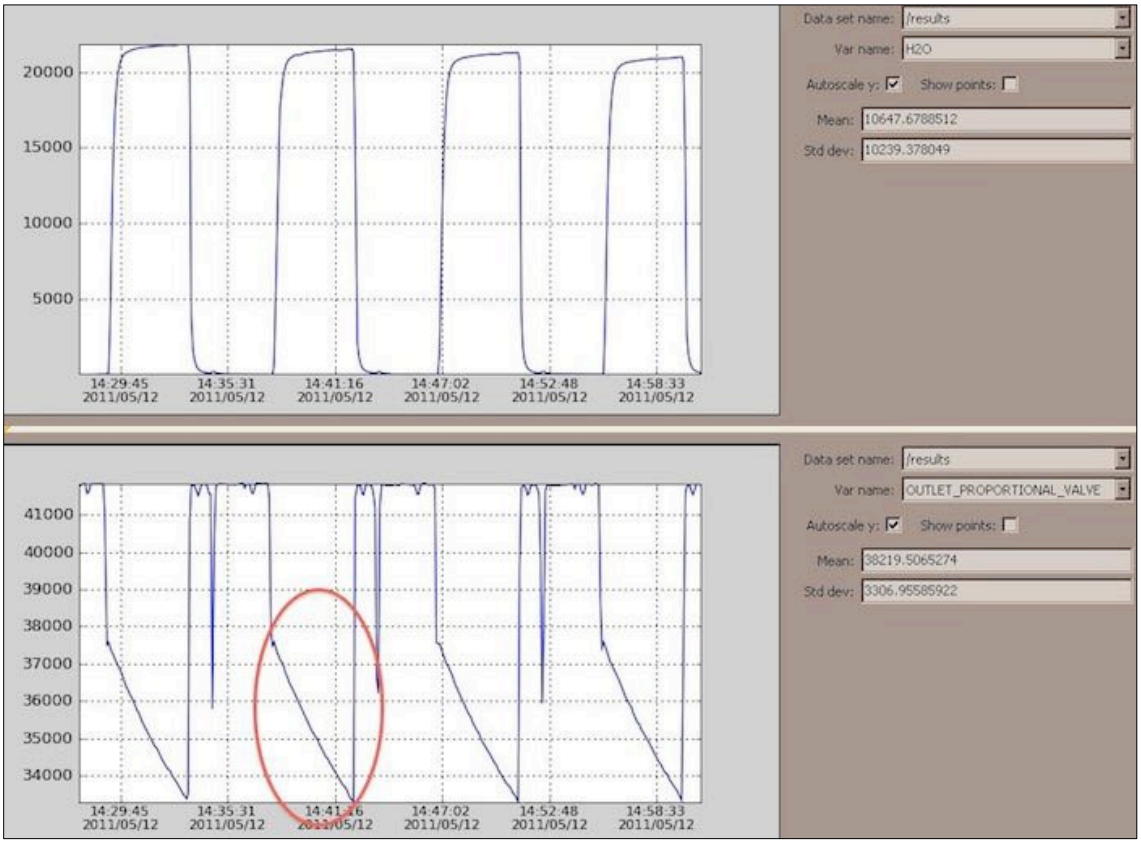


Figure 67: Ideal Water Concentration and Outlet Proportional Valve Graphs

For a proper analysis, the concentration of the dry gas (between the pulses) should be < 500 ppm H_2O. The peak height of the pulse should be reproducible (within ± 1,000 ppm) and between approximately 17,000 and 23,000 ppm.

14.5 Water Concentration and Outlet Proportional Valve Graph Problems and Potential Causes

Problem: Extra Pulses after the Main Sample Pulse

The image below shows extra little "pulses" after the main sample pulse. Note that the peaks for the main pulses appear normal, and the outlet valve is operating normally. The problem is during the cleanout cycle of the vaporizer, not during sample delivery.

There are three potential causes of this problem:

1. Leaky vaporizer septum. This should be changed after every ~ 300-400 injections.
2. Bad vaporizer vacuum pump. The pump may be starting to fail if it has more than 10,000 hours of use.
3. Bad connection between the vaporizer vacuum pump and the vaporizer. Check the tubing and swage connections for cracks near the metal connections. Be careful not to over-tighten the swage fittings.

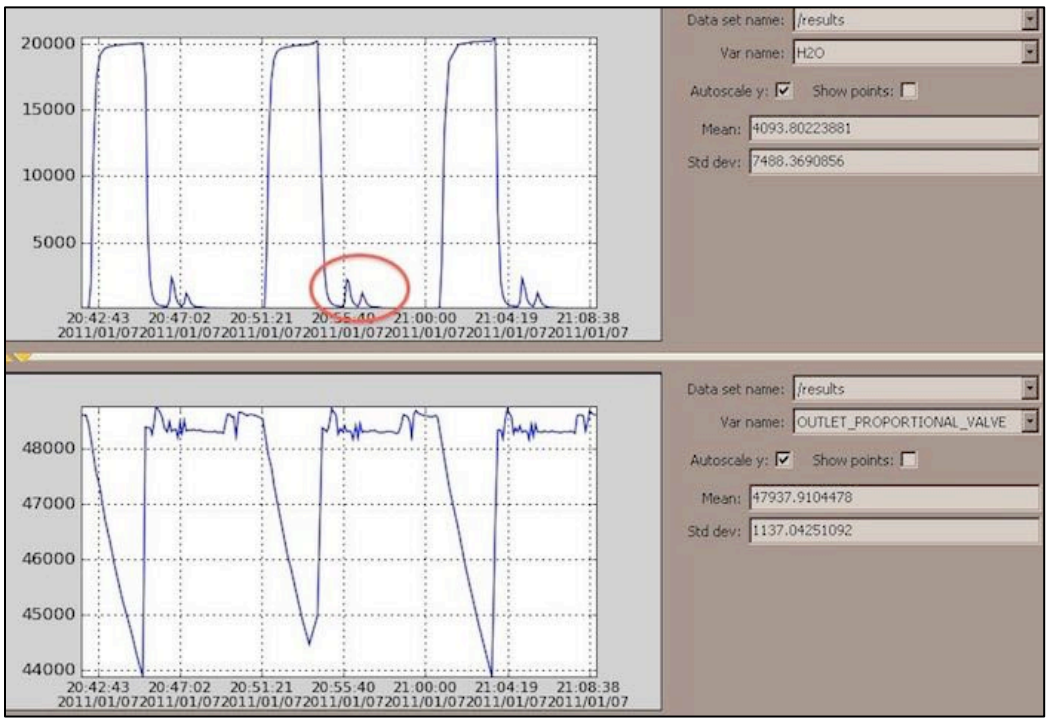


Figure 68: Extra Pulses after the Main Sample Pulse

NOTE

When reattaching 1/4" Swagelok fittings, the nut should be hand-tightened and then turned an additional 1/8 of a turn using a wrench.

Problem: Extra Peaks Before and After the Main Sample Pulse

The water concentration graph below has two abnormalities: an extra little peak after the main peak, and a "spike" at the beginning of the main peak. Note also that the outlet proportional valve is flat. This indicates that the outlet valve is constant during the time the analyzer is drawing air from the vaporizer's internal fixed volume. Because the outlet valve is constant, the pressure on the inlet of the analyzer is not changing. This indicates there is a leak between the analyzer and the vaporizer.

The spike at the beginning of the main pulse could be moist ambient air entering through the leak. In this particular example, the spike peaks at ~ 12,000ppm. In a dry environment, a leak might look like a slope going upwards from left to right with a dependence on the ambient conditions relative to the nominal 20,000 ppm concentration of the vaporized sample. A very leaky septum could also look similar.

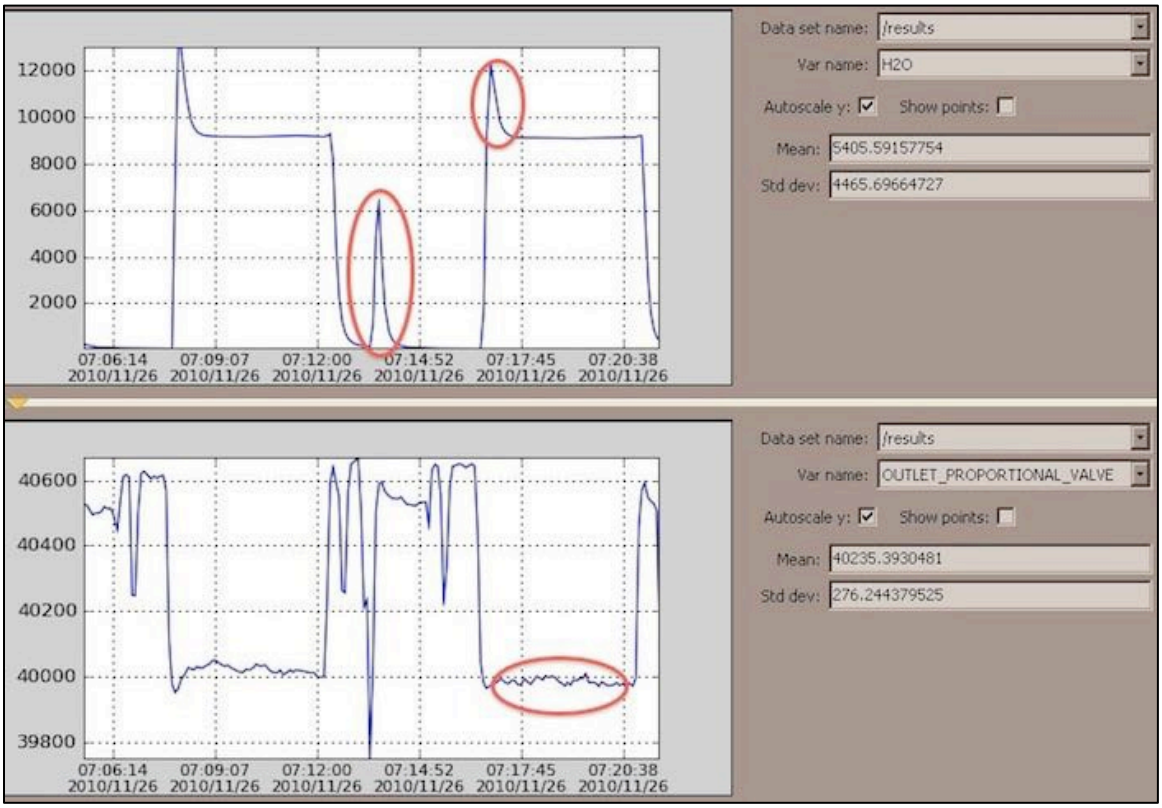


Figure 69: Extra Peaks Before and After Main Sample Pulse

Problem: Decreasing Concentration in the Main Pulse

In this example, the outlet valve is constant during the pulse, but the pulse has a decreasing concentration. This is consistent with a leak of lower-concentration ambient air into the analyzer during analysis. This leak is likely at the connection from the vaporizer to the analyzer.

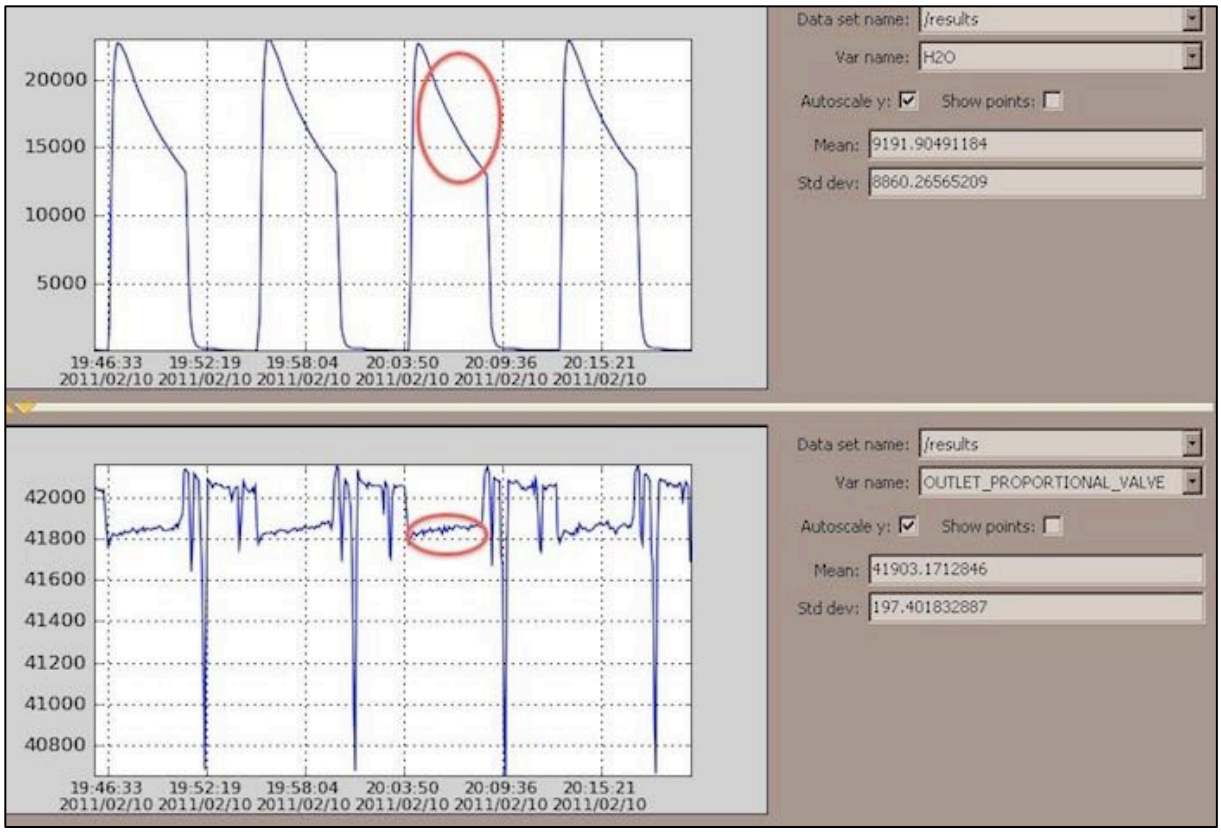


Figure 70: Decreasing Concentration in Main Pulse

Problem: Water Pulse Is Sloped

The slope of the main pulse in the water concentrations, particularly one going upwards as in the first example shown below (Figure 71), indicates poor mixing inside the vaporizer. This can happen if the valve that injects dry gas into the vaporizer is not working perfectly. In this case, the outlet valve position is normal and therefore a leak between the vaporizer and analyzer is excluded as the cause of the problem.

In the second example (Figure 72 below) however, note the change in the nominal outlet valve position. This shows the vaporizer is filling to different pressures with each pulse, so there is inconsistent filling of the vaporizer.

If you see either:

- **Variation in the nominal stopping position of the outlet valve, or**
- **Large increases in water concentration during a pulse**

Contact Technical Support (support@picarro.com) and we can help diagnose and repair the fault, if necessary. Please always provide your analyzer and vaporizer serial number when contacting Picarro.

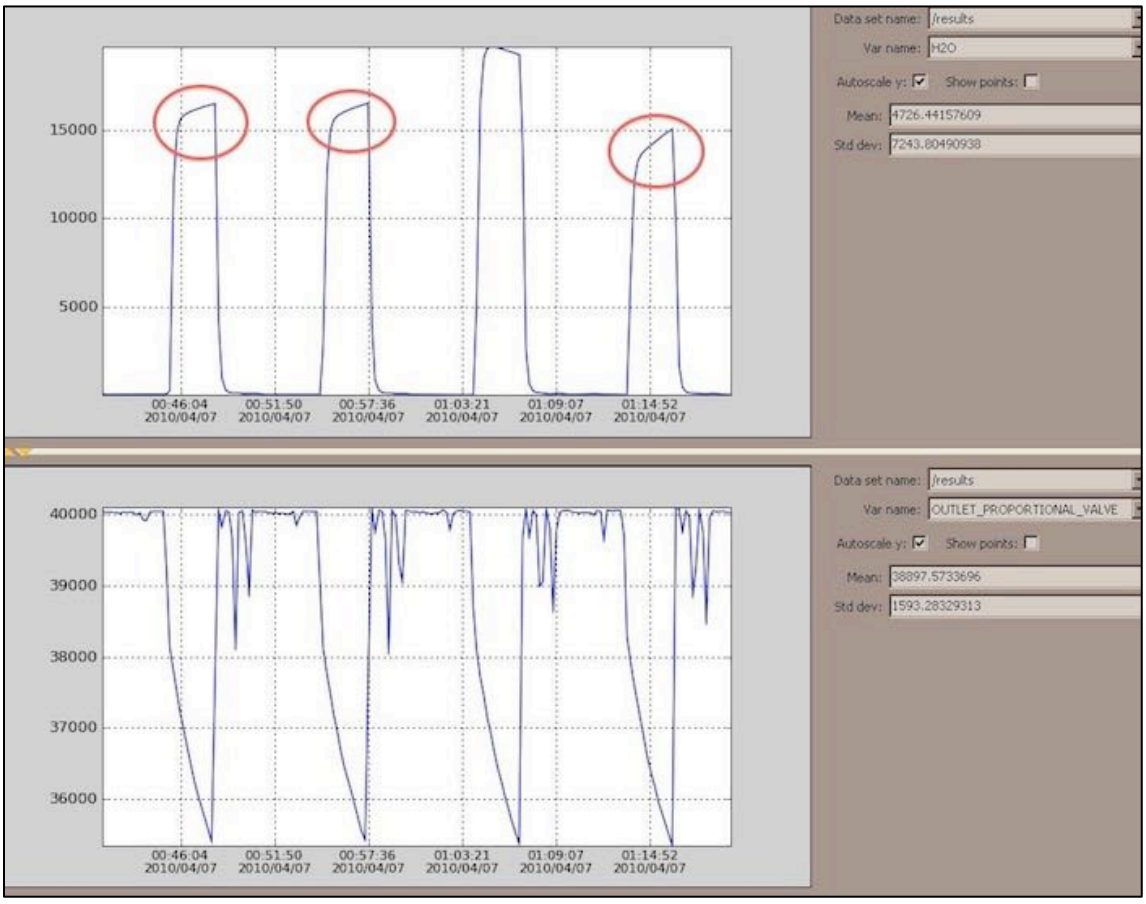


Figure 71: Water Pulse Sloped – Poor Mixing in Vaporizer

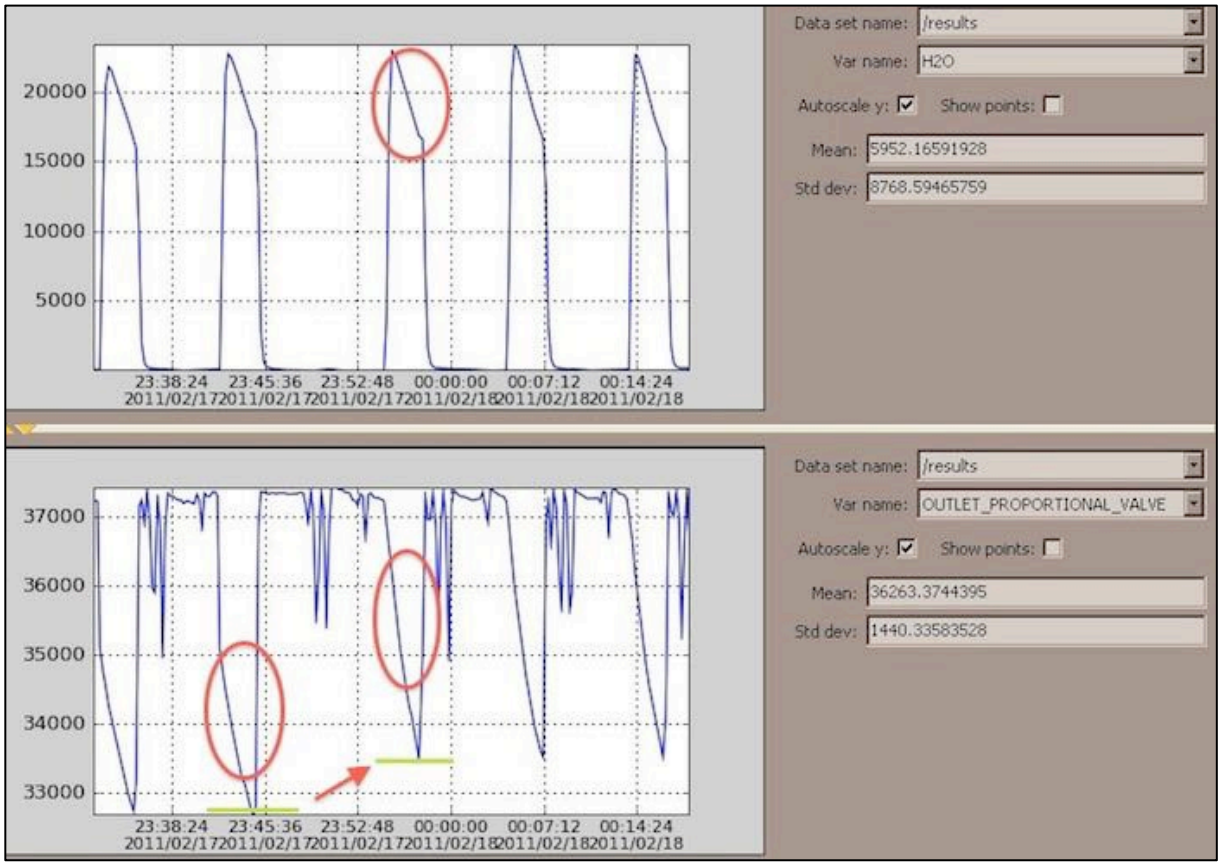


Figure 72: Water Pulse Sloped – Inconsistent Filling of Vaporizer

Problem: Variability in Measured Water Concentration

The measured water concentration should consistently be near 20,000 ppm (±1000 ppm). The circled areas in the water graph below shows values that are higher or lower than expected. The outlet valve behavior is normal.

This can happen if the syringe is clogged, causing inconsistencies in the injected volume. Another problem is an inconsistent gas supply, perhaps due to a failing regulator or another piece of equipment using the same dry gas supply. This causes inconsistent pressure or flow at the inlet dry gas supply.

Other problems associated with sample delivery are:

- Overfilling or pressurizing the liquid in the vials
- Significant contamination of the samples
- Insufficient needle depth resulting in the collection of air, rather than liquid
- Variable volume bubble in the syringe

A test injection is recommended before each run, when you change a syringe, or if water concentrations during the pulse are consistently outside of the ideal ~ 17,000 to 23,000 ppm range. It is possible to scale the injection volume by the

appropriate percentage to target the ideal water concentration range (see section ***15.2 Adjusting Injection Volume*** in section ***15 Best Practices and Operational Tips***).

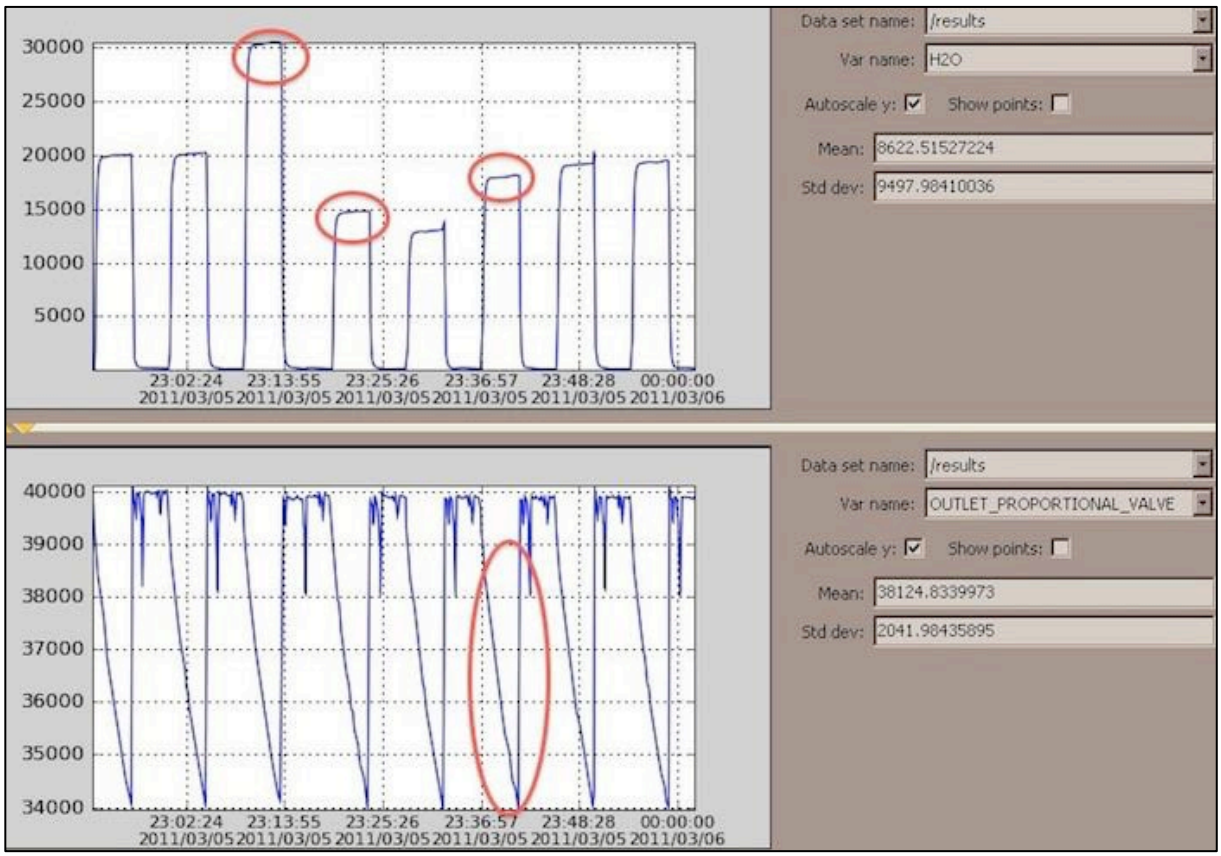


Figure 73: Water Pulse Sloped – Water Concentration Variability

Problem: Water Concentration Suddenly Decreases

In this example, the measured water concentration drops to near the baseline. This can happen if the needle penetration depth into the vaporizer changes and is not deep enough to get the sample into the vaporizer. The tall peak at left is a partial injection, but the subsequent peaks indicate that little water was injected into the vaporizer.

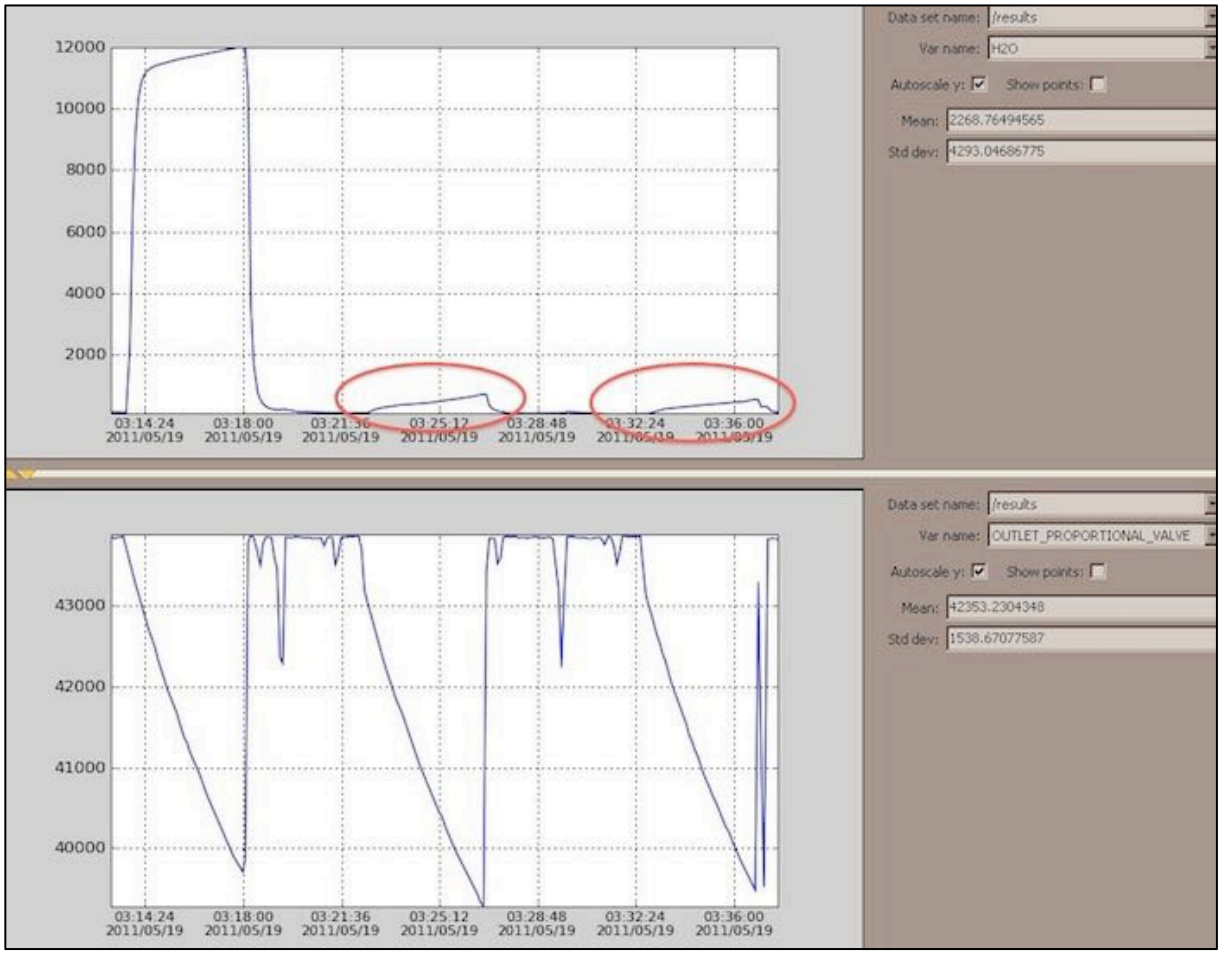


Figure 74: Water Pulse Sloped – Sudden Decrease in Water Concentration

Problem: Baseline of Water Concentration and Outlet Valve Change

This is what happens when a normal analysis runs out of dry air from the dry air cylinder. The same behavior is also possible if there is a large gas leak in your cylinder. As the cylinder gas pressure goes to zero, the vaporizer is forced to take in moist room air, either from the leak or backwards through the Wavelength Monitor (WLM) purge line. The result is that the nominal dry baseline rises to the level of the room air. Also, the outlet valve position decreases since the vaporizer experiences less pressure from the cylinder gas.

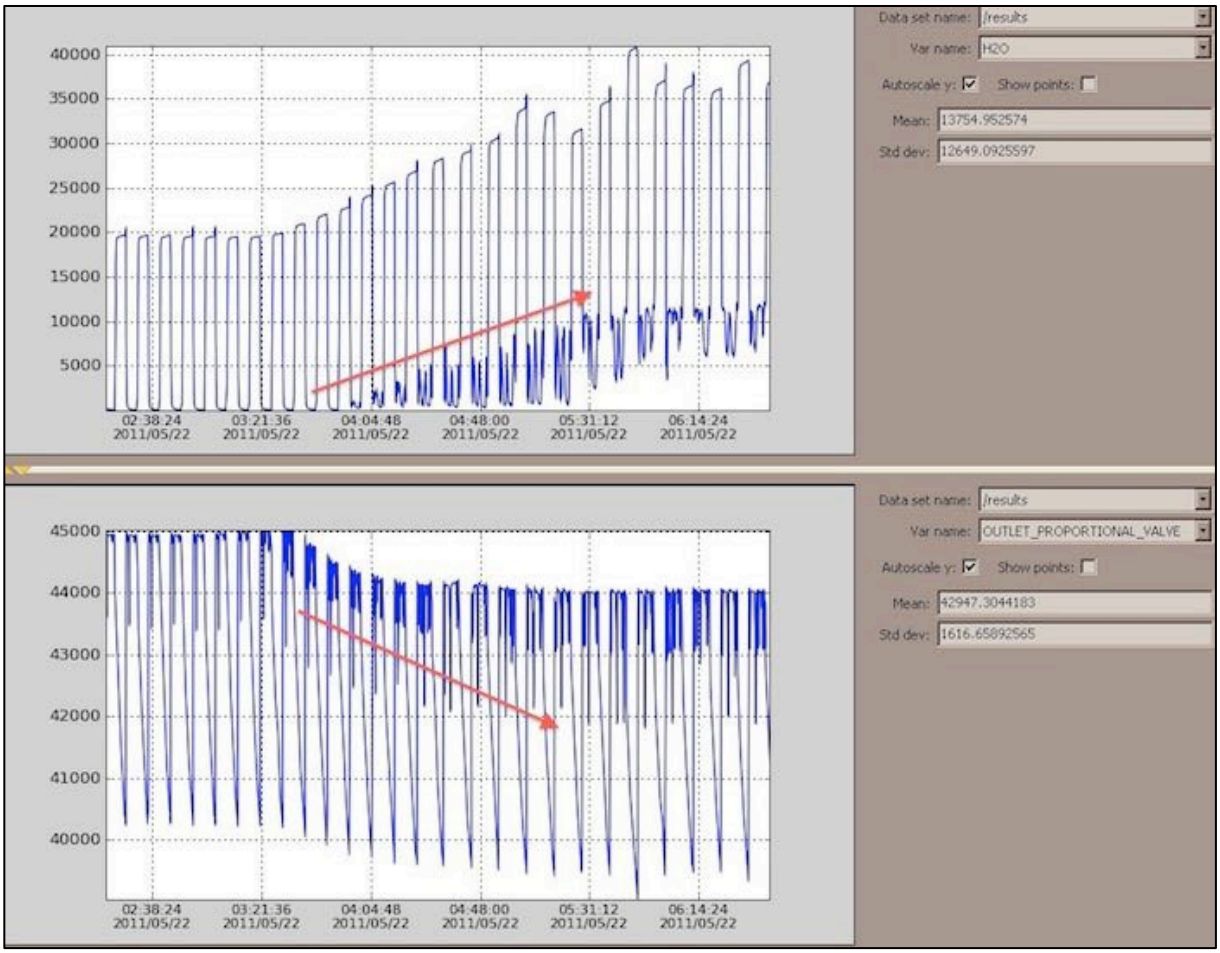


Figure 75: Baseline of Water Concentration and Outlet Valve Change

Problem: Water Pulses Split Into Multiple Peaks

The final example shows what happens if the analyzer's solenoid valve sequencer is running at the same time the coordinator is. The solenoid valve sequencer should be disabled by default for Picarro water isotope analyzers. If the sequencer runs at the same time as the coordinator, the two components send conflicting signals to the valves that control the vaporizer. In this example, the sequencer is turned off following the third pulse, and the final pulse returns to normal.

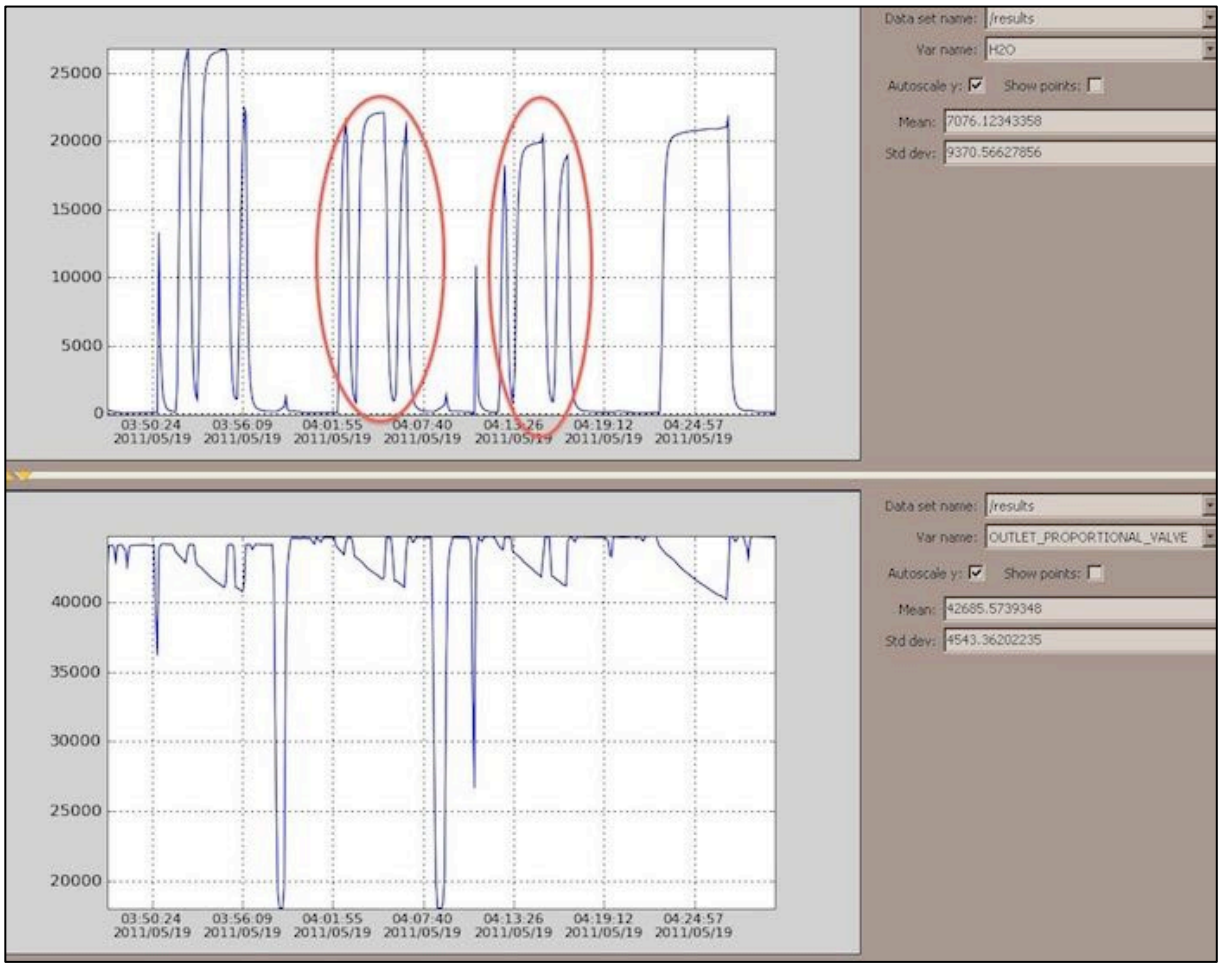


Figure 76: Water Pulses Split Into Multiple Peaks

15. Best Practices and Operational Tips

15.1 Pulse Customization

Pulse Analysis

There is a delay of a few seconds at both the beginning of the pulse and the end of a pulse where the pulse analysis ignores incoming data. Therefore, only the most stable center portion of the pulse is included in the pulse analysis. Although the default settings should be adequate for most uses, one can adjust the delays by editing the appropriate Coordinator .ini script. Please be sure to keep a copy of the original file in case of any mistake. The example below is for the High Precision Mode Coordinator on a L2130-*i* with a Picarro Autosampler.

- Edit the `validTimeAfterTrigger` or `validTimeBeforeEnd` fields in the following file:

  C:\Picarro\G2000\AppConfig\Config\Coordinator\CoordinatorLIMS_G2000_A0340.ini (**Note:** for A0325 Autosampler, find file "…G2000_A0325.ini")

  The default settings are: `validTimeAfterTrigger = 100`, `validTimeBeforeEnd = 15`

- One can similarly adjust the level that triggers a pulse analysis event by changing the 6500 value in the upslope or downslope trigger in the following file:

  C:\Picarro\G2000\AppConfig\Config\Coordinator\CoordinatorLIMS_G2000_A0340.ini (**Note:** for A0325 Autosampler, find file "…G2000_A0325.ini")

  The default settings are: `thres1Pair = [6500, 30000]` and `thres2Pair = [5500, 30000] #this is the downslope trigger`

15.2 Adjusting Injection Volume

For best results, liquid sample injections should be provided to the instrument at a concentration of **18,000 ± 3,000 ppmv (parts per million by volume)**. Each liquid injection will be labelled as "good" in the coordinator if this concentration is between **15,000 - 21,000 ppmv**. If the concentration is significantly above or below this range (i.e., < 15,000 ppmv or > 25,000 ppmv) or if the dry background is > 500 ppmv, the pulse will not be analyzed, and the data will not appear in the coordinator.

To achieve the appropriate injection concentration:

1. Dry nitrogen or zero air (< 50 ppmv water concentration) should be supplied to the instrument at 2.5 ± 0.2psi (17.2 ± 1.4kPa), with a flow of approximately 200 sccm (Standard Cubic Centimeters per Minute). If Drierite (or similar) is used for the dry air (rather than a nitrogen or zero air tank) supply, a measured background level of ~ 100-200 ppmv will produce satisfactory data. Remember to select the Measurement Mode appropriate to your background gas matrix (see the section ***Switching Between Measurement Modes***.)
2. Sample injection volume (controlled by Autosampler) should be set at ~ 1.8µL.

If the resulting concentration peak after the 2nd or 3rd liquid injection is substantially different from 20,000 ppmv:

1. **The injection volume may need to be scaled appropriately:** For example, if the resulting concentration peak of an initial 'test' injection is 16,000 ppmv, then the injection volume needs to be adjusted by the factor 20,000/16,000 = 1.25. To accomplish this, multiply the current injection volume in the Autosampler method by 1.25.
2. **The injection quality may need improvement.** Bad Injections can cause incorrect injection concentrations. Bad injections can be from a clogged needle, damaged vaporizer septum, or incorrect dry gas pressure/flow restriction.

NOTE

Five failed injections will lead to a Time Out: Every time there is a liquid injection into a vaporizer by the Autosampler, a pulse of water vapor should enter the cavity and be analyzed. If something goes wrong (e.g., syringe breaks), and the pulse analysis fails, the software will try injecting five times in a row. After 5 failed injection pulses, the coordinator will time out. You will need to restart the coordinator to continue the experiment. This is a built-in safety mechanism that helps prevent un-intended sample contamination following multiple pierces of the vial septum.

15.3 Syringe Lifetime

A common failure in liquid water analysis is syringe breakage. These consumable parts, although replaceable, can be expensive. We recommend the following best practices for enhancing syringe lifetime.

Summary

- **Recommended syringe size: 10 µL**
- **Manually clean syringe between each autosampler run with deionized water**

- **Make sure plunger moves smoothly in the barrel**
- **Use a lubricant, like N-Methyl-2-pyrrolidone (NMP), if necessary**
- **Use the Autosampler Training program (rather than the Autosampler Controller program) to change the syringe**
- **Check syringe injection and fill speed, and the injection depth**

Syringe Details

Picarro analyzers ship with 10 µL syringes from SGE Analytical Science (10 µL syringe part # 002982, 10R-C/T-5/0.47C). The thicker plunger on these syringes makes them more robust than 5 µL syringes.

Samples with Precipitates

The High Precision Vaporizer can operate with liquid waters containing as much as approximately 200 g/kg total dissolved solids (TDS). In principle, water samples can be analyzed without filtration, especially if the precipitate has settled and the syringe is collecting water from near the top of the vial. However, running samples with high TDS will decrease syringe life, require more vaporizer maintenance, and possibly decrease the lifetime of the vaporizer valves.

Therefore, samples should be filtered or centrifuged when possible. The "purer" the liquid being injected into the vaporizer, the longer the syringe, septa, and vaporizer can go without replacement or maintenance.

Dissolving the precipitate by lowering the pH of the fluid is not recommended for these reasons: (1) the sample will fractionate, and (2) introducing acid to the vaporizer, stainless steel tubing, and potentially the cavity, may result in corrosion that requires repair.

15.4 Memory Effect

Memory refers to the effect of the previous sample on the current measurement due to carryover of trace amounts of the previous sample. Water is especially subject to this effect because it adheres to surfaces even at temperatures well above the boiling point. It is a common problem encountered by all methods of isotopic analysis.

In Picarro analyzers, the memory is a function of the entire assembly (vaporizer, connection to the analyzer, and the analyzer itself). It is commonly accounted for by performing multiple injections of the same sample.

The simplest way to correct for memory is to ignore the first 2 or 3 injections of a sample and only use the later injections. For waters with closely clustered isotopic values, this usually means running 6 injections per sample and ignoring the results of the first two injections. In more extreme cases, running 8 injections and ignoring the first 3 or 4 will yield better results.

The effect of memory is stable over time. This means that the same percentage of the previous sample is carried over to the new sample each time.

However, memory should be characterized every one to two months, particularly if samples with high levels of insoluble material or high dissolved solids are frequently analyzed. These materials build up in the vaporizer and can increase the retention of old sample.

This effect can be quantified using the following procedure:

1. Inject a sample of water at least 20 times (40-50 times is preferable).
2. Switch to a new sample with significantly different (> 100‰ for δ^2H) isotopic value and inject the new sample the same number of times as the previous sample.
3. Switch back to the original sample and again measure that multiple times.
4. Calculate the 'true' value of each sample by averaging the last 5 to 10 injections of that sample.
5. Then subtract an individual injection from the 'true' value of the previous sample and divide this by the difference in isotope space between the 'true' value of the current sample and the previous sample.

   This will yield a memory coefficient (in percent) for each injection, x, where, for example 99% means that 99% of the true isotope difference between two samples of water has been attained after x injections. The first injection of sample will be in the range of 94% to 97%. By the 4^{th} injection, it will be approximately 98% for δ^2H and 99% for $\delta^{18}O$. Typically, the memory effect is larger for δ^2H than for $\delta^{18}O$.

15.5 Analyzing Samples with High Total Dissolved Solids

Picarro's High Precision Vaporizer can be used to measure saline samples. However, these samples present two unique challenges to instrument performance and lifetime:

1. Salty samples generate residue in the syringe, which decreases syringe lifetime. See previous section ***15.3 Syringe Lifetime*** for more information on increasing syringe lifetime when running salty samples.
2. Upon vaporization, dissolved solids create a residue in the vaporizer, which can increase the memory effect and influence data quality.

If you are running salty samples and you see a decrease in the memory coefficient, Picarro recommends cleaning the vaporizer. The vaporizer might need cleaning every 200 mg of salt injected, and the cleaning will take about 12 hours

of downtime. Contact Picarro to receive instructions on cleaning the vaporizer, or to order the Vaporizer Cleaning Kit (part number C0211).


NOTE

Although vaporizer cleaning will improve the performance of your High Precision Vaporizer, salt build up can decrease the lifetime vaporizer valves and eventually lead to valve failure. This is particularly true if salts get into the valves themselves, preventing good seals at the valves.

15.6 Sample and Standard Handling

Sample Storage

Whenever samples should be stored in sealed vial in a refrigerator or freezer. If samples are frozen prior to analysis, it is essential to have sufficient headspace in the vial to prevent breakage during phase change, and to ensure the entire sample is returned to liquid form prior to isotope analysis. Parafilming the cap of the storage container is also recommended. If samples are stored in 2 mL autosampler containers, the cap with septa should be replaced once pierced.

Two types of autosampler vial are recommended for use with your Picarro Autosampler:

- **2 mL glass vial with cap and septa (Picarro part number C0322, or as part of a consumables kit, C0328 or C0329)**
- **If samples or standards are limited, it is also possible to use 2 mL vials with 250 µL inserts. These vials act to limit headspace for small samples. Picarro recommends the use of fixed inserts to avoid water vapor passing between the insert and the wall of the larger 2 mL vial. For example, Agilent LS Screw Vial (Agilent part number 5188-6591, available from Fisher Scientific).**

Storage of Secondary Isotopic Water Standards

Selecting the proper containers for long term storage is critical to avoid any change of isotope composition with time due to evaporation or exchange. The following is a list of storage methods for isotope standards.

Glass ampoules: The most reliable containers are glass ampoules that are sealed with a gas torch, such as those provided by the International Atomic Energy Agency with VSMOW2 and SLAP2. After filling and sealing, ampoules can be sterilized by heating the ampoules to about 105°C overnight. This will eliminate the possibility of the growth of algae or other biological activities. Leaking ampoules should be discarded.

Stainless steel barrels: Internal laboratory standards can be stored in stainless steel barrels (25 to 50 liters). These barrels can be obtained from suppliers for the juice, wine, and beer processing industries. When using this method, water

standards should be kept under a slight overpressure of argon or nitrogen gas. The dispensing system ideally consists of a valve with a tube down to the bottom of the barrel to extract the water and a second valve with a manometer and tube connector to keep a headspace overpressure of inert gas in the barrel. Due to the overpressure in the barrel, water can be dispensed by opening the first valve. The laboratory standard has no contact with the atmosphere and therefore no risk exists of any evaporation during storage.

Amber vials and glass bottles: For routine work, a 250 mL glass bottle can be filled from the appropriate internal laboratory standard barrel. 2 mL aliquots of these standards can then be moved to a standard autosampler vial with septa cap for routine, daily calibration. Glass bottles should be filled from their source on a regular basis (every few weeks), without discarding the remaining portion of the standards. This handling method minimizes isotope fractionation during evaporation and exposure to air while the bottle is open.

NOTE

Picarro recommends that once an autosampler vial is pierced by a needle, the vial should be discarded and not used repeatedly. For example, if a multi-day autosampler run is set up, the first standard water should not be used again for the last standard water in the sequence. Exceptions can occur if the cap with septa is replaced between the first and last analysis. Once a septa is pierced the sample is susceptible to isotopic fractionation due to evaporation and loss of the water through the cap.

Recommended Reading:

Groening, M. (2018) "***TEL Technical Note No. 03 Stable Isotope Internal Laboratory Water Standards: Preparation, Calibration and Storage***", Terrestrial Environment Laboratory, International Atomic Energy Agency, Vienna, Austria.

16. Troubleshooting

The following section lists problems that may be encountered during installation and operation of the analyzer. The corresponding step-by-step procedures provide resolution in most cases. If, after attempting these procedures, the problem remains unresolved, contact Picarro Customer Service at (408-962-3991), EU Technical Support (31-85-888-1650) or support@picarro.com.

16.1 Power LED on Analyzer Does Not Illuminate

Context: Turning on the analyzer by momentarily depressing its front panel power switch should apply power. The green power LED is illuminated when it detects the correct power levels.

1. Check that the AC power cord is attached and plugged into a working outlet.
2. Check that the rear on-off switch near the AC power cord is in the ON position (**I**).
3. Press and hold the front panel power switch for at least 5 seconds as the analyzer may take several seconds to respond.

16.2 User Interface Program Does Not Start

Context: The computer may be configured to start the instrument and the associated user interface program automatically after it completes its boot-up sequence, or the program may be launched using the "**Start instrument**" icon on the desktop.

Communications problems with the analyzer may occur if the analyzer fails to initialize correctly on power up. Should the analyzer initialization process not complete correctly, shut down the instrument by shutting down the Windows operating system on the control computer:

NOTE

Do not simply restart Windows by selecting "Restart" in the drop-down box on Step 3, since this does not cycle the power to the analyzer.

1. Using the Start menu, select the red Shut Down button and select "Shut down" in the drop-down box under "What do you want the computer to do?"
2. Wait for the shutdown to complete normally and for the computer and analyzer to turn off completely.

3. After a few seconds, restart the computer by momentarily depressing the power button.

16.3 Sample Pressure not Controlled to Appropriate Value for Concentration Measurements

Context: Under normal operation, the cavity pressure is automatically locked to the correct value by means of electronically controlled inlet and outlet valves. The message “Pressure Locked” on the front panel display and the user interface indicates that the cavity pressure is at the appropriate value. Should either of the messages “Pressure high” or “Pressure low” be displayed, the cavity pressure is out of its correct operating range.

1. The “Pressure low” message indicates that there is insufficient gas available at the inlet of the analyzer. Check the inlet plumbing to the analyzer and ensure that the pressure at the inlet is within the specifications. Check for blockages in the lines, or regulators that are turned off, especially by removing all items upstream of the inlet to see if the pressure returns to the spec. If removing plumbing from upstream of the instrument inlet doesn’t work, the inlet particulate filter may need to be replaced. See section ***17, Maintenance*** for more information.
2. The “Pressure high” message indicates that gas cannot be removed from the analyzer at a sufficient rate. Check the vacuum line between the analyzer and the power vacuum unit for leaks. Failure of the vacuum pump, injecting dilution gas at excessive pressure, or excessive pressure at the inlet can also cause this problem.

16.4 User Interface Program “Freezes”/Won’t Update Graphs as Data are Collected

Context: The computer may become unresponsive causing the programs that control the analyzer to stop functioning. The computer and analyzer should be shut down and restarted.

If the computer responds to the mouse, a normal Windows shutdown may be carried out:

1. Using the Start menu, select the red Shut down button and select “Shut down” in the drop-down box under “What do you want the computer to do?”
2. Wait for the shutdown to complete normally and for the computer and analyzer to turn off completely.
3. After a few seconds, restart the computer by momentarily depressing the power button.

If the computer does not respond to the mouse:

4. hold down the power switch on the front panel for a few seconds until the computer and the instrument turn off.
5. After another few seconds, restart the analyzer by momentarily depressing the power button.

16.5 ChemCorrect Troubleshooting

This section lists solutions to a common problem that may be encountered while using the ChemCorrect software.

ChemCorrect Processing Software Hung Up (frozen).

Recommendation: Check that you ran a coordinator compatible with ChemCorrect. Coordinators for the ^{17}O-excess mode are not compatible with ChemCorrect. Coordinator output csv files should contain columns with baseline_shift for L2130-*i* and L2140-*i*.

If the above checked out, the other usual cause is syntax error and/or missing/empty row(s) in the coordinator output file. The three files listed below are user-editable:

- Instruction Set: C:\Picarro\ChemCorrectExe\chemcorrect_inst xx.csv

  The instruction set is usually not edited unless you're an avid user.

- Standard Library: C:\Picarro\ChemCorrectExe\standards file.csv

  The standards file syntax is not too complicated to follow.

- Coordinator Output csv file or source file: HIDSxx _CC_IsoWater_xx.csv

The most common errors occur in the Coordinator Output file. These are the items to check:

- The number of injections that you set ChemCorrect Analysis to ignore has to be less than the total injections/sample.
- There can't be any empty row or blank value (as a result of broken/bent needle, or sample ran out of liquid). This is not an issue if you have ChemCorrect version 1.2.0 or later.
- "Line" column has to be sequential and start at 1
- "Time Code" column has to be chronological.
- Port number should correspond with the correct sample number.

17. Maintenance

The advanced, rugged design of Picarro analyzers provides stable, long-term operation with minimal service or maintenance. With the exception of the following items, the analyzer and pump are not user serviceable. Should either appear to malfunction, please refer to the Troubleshooting Guide or contact Picarro Support.

As described below, users may obtain preventive maintenance components as part of a service plan, as part of a designated PM kit, or individually from the Picarro store.

17.1 Service Plans

In addition to basic telephone and email support and remote diagnostics, service plans include an annual preventive maintenance kit and can be purchased by contacting sales@picarro.com. The three service plans are as follows:

- **W3101 Essential Service Plan:** Free yearly maintenance kit; 50% discount on Field Replaceable Parts; 10-20% Discounted factory repair. See data sheet for complete terms and conditions.
- **W3102 Premium Service Plan:** Free yearly maintenance kit; Extended warranty; Free factory repair; Free Field Replaceable Parts. See data sheet for complete terms and conditions.
- **W3103 Commercial Service Plan:** Free yearly maintenance kit; Extended warranty; Free factory repair; Free Field Replaceable Parts; Loaner instrument; Free yearly prevention maintenance visit; Complimentary remote refresher training. See data sheet for complete terms and conditions.

17.2 Preventive Maintenance Kits

Preventive maintenance kits can be purchased by contacting support@picarro.com. The maintenance kits all include the following elements:

Replacement CPU Fan; particulate filter (Stainless Steel or Teflon); dust filter; replacement screws for instrument cover panels; Ball-Point Hex L-Keys; Anti-Static Wrist Strap.

The kits come in three forms depending on the instrument being serviced.

- **S3092:** Yearly Maintenance Kit for GHG, L2xxx, and EtO

17.3 User-replaceable Hardware – Individual Components

Inlet Particulate Filter

The inlet particulate filter is user-replaceable. Use the following links to order replacements and to find an instructional video and supporting maintenance document.

Picarro Store Ordering Links:

- **Stainless Steel Filter:** For all models except those that measure HF, NH_3, CH_2O, HCl and H_2O_2

  S1020 Particulate Filter Kit – If viewing this manual as a paper hard copy, enter the following URL in your browser:

  http://store.picarro.com/For-Analyzer/Parts/Particulate-filter-kit-all-models-except-HF-NH3.html

Filter Replacement Instructional Video and Document:

- **Filter Replacement Instructional Video:** https://vimeo.com/375518688

  This video covers replacement of both stainless steel and Teflon filters. Note that this video does not currently cover replacement of externally mounted particulate filters.

- **Filter Replacement Maintenance Guide:** https://www.picarro.com/support/documents/inlet_particulate_filter_maintenance_guide

  This guide covers replacement of both stainless steel and Teflon filters for analyzer models that have either internally or externally mounted filters.

A2000 Pump Rebuild Kit

The pump rebuild kit is the only component not currently sold as part of a preventive maintenance kit because the replacement frequency is not strictly annual (frequency depends on pump usage).

The A2000 pump diaphragms and valves are user-replaceable. Use the following link to order rebuild kits and to find the instructional video and supporting maintenance document.

- Pump Rebuild Kit: Used with SI2xxx, G2xxx analyzers (except Flight and Flux analyzers)

  S2009 Rebuild Kit for A2000 Vacuum Pump – If viewing this manual as a paper hard copy, enter the following URL in your browser:

  http://store.picarro.com/For-Analyzer/Pump/Rebuild-kit-for-Picarro-A2000-vacuum-pump.html

17.4 A0211 Vaporizer Injection Port Septum Replacement

For instructions on replacing the injection port septum and salt liner (if used), refer to the Maintenance section in the **A0211 High-Precision Vaporizer User Manual** (PN 40-0044).

17.5 Cleaning

Clean the outside of the analyzer with a clean dry cloth. Only certified service technicians should access or clean the inside of the analyzer.

18. Transportation and Storage

If the analyzer will be transported or stored, use the following procedure to prepare and repack it into the original packaging.

CAUTION

When shipping or relocating the analyzer, it is important to protect it from mechanical shocks. Failure to do so can compromise its performance. When shipping the analyzer, use its original packaging only.

18.1 Shutdown and Preparation

CAUTION

A flow of clean, relatively dry gas should always be directed to the instrument for several minutes prior to shutting down. Trapping a high-moisture content gas sample in the cavity can cause condensation damage to the mirrors as the instrument cools from its operating temperature. See section *7.2, Shutdown* for specific shutdown instructions for your model analyzer.

1. Click on the **Shutdown** button located on the left side of the Data Viewer window.
2. A window will pop-up (Figure 77) prompting the user to confirm the shutdown. Once confirmed, the analyzer software and hardware will turn off.

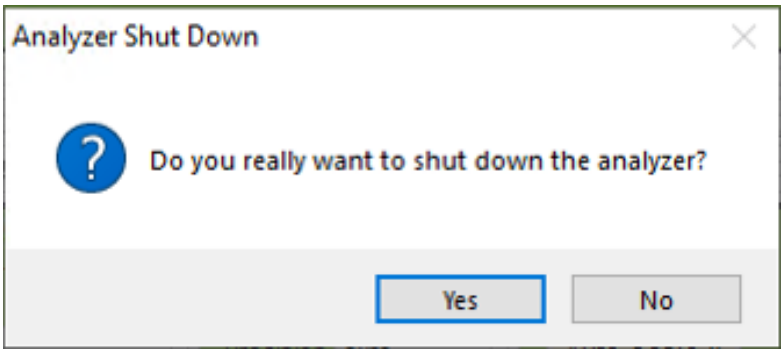


Figure 77: Shutdown Confirmation Pop-Up Dialog

3. Manually turn off the pump(s) and dry gas (if used).
4. Disconnect all tubing and electrical connections from the analyzer.
5. To prevent contamination and possible damage to the connector threads, place protective caps on all gas connections.

18.2 Packing

1. Place the analyzer in a plastic bag with a package of desiccant. Seal the bags with tape. If shipping the pump, do the same for it.
2. Pack the analyzer and pump in the original shipping containers ensuring that all the foam pieces are in place to protect the analyzer during shipping.

APPENDIX A – Setup Tool and Communication

A.1 Setup Tool

In the desktop folder called **Picarro Utilities**, the **Picarro Analyzer Setup Tool** can be launched by double clicking on its icon. This tool allows the user to configure data file saving details, including which data elements are written to data files, digital data output (via serial port or TCP/IP), remote data delivery (via email), and general GUI properties.

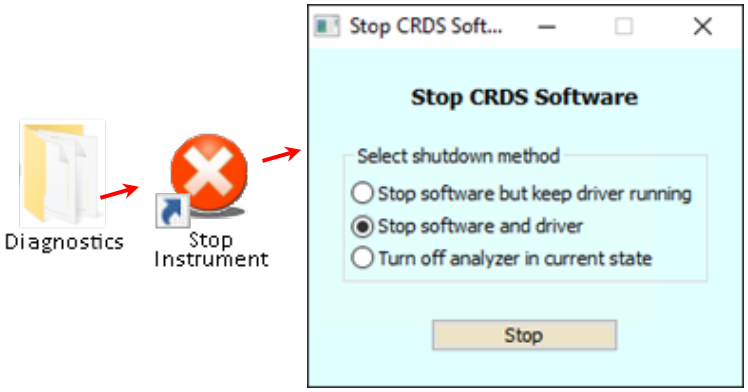
Seven tabs of the Setup Tool Window are explained in the next pages in brief. A more in-depth description of the material is provided in the subsequent section. If you have any questions about the Setup Tool, please contact Picarro or refer to Picarro Community for further details.

https://www.picarro.com/support/community

NOTE

Before running the Setup Tool, the instrument software and drivers must be stopped.

From the desktop, open the *Diagnostics* folder, double-click on the *Stop Instrument* icon. The *Stop CRDS Software* window appears. Select the radio button "*Stop software and driver*," then click the *Stop* button.



Data Logger Tab

Configuring Data File Saving Details with Data Logger

The **Data Logger** tab (Figure 78) allows the user to configure various data file saving details, including which data elements are written to data files.

- **Data Columns:** Controls which data elements are written to data files.
- **Hours of Each Log File:** Controls the size of each data document.

- **Enable Mailbox Archiving:** Enables archiving of data in the mailbox folder – C:\Picarro\G2000\Log\Archive\DataLog_Mailbox
- **Archived Directory Structure:** Specifies part of naming convention for data documents.
- **Total User Log Storage Size (GB):** Specifies the size of storage allowed for User Data (Recent Data).
- **Mode:** Changes the way the analyzer fits and displays data in the data viewer on the basis of gas matrix, species reported, precision, and dynamic range.

After making the appropriate edits, click **Apply** to put changes into effect and then **Exit** to close the window.

Figure 78: Data Logger Setup Window

Port Manager Tab

Managing Ports for Digital Data Output/Input and Serial Communication with Port Manager

The **Port Manager** tab (Figure 79) allows you to control digital data output/Input via serial port or TCP/IP.

On this window, you can specify:

- **Data Streaming:** The port you want your data to stream through (COM1/COM2/Off),
- **Valve Sequencer MPV (Multi Position Valve):** The port you want to connect your MPV to (COM1/COM2/Off)

  For more information on the configuring for external valves, contact Picarro Support.

- **Command Interface:** (COM1/COM2/TCP/Off).

  Make sure there are no COM port conflicts before clicking **Apply**.

After making the appropriate edits, click **Apply** to put changes into effect and then **Exit** to close the window.

To learn more about Serial Communication, see ***Remote Data Access*** in ***APPENDIX A – Setup Tool and Communication***.

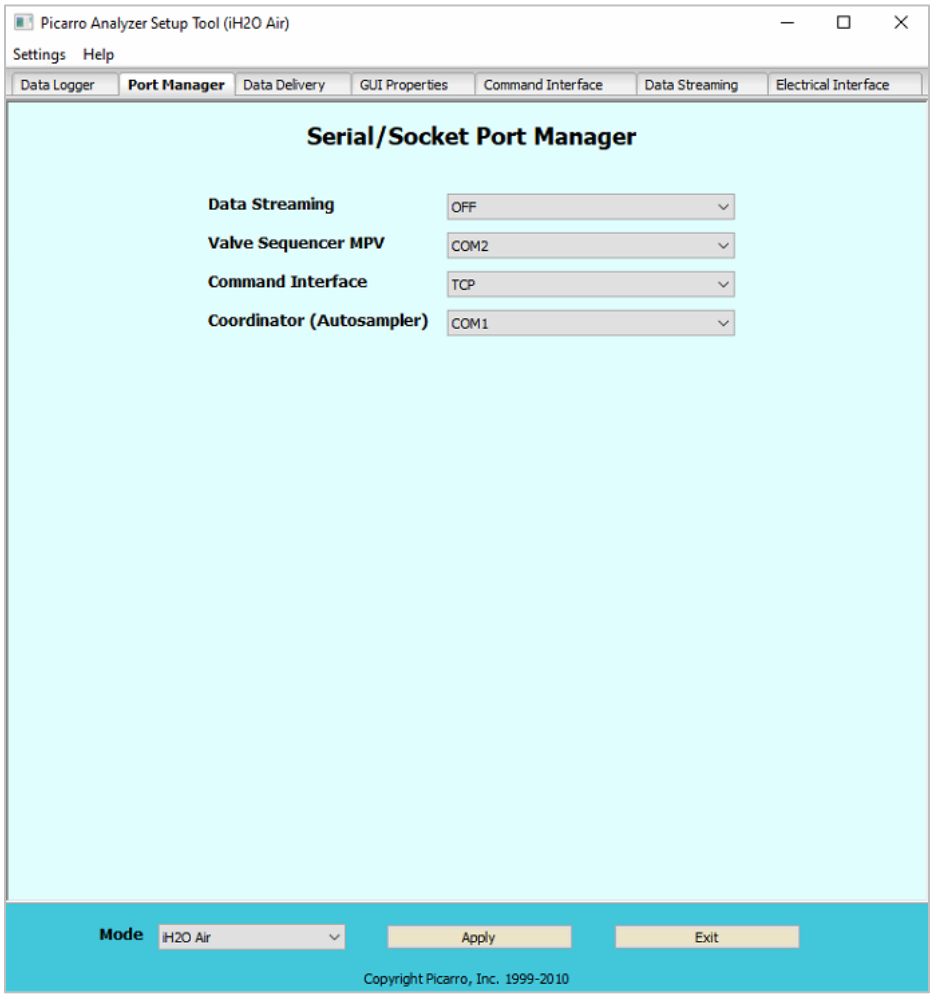


Figure 79: Serial/Socket Port Manager Window

Data Delivery Tab

The **Data Delivery** tab (Figure 80) allows the user to schedule remote data delivery (email).

- **Delivery Start Time:** Time of the day when data will be sent.
- **SSL:** Depending on the sender's email server, the sender can activate the Secure Sockets Layer (SSL).
- **Use Authentication:** Turning this on will require the receiver to provide a password and a username to access data. Set up the password and Username from this window.
- **From:** Sender's email
- **To:** Receiver's email.
- **Subject:** subject line of the email.
- **Data Directory:** Location of the data you want email.

After making the appropriate edits, click **Apply** to put changes into effect and then **Exit** to close the window.

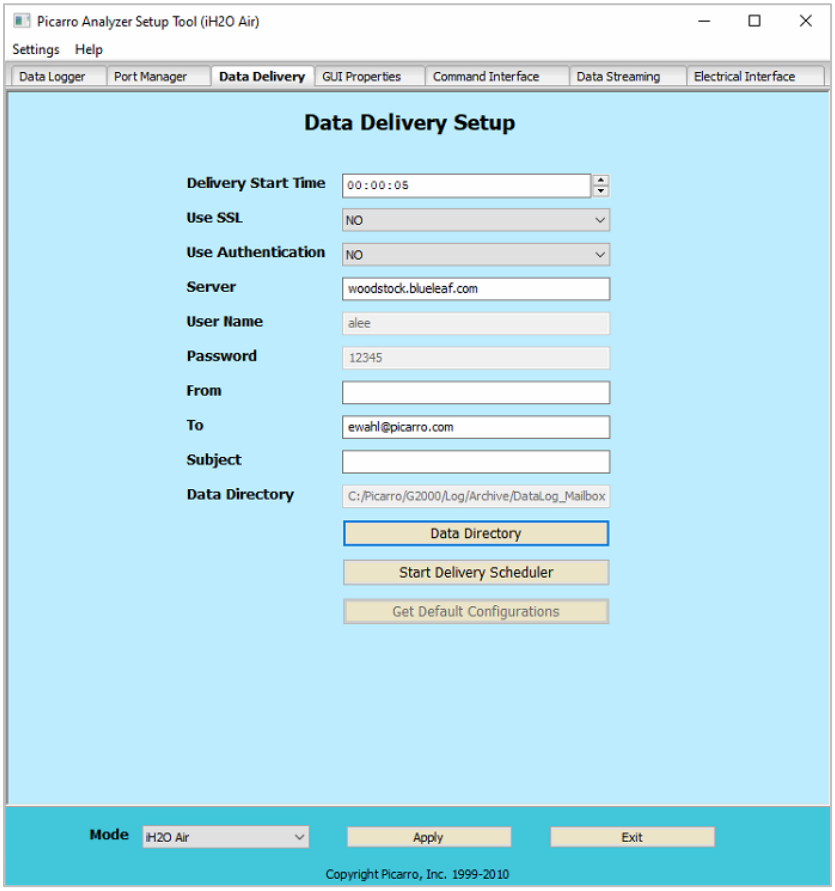


Figure 80: Data Delivery Settings Tab

GUI Properties

The **GUI PROPERTIES** tab (Figure 81) allows you to set the number of graphs displayed and to enable the control of Valve Sequencer from the main GUI.

Number of Graphs: Set the desired number of line graphs to be visible on the main GUI.

Enable Control of Valve Sequencer: To make the Valve Sequencer menu item visible under the **Tools** menu of the main GUI:

3. Click on **Settings** of the **Setup Tool** window, and then **Switch to Service** mode.
4. Choose Yes next to Enable Control Valve Sequencer drop down menu on the GUI Properties tab.
5. Click **Apply** to put changes into effect and then **Exit** to close the window.

You should now be able to access the **Show/Hide Valve Sequencer GUI** menu from the main GUI under the **Tools** menu**.**

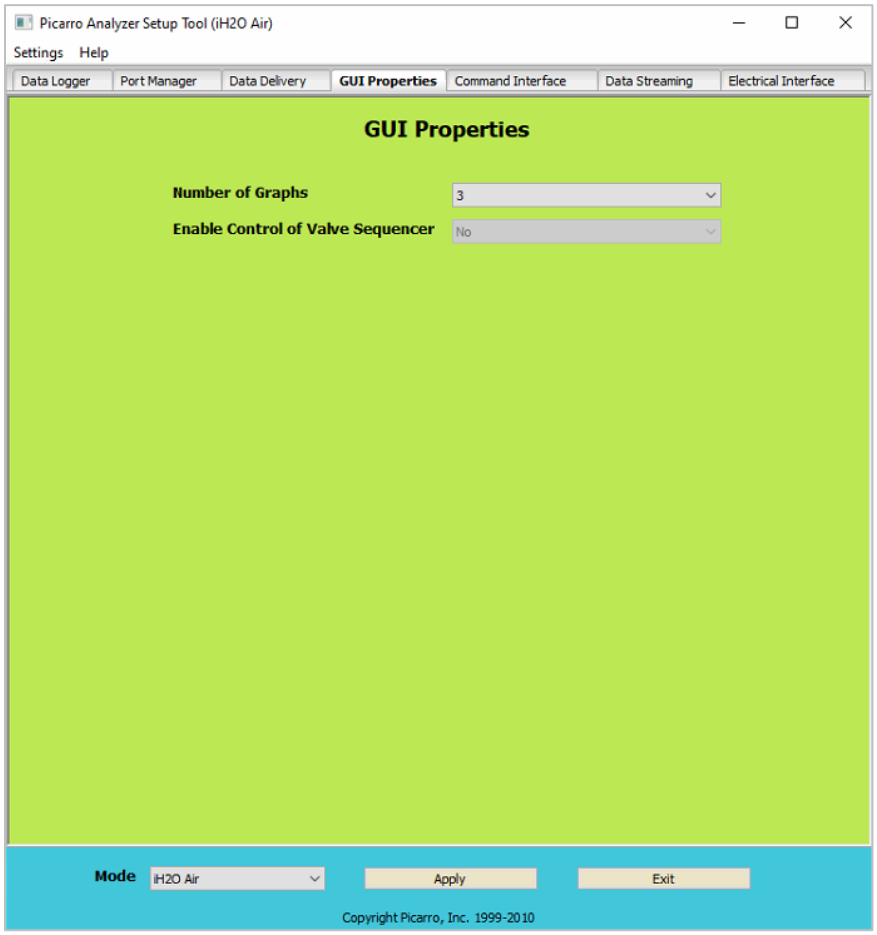


Figure 81: GUI Properties Settings Tab

Command Interface – Specifying Digital Data Output

The **COMMAND INTERFACE** tab allows you to specify the data elements that are sent via COM port/TCP (specified in the **PORT MANAGER** tab). Two types of data can be specified here:

Output Data Source:

- Datalog_User
- DataLog_User_Sync (Relevant only for Flux G2311-f analyzers).

Output Data Columns:

- The data columns are output in the order they are checked, e.g., CH_4, comes before CO_2. Command Interface enables an external device to send a set of predetermined commands to a Picarro analyzer. The Picarro returns data or metadata on the basis of the command received.

After making the appropriate edits, click **Apply** to put changes into effect and then **Exit** to close the window.

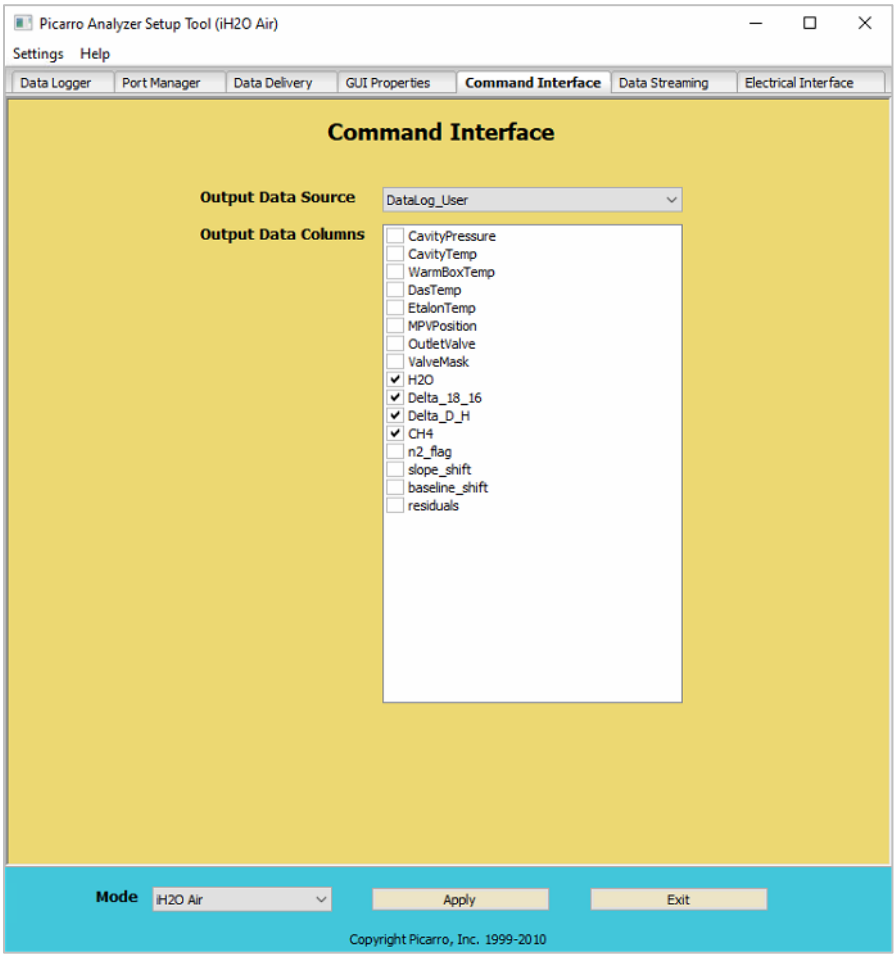


Figure 82: Command Interface Settings Tab

Data Streaming – Specifying Digital Data Output

The **DATA STREAMING** tab allows you to specify the data elements that you want to send via COM port (specified from the **PORT MANAGER** tab). Two types of data can be specified here:

Output Data Source:

- Datalog_User
- DataLog_User_Sync (Relevant only for Flux G2311-f analyzers).

Output Data Columns:

The data columns are output in the order they are checked, e.g., CH_4, comes before CO_2. Command Interface enables an external device to send a set of predetermined commands to a Picarro analyzer. The Picarro returns data or metadata on the basis of the command received.

Data Streaming outputs data continuously, whereas the Command Interface needs commands to output data.

After making the appropriate edits, click **Apply** to put changes into effect and then **Exit** to close the window.

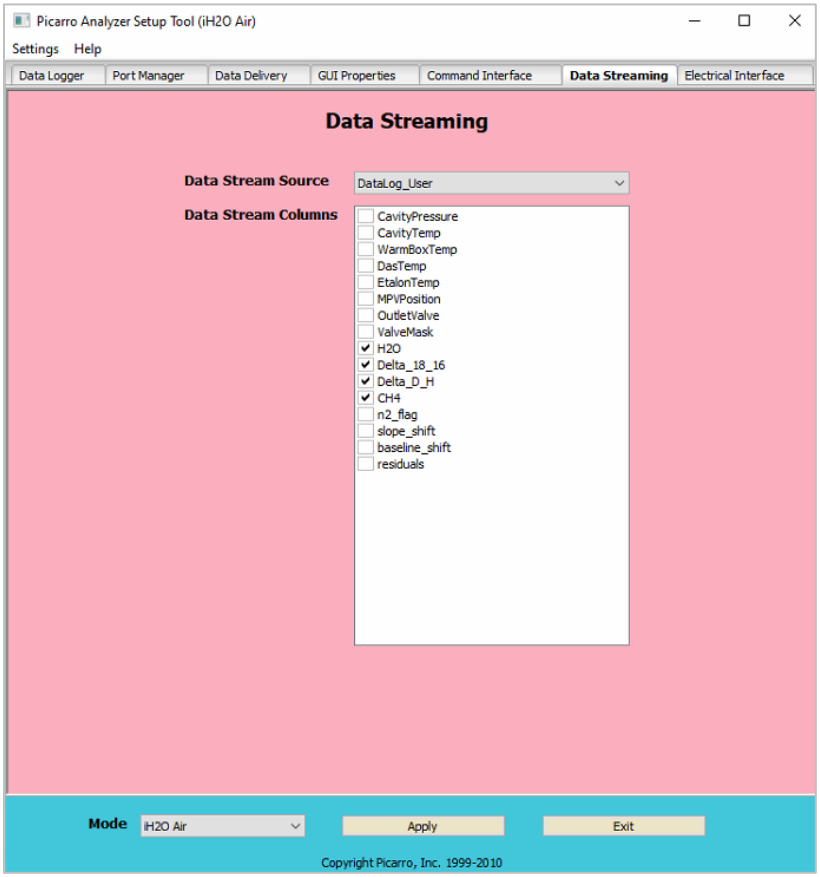


Figure 83: Data Streaming Settings Window

Electrical Interface – Customizing Analog Output Channels

The Picarro analyzer may be optionally configured with an **Electrical Interface Card** (EIC) that provides up to 8 analog signals available to the user for monitoring various measurements results and analyzer parameters.

The **ELECTRICAL INTERFACE** tab (Figure 84) allows you to customize each analog output channel.

After making the appropriate edits, click Apply to put changes into effect and then **Exit** to close the window.

NOTE

This tab will be disabled if your analyzer was not configured to work with an analog peripheral.

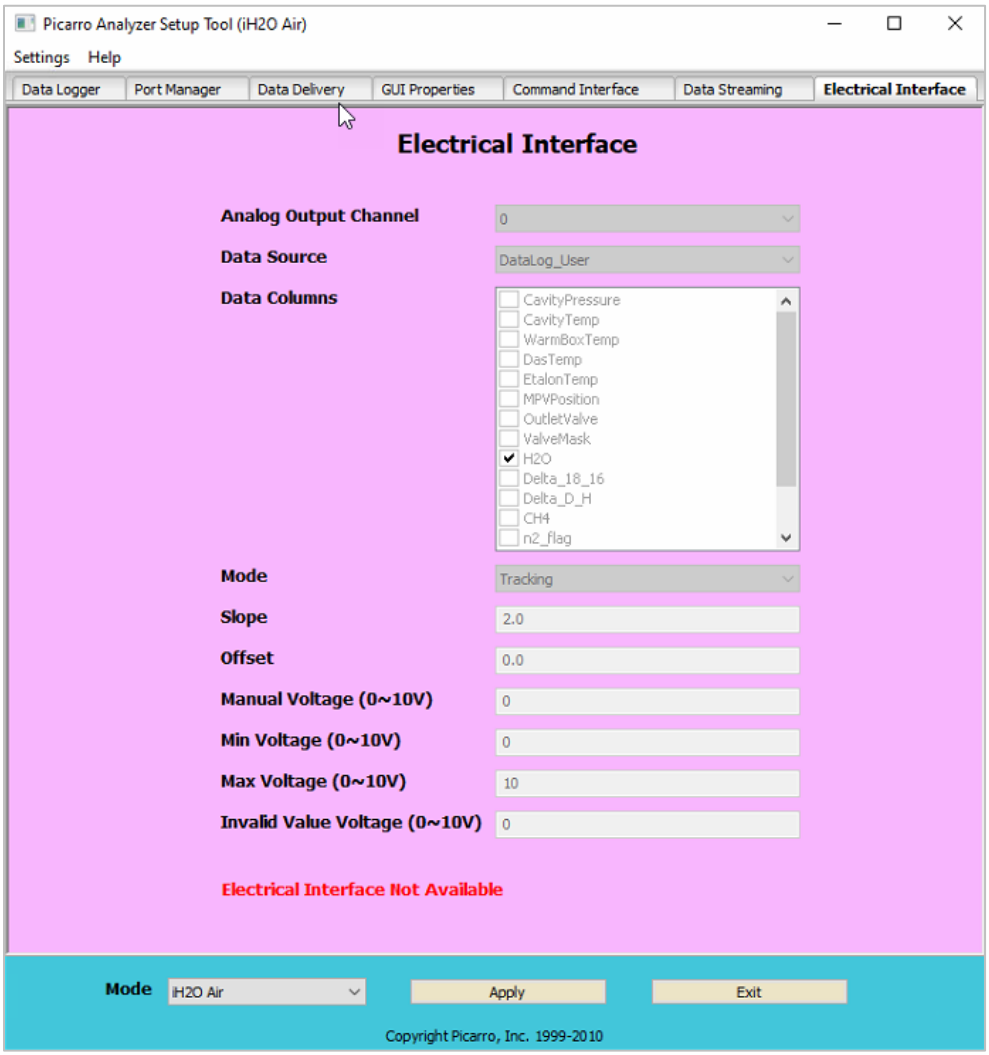


Figure 84: Electrical Interface Settings Window

A.2 Remote Data Access

Picarro Serial Communication

The analyzer supports an RS-232 physical command interface, which can be used to control the instrument and to retrieve concentration data. Not all features of the instrument are available on the serial interface.

For details on using the serial command interface, please see the Picarro analyzer ***Remote Interface Programming Guide***.

To Download:

1. Go to ***https://www.picarro.com/***.
2. Under the ***Support*** tab (near the home page upper-right corner), select ***Document Library***.

NOTE

Registration/Login Required: Access to online User Manuals is available to all registered Picarro customers with login credentials. If you do not yet have an account, please email us at support@picarro.com to request access to the document library.

3. When the Document Library page opens, enter the search terms, "*Remote Interface*" in the ***Search*** field.
4. In the results, click on the link titled "***Remote Interface Programming Guide 40-0063***" to open the manual in your browser. From there you can also download and save it to your PC.

This command set may also be used across a TCP/IP interface through an Ethernet connection. Please contact Picarro for further details if needed.

Remote Data Access

Using the *RemoteAccess.ini* file, the analyzer can be configured to automatically:

- Send data from the instrument to a list of e-mail accounts.
- Measure the offset of the host computer system clock from a set of Internet time servers and (optionally) to resynchronize the clock based on this information.

The Internet connection need not be permanent and may be a dial-up connection accessible via a user-supplied USB modem. The task of sending data and/or synchronizing the clock on the analyzer is performed using the *C:\Picarro\G2000\HostExe\RemoteAccess.exe* program. This program can be set up to run periodically using the Windows task scheduler at a user-configurable frequency. If a dial-up connection to the Internet is employed, it is used only on demand to minimize the connection time.

Each time that the *RemoteAccess.exe* program runs, it appends information to a log file, which keeps a record of the results of the time synchronization and of the files sent by e-mail. The RemoteAccess.exe program is configurable by means of an initialization file, which includes information such as the login credentials for the dial-up connection, the e-mail account, and the list of time servers.

The initialization file is:

C:\Picarro\G2000\AppConfig\Config\UtilitiesRemoteAccess\RemoteAccess.ini

It should be placed in the same directory as the executable *RemoteAccess.exe*. The file has one required section named **LOGGING** and optional sections named **NTP** and **EMAIL**. The logging section has a single key Logfile whose value is the path to the log file. Once this log file exceeds 64 Kbytes in length, it is backed up, appending a numeric extension to the file name, and a new file is opened. A total of ten backup log files are kept.

NTP

The NTP section controls querying the Internet time servers using the SNTP protocol (RFC4330) and the resetting of the clock on the host computer. If the section is not present, time synchronization is not carried out. The keys Server1, Server2, etc., are used to specify the URLs of the time servers. If the UpdateClock key is set to “true,” the offset is applied to the host clock. Otherwise, the offset is recorded, but the host clock is not changed.

Email

The EMAIL section controls the sending of the data files as e-mail attachments. If the section is not present, e-mail messages are not sent. The key Directory specifies the directory that contains the data files. When the program is run, files in this directory are sent to the specified recipients and the files are deleted. To avoid problems with incomplete files, programs that place files into this directory should do so using an atomic operation, such as a rename. The Server key is set to the name of an RFC2821- compliant SMTP server that sends the e-mail messages.

The From key is the e-mail address from which the messages are sent. Note that some SMTP servers check that the source is permitted to send email while others allow any name in this field. The collection of e-mail addresses to which copies of the e-mail is sent is specified by the keys To1, To2, etc. The Subject key is used to fill the subject field in the email header and may be set to any string. Depending on the SMTP server, it may be necessary to use authentication before e-mails can be sent, as described in RFC2554. If such authentication is not needed, the key UseAuthentication is set to false. If this key is set to true, two additional keys Username and Password must also be specified for the e-mail account.

APPENDIX B – Data File Viewer

B.1 Quick Start Guide

The following sections introduce the user to all functionalities of the Data File Viewer in detail. This section describes the most common, simple use case.

The Data File Viewer software allows the user to concatenate multiple one-hour files into one larger file, enabling the user to observe trends over several days of measurements.

1. To start, translate the UserData files from DAT to H5. The Batch Convert option (B) allows users to select any folder containing instrument data from a given day.

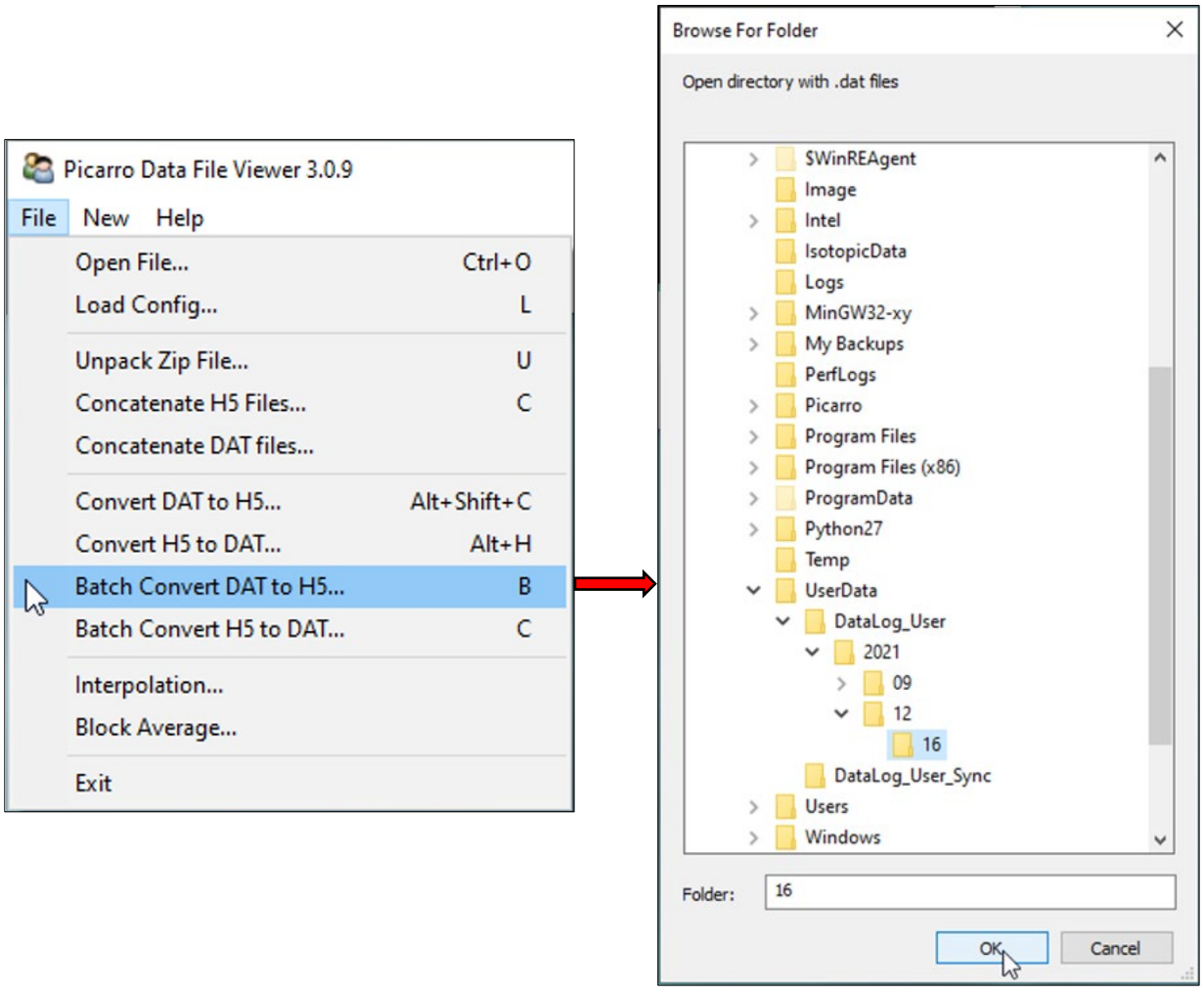


Figure 85: Batch Convert DAT to H5 – Navigation

2. In the source folder there are now copies of the original files translated into the H5 format.
3. From **File** menu select **Concatenate H5 Files** (C) to combine the H5 files into a time series. Take care to select exactly the same folder in the file viewer window.
4. In the Select Variables window, click **All** to move over all variables for concatenation. If concatenating very long records, the user can instead select only a few variables by clicking the variable name on the left dialogue, and clicking the double arrow button. Confirm by clicking **OK**. (Figure 86).

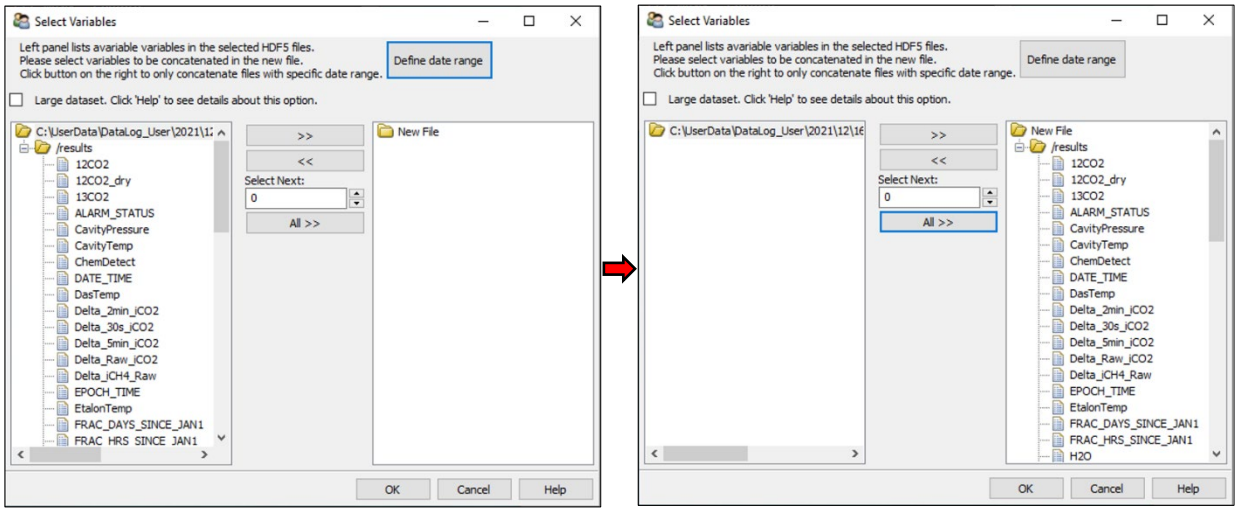


Figure 86: Selecting Variables for Concatenation

5. The user will then be asked to confirm the file name for the concatenated data. The default location will be in the parent folder for the selected day, and the filename will by default describe the time span of the measurements within. Successful concatenation will lead to the filename automatically being displayed in the main data file viewer window.

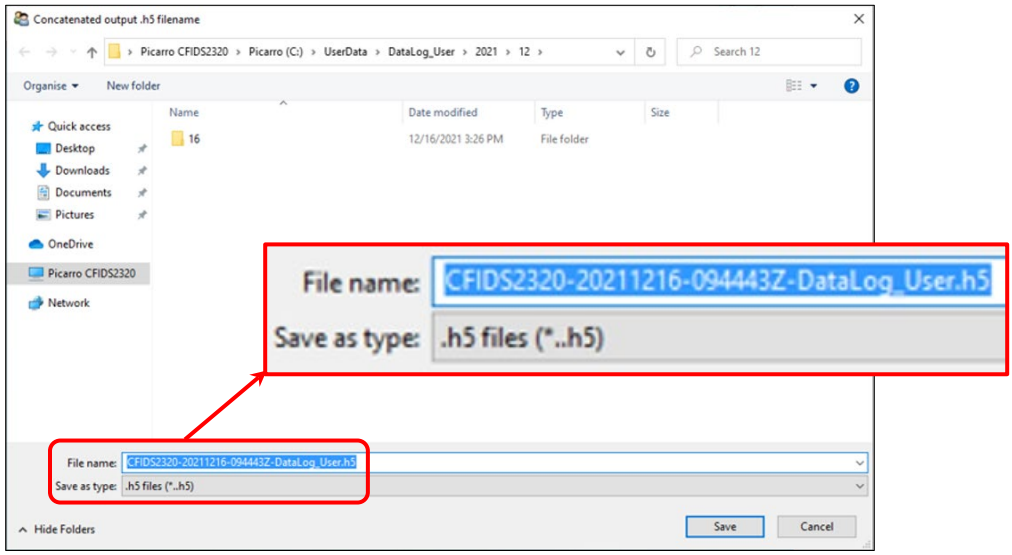


Figure 87: Concatenated Output .h5 Filename

NOTE

You can concatenate several days into one larger file, either by following steps 1-3 for selected folders, or by copying all their DAT files into a new folder and performing steps 1-5 just once.

6. With the file now opened, the user can select how many **Time Series** to display on the screen.

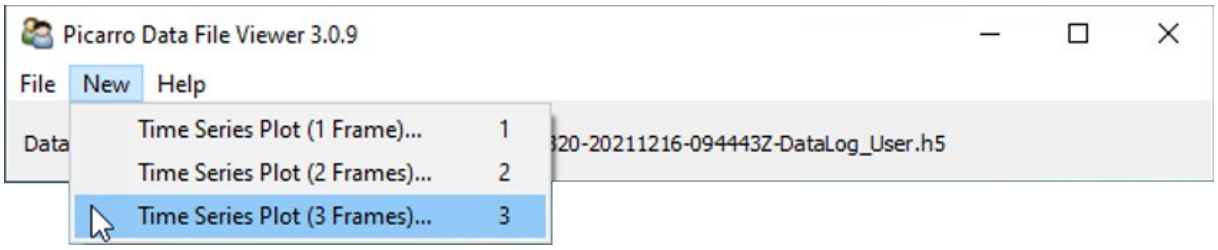


Figure 88: Time Series Selection Options

7. In the new window that appears, select the variables from the **Var Name** dropdown on the right of each plot. Deselect **Autoscale y** if the data stream has a large amount of variability in the Y-axis.
8. Please read the following sections to learn more about features of the Data File Viewer.

B.2 Data File Viewer Overview

The Picarro Data File Viewer software is located on the desktop of the Picarro instrument. The software allows the user to graph and to conduct statistical analysis of the raw data. Additional functions include Allan Variance plot and quadratic or polynomial fittings. The Picarro Data File Viewer includes two main menus: File and New (Figure 89).

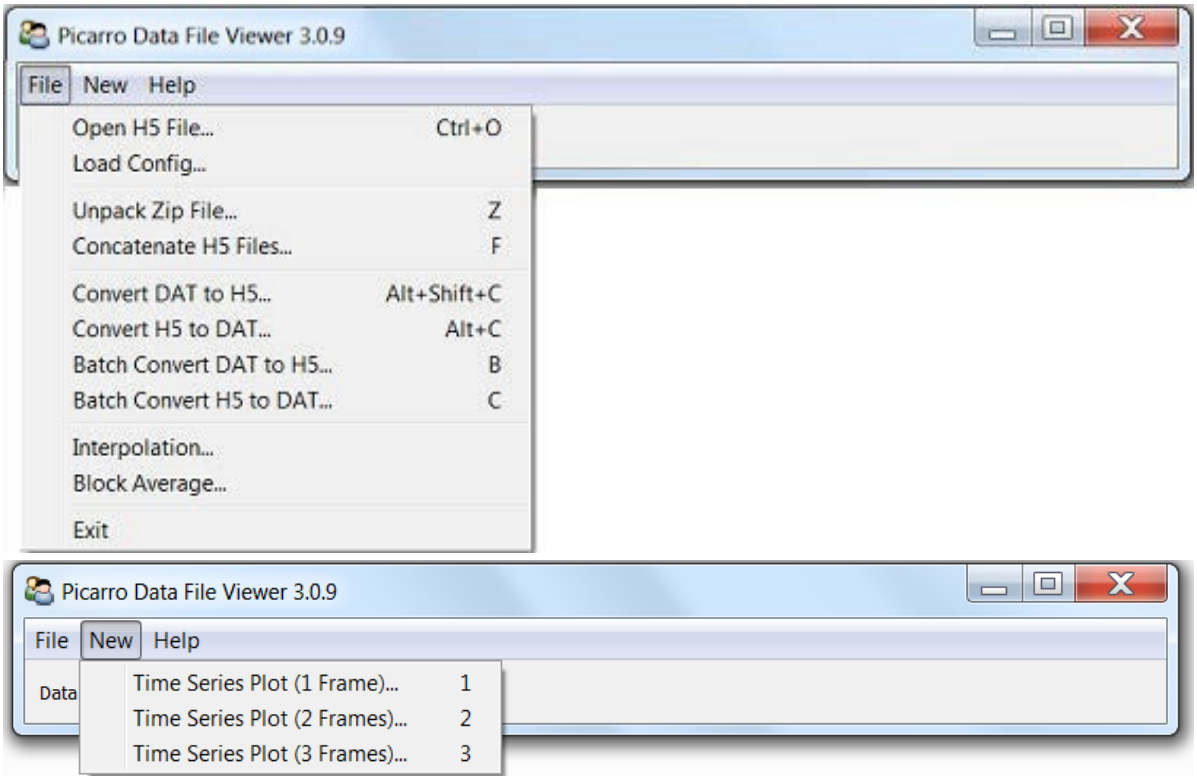


Figure 89: Picarro Data File Viewer – File and New Menus

B.3 File Menu

This section describes the functions available from the Data File Viewer File menu.

Open H5

File > Open H5 File: Opens a Picarro data file (HDF5 format) for data analysis and visualization. After opening the data file, you can create a new time series plot. Refer to section ***B.4, New – Time Series Plot*** for more information.

Load Config

File > Load Config: Loads a configuration file (ini format) to restore parameters of a workplace. Refer to ***Save Configuration*** on Page 165 for more information.

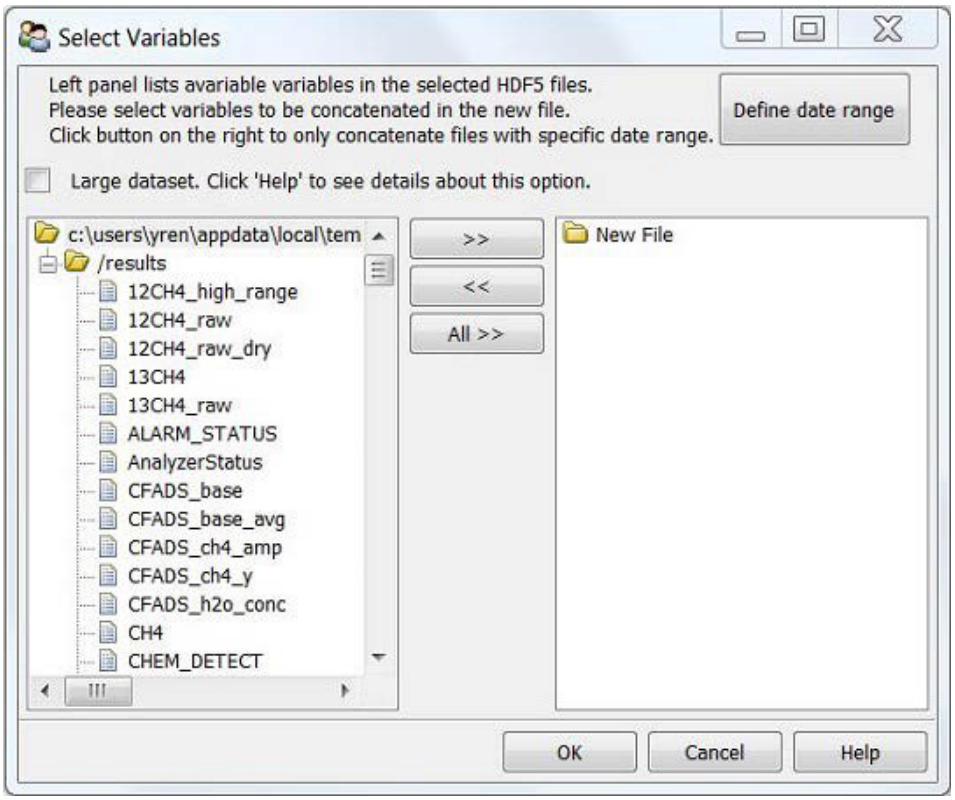
Unpack Zip File

File > Unpack Zip File: Use to concatenate all H5 files inside the zip file into a single H5 file. Refer to Concatenate H5 Files below for details.

Concatenate H5 Files

File > Concatenate H5 Files: Use to concatenate multiple files and zip archives of H5 files into a single H5 file. Navigate to the desired folder or use the **Define Date Range** button to specify a date range of files to concatenate. (See next section.)

After selecting the path of the data files, Data File Viewer will automatically search an H5 file in the specified zip/folder and look for all available variables in the H5 file. The variables are then listed in the ***Select Variables*** window in the left panel (as shown in Figure 90), and users can use the "**>>**" button to move variables to the right panel for concatenation.



Note: This screenshot is for example only. The species selections shown on your analyzer may vary.

Figure 90: Select Variables Form

Define Date Range

Data File Viewer can search data files within the desired date range and then concatenate such files into an H5 file.

By default, TimeZone is set to your local time zone. However, if data were taken elsewhere, select the time zone where data were taken.

Select File > Concatenate H5 Files, then click **Define Date Range** to specify the desired date range as shown in Figure 91.

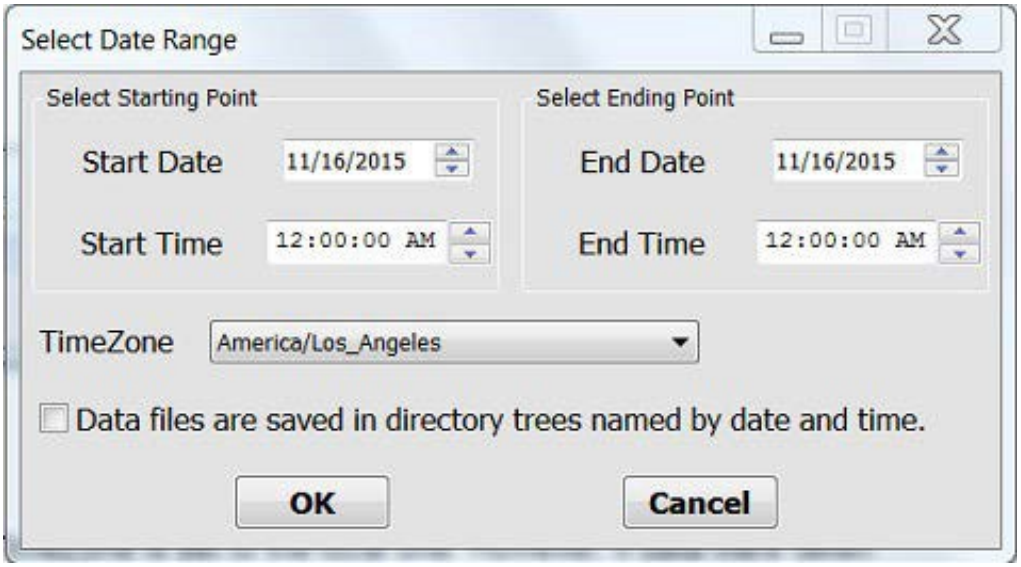


Figure 91: Define Date Range Dialog

Data files are saved in directory trees named by date and time option.

Picarro software saves data in a directory tree that is named by the creation year, month, and day as shown in Figure 91. Select this option if the target folder has this file structure. This way, Data File Viewer will only search folders within the desired date range, which can substantially reduce processing time.

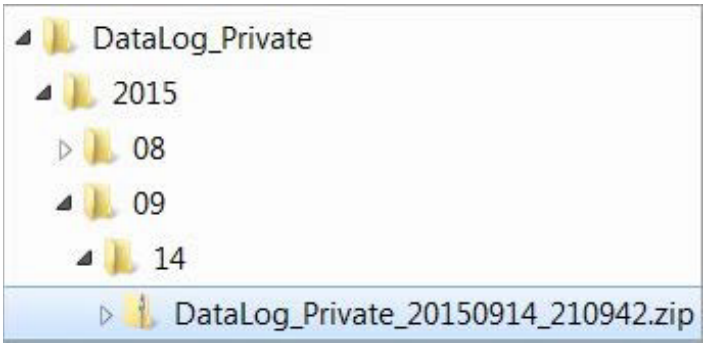


Figure 92: File Structure of Data File Viewer

NOTE

To save processing time, Data File Viewer does not open data files, but only determines data acquisition time based on the file name.

CAUTION

Do not define a time range for data files whose names have been changed.

NOTE

Data File Viewer does not concatenate data files exactly within the defined time range. This is because the time extracted from file name is different from the data acquisition time. To not miss data points, Data File Viewer expands the specified time range, so the resulting dataset normally has a wider time range than the user specification.

Convert DAT to H5

Select File > Convert DAT to H5 to convert a file in DAT format to HDF5 format. These formats are described below:

- DAT format: DAT files accepted by DatViewer store tabular data (numbers and text) in plain text.
- Each line of the file is a data record. Each record consists of one or more fields separated by whitespaces.
- The first line of the data file indicates column names.
- There must be a field “EPOCH_TIME” to store the acquisition epoch time (expressed as seconds since Jan 1, 1970) of the data. Otherwise, the first and second fields must be “DATE” and “TIME.” The “DATE” field must have the format “mm/dd/yyyy” or “yyyy-mm-dd,” and the “TIME” field must have the format “HH:MM:SS(.sss)” where (.sss) is an optional fraction of seconds.
- **HDF5 Format:** HDF5 is a data model, library, and file format for storing and managing data. (See the HDF5 Home Page on the HDF Group website https://www.hdfgroup.org/ for more information.) When converting DAT to HDF5 format, Data File Viewer creates a table named “results” to the contained data.

Convert H5 to DAT

Select **File > Convert H5 to DAT** to convert a file in a HDF5 format to DAT. These formats are described in Convert DAT to H5.

NOTE

Data File Viewer does not concatenate data files exactly within the defined time range. This is because the time extracted from file name is different from the data acquisition time. To not miss data points, Data File Viewer expands the specified time range.

Interpolation

Interpolation describes the method for constructing data points with a range of a discrete set of known data points. Select **File > Interpolation** to perform interpolation on a time grid with a constant interval.

Block Average

Select File > Block Average to divide a dataset into small blocks based on a user-defined block size. The average is calculated for data in each block, and the results are saved in a new H5 file.

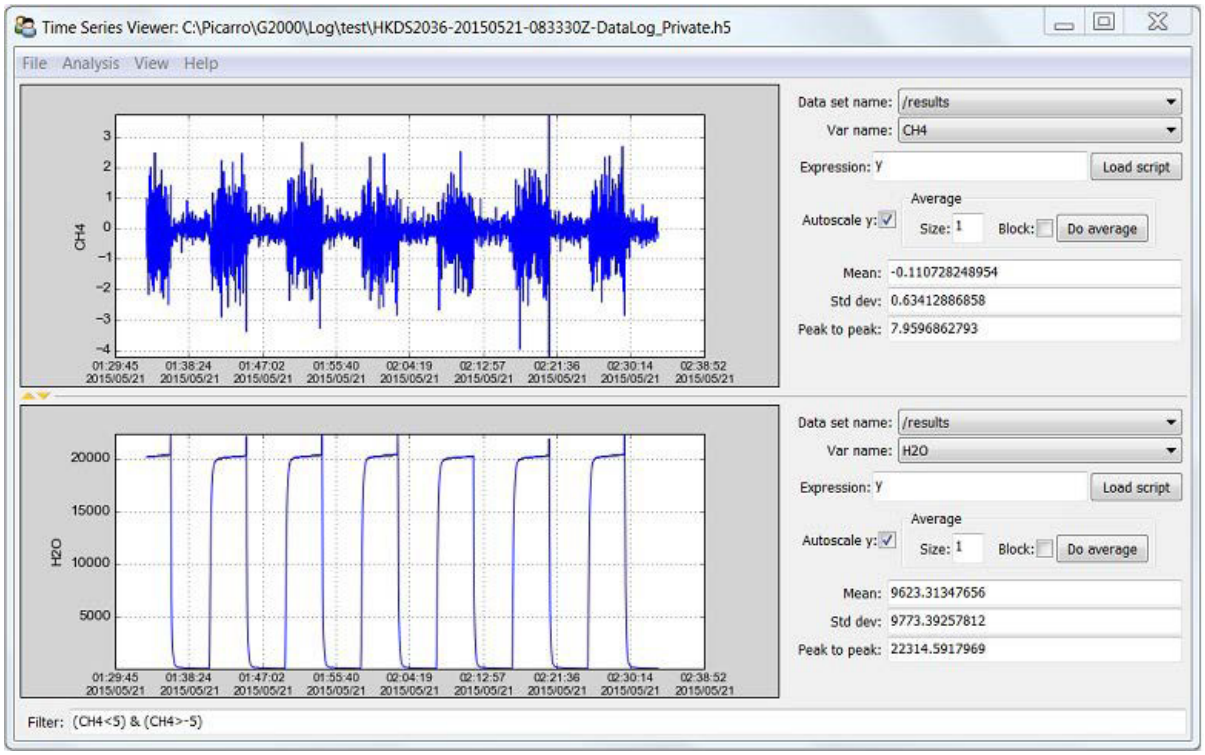
NOTE

The specified block size must be greater than the average data interval.

Because the data interval is normally not a constant (unless interpolation is performed), fluctuations in the data interval will affect block averaging if the block size is comparable to the average data interval.

B.4 Time Series Plot

You can create a time-series plots with one, two, or three frames. The additional plots display in the Time Series Viewer.



Note: This screenshot is for example only. The species shown on your analyzer may vary.

Figure 93: Time Series Viewer

The next section describes the options available on the *Time Series Viewer* menu bar. Refer to The Time Series Viewer Canvas on Page 89 for more information on the Time Series Viewer UI features and options.

B.5 Time Series Viewer Menus

The Time Series Viewer form includes the following menus:

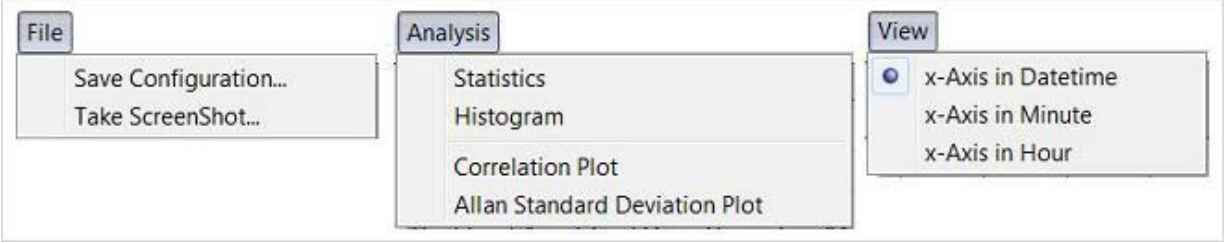


Figure 94: Time Series Viewer Menus

Time Series Viewer File Menu

Use the **File** menu to save a configuration or take a screenshot.

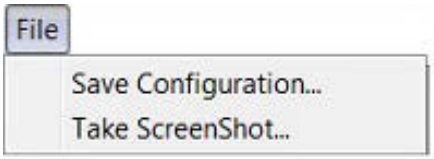


Figure 95: Time Series Viewer – File Menu

Save Configuration

Click **File > Save Configuration** to open the **Feature Capture** form. With this form, you can save figure properties, expressions, filters, and other settings to a configuration file so that it can be easily loaded in the future.

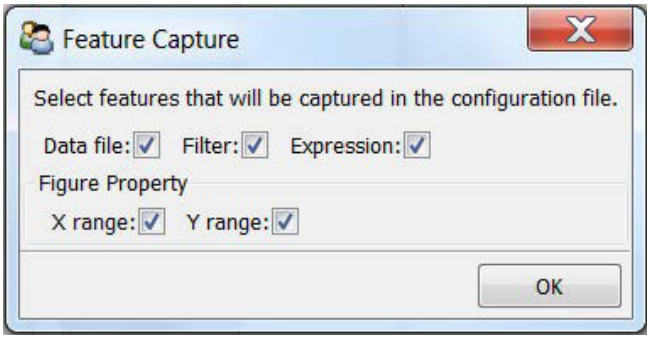


Figure 96: Time Series Viewer – Feature Capture

CAUTION

If a feature is not captured, it will be omitted when the configuration file is loaded.

Depending on the features captured, loading a configuration file can have different effects. For example:

- If all features are captured, a saved workplace is reproduced.
- If Data file is not captured, saved parameters will be applied to the data file in memory.
- If Expression is not captured, plots will not be transformed.
- If X (Y) range is not captured, figures will be auto-scaled on the x (y) axis.

Take Screenshot

Use **File > Take ScreenShot** to take a screenshot of the Time Series Viewer and save it as a .png to a specified file.

Time Series Viewer Analysis Menu

Use the Analysis menu to calculate statistics, generate a histogram, and to plot correlations and Allan Standard deviations.

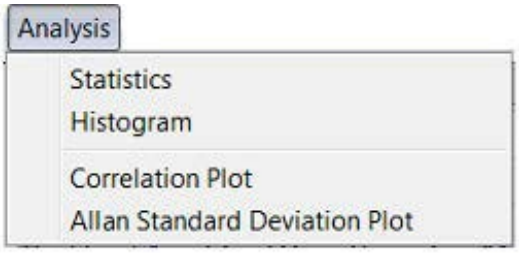


Figure 97: Time Series Viewer – Analysis Menu

Statistics

Use **Analysis > Statistics** to calculate mean, standard deviation, and peak to peak for all plots in the current window.

Histogram

Use **Analysis > Histogram** to generate a histogram of data as shown in Figure 98 below.

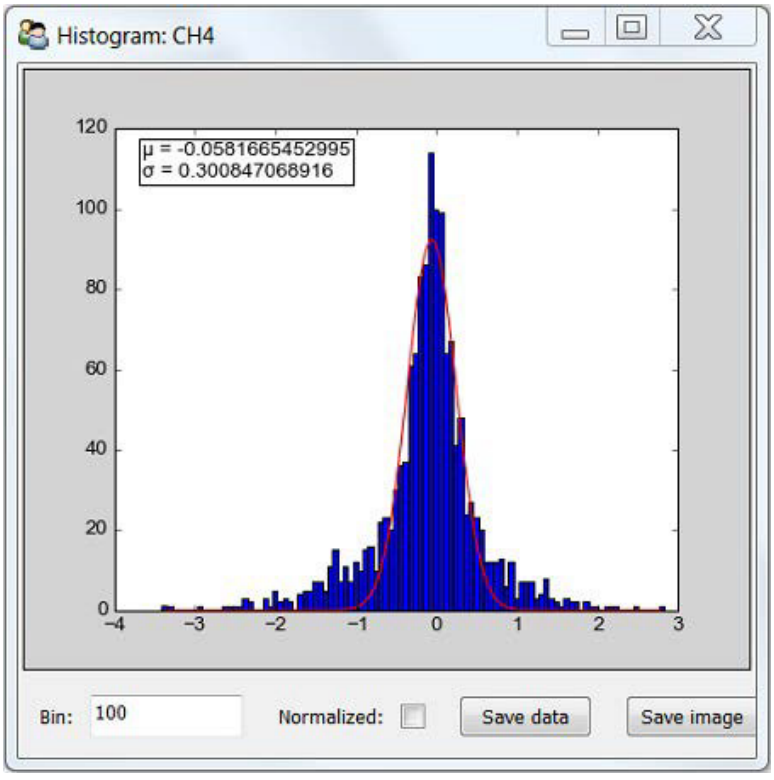


Figure 98: Histogram Window – CH4

Histogram Window Features

- **Red Line:** A Gaussian function fitted to the histogram. Fitting results of μ and σ are shown in the top-left corner of the plot.
- **Bin:** Specifies the number of intervals that the range of values is divided into.
- **Normalized:** When selected, the sum of the histograms is normalized to 1.
- **Save data:** Saves histogram data to a CSV file.
- **Save image:** Saves the histogram image as a JPEG/PNG/PDF file.

Correlation Plot

Use **Analysis > Correlation Plot** to plot Y-axis data in one frame versus that in the other. This can be used when two or more frames exist in the current Time Series Plot window. See the section, ***Correlation Plot*** on Page 167 for details.

Allan Standard Deviation Plot

Use **Analysis > Allan Standard Deviation Plot** to create an Allan Standard Deviation plot (versus a standard deviation plot) for data in the current window. See Allan Variance Wikipedia page for more information.

Time Series Viewer View Menu

Use the View menu to view X-axis information in date-time, minute, or hour format.

Figure 99: Time Series Viewer – View Menu

NOTE

When switching from Datetime to Minute or Hour, the X-axis data is subtracted from the earliest point shown in the panel and then converted to the desired unit.

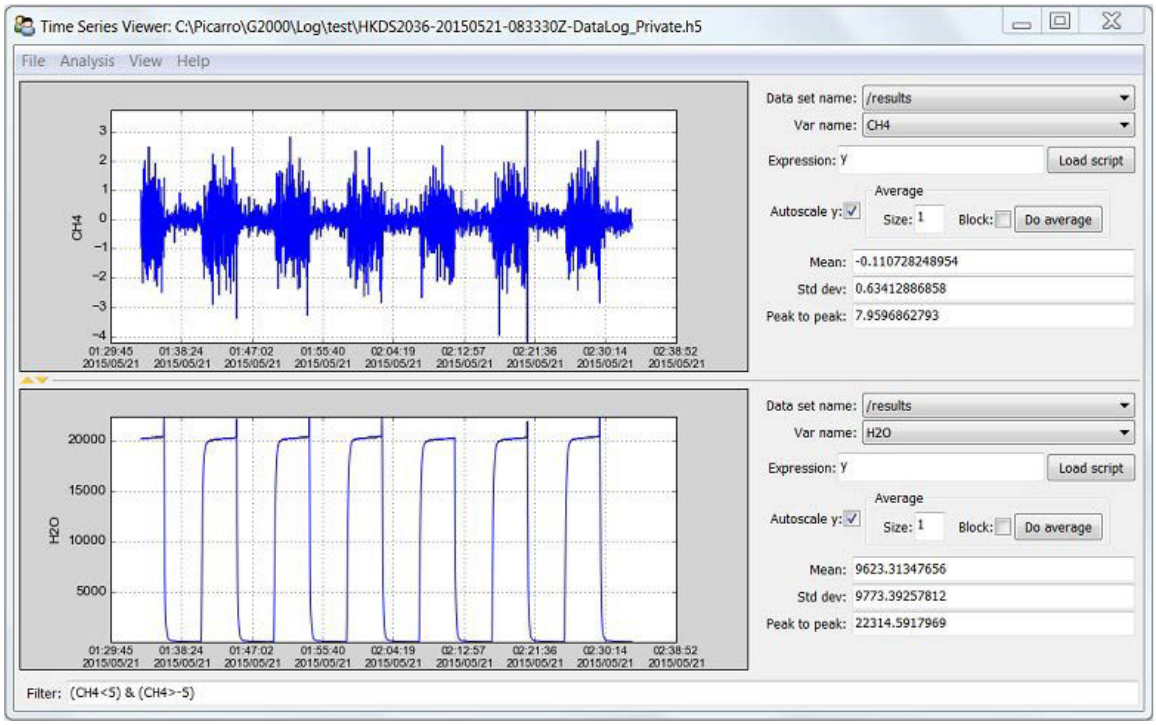
The Time Series Viewer Canvas

The Time Series Viewer canvas (Figure 100 below) is comprised of interactive graphs and a variety of configuration options.

Mouse Options and Graph Transform

The following mouse actions can be used in the canvas graphs:

- Left click and drag: Zooms into the selected area of the plot.
- Left click and drag with the SHIFT key down: Pans the plot.
- Left click and drag with CTRL key down: Zooms out from the plot.
- Left click and drag with ALT key down: Stretches the plot.
- Right-click: Opens an additional menu. Refer to the Right-click Menu below in the next section.



Note: this screenshot is for example only. The species shown on your analyzer may vary.

Figure 100: Time Series Viewer Canvas

Right-click Menu

Right-clicking on the canvas opens a pop-up menu:

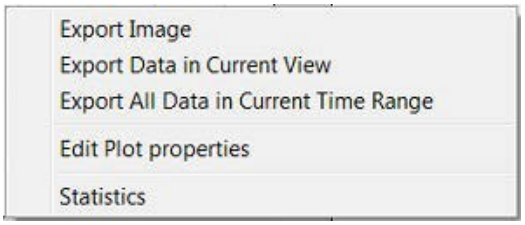


Figure 101: Canvas Right-click Pop-up Menu

Export Image: Exports the current plot as a jpeg, png, or pdf file.

Export Data in Current View: Exports only date/time and the selected variable in the current view to an HDF5 or CSV file.

Export All Data in Current Time Range: Exports all variable columns of the selected dataset in the current time range to an HDF5 file. Refer to Concatenate H5 Files on Page 81 for more information.

Edit Plot properties: Opens the **Image Editor form** (Figure 102 below), where the following options can be specified.

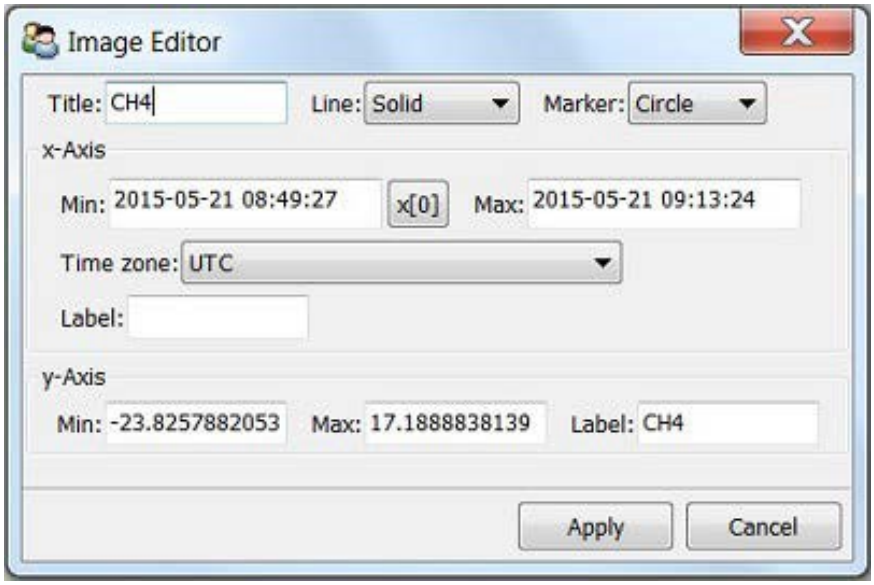


Figure 102: Image Editor Form

Image Editor Form Options:

- **Title:** Edits the title of the plot.
- **Line:** Specifies the line pattern of the plot. If None is selected, the data points will be plotted without connecting lines.
- **Marker:** Specifies the marker type to indicate data points. If None is selected, data points will not be shown.
- **x-Axis: Min and Max:** Specifies the minimum and maximum of date range for the X-axis.
- **x[0]:** Sets the earliest time of the dataset as the minimum of the X-axis.
- **Time zone:** Sets the time zone for date/time variables. This defaults to the local time zone.
- **Label:** Specify labels for the X-axis and the Y-axis.
- **y-Axis: Min and Max:** Specifies the minimum and maximum of data displayed on the Y-axis.

Dataset Name and Var Name

An HDF5 file can store one or more tables. Each of these tables is called a Dataset. A table can contain one or more columns. Each column is called a variable (Var).

Use the **Dataset name** drop down (Figure 103) to select the dataset that will be used for this time series graph. Use the **Var name** drop down to select the column in the dataset to use in the graph.

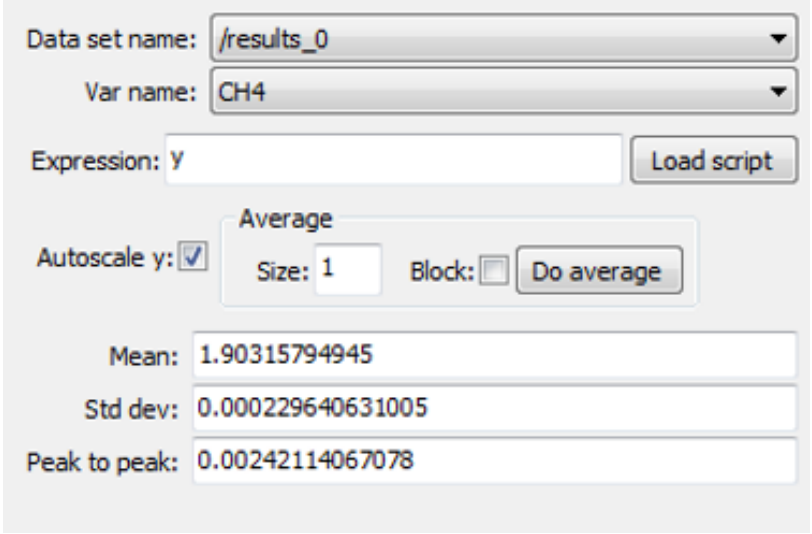


Figure 103: Time Series Viewer Dataset Options

Autoscale Y

When the **Autoscale Y** option is selected, the Time Series Viewer will autoscale on the Y-axis to make sure that all data within the range of the X axis is displayed. This feature can make it hard to see small signals when large signals blow the Y axis out, so it is often advisable to deselect this checkbox for dynamic or spikey datasets.

Average

If **Block** is selected, a block average is calculated when you click the **Do average** button. Otherwise, a moving average is calculated.

For a block average, **Size** specifies block size in unit of a minute. For a moving average, **Size** specifies subset size in unit of data points.

REMINDER

Averaging is performed after the Filter and Expression are performed.

Mean, Std Dev, and Peak to Peak

The **Mean, Std dev** (Standard deviation) and **Peak to peak** fields (Figure 103) provide all the statistical information of data in the current view.

Correlation/XY Plot

The Correlation/XY Plot window (Figure 104) includes two menu items: File and Analysis. For details about the File menu, see ***Save Configuration*** on page 165.

REMINDER

The canvas in this plot is interactive. For details about the plot canvas, see *The Time Series Viewer Canvas* on Page 167.

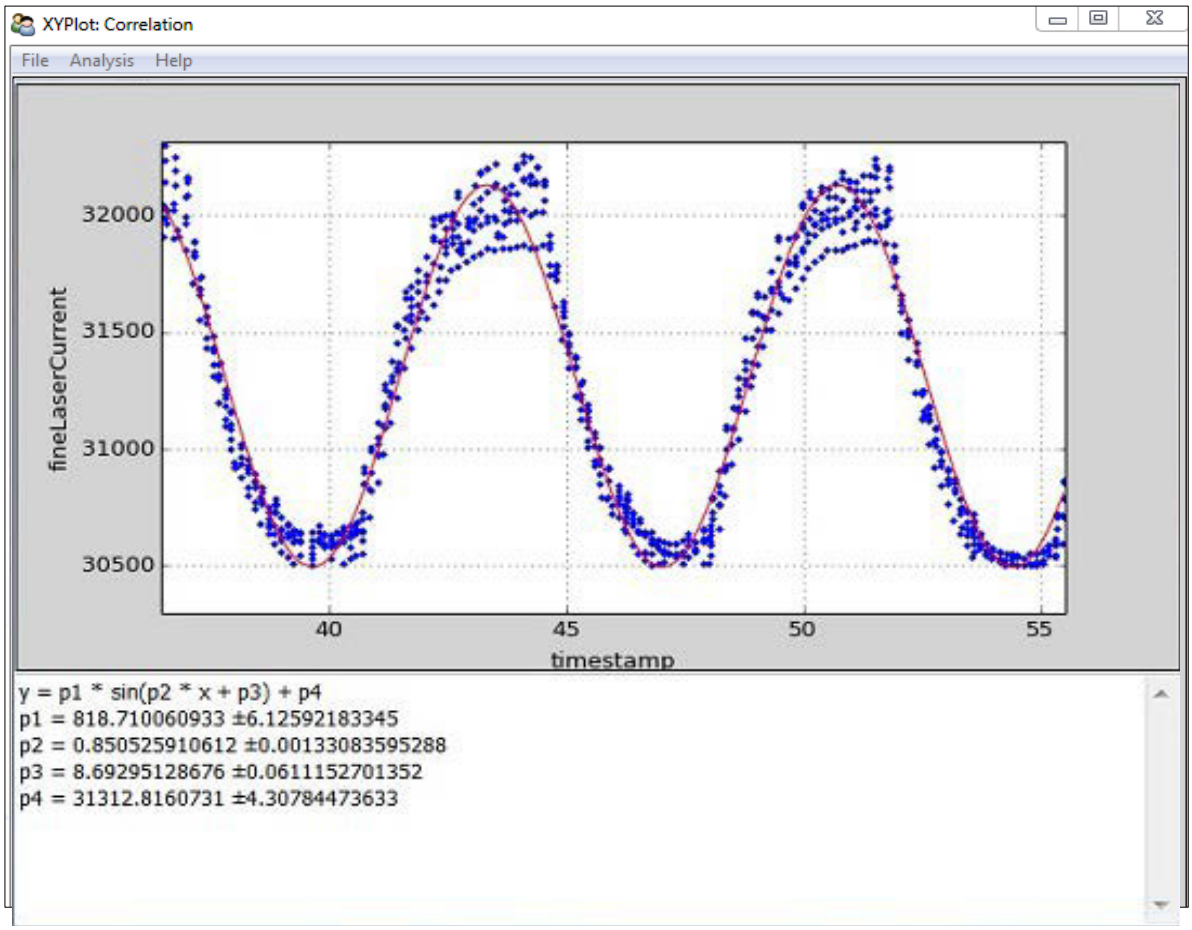


Figure 104: Correlation XY Plot

Analysis Menu

The Analysis Menu (Figure 105) includes three options: **Fitting, Integration**, and **Statistics.**

Fitting allows you to specify one of four fitting methods to include in the Correlation/XY plot:

1. **Linear fit:** Specifies to fit to linear function:

   y = c1x + c0

2. **Quadratic fit:** Specifies to fit to quadratic function:

   y = c2x2 + c1x + c0

3. **Polynomial fit:** Specifies to fit polynomial function of degree n:

   y = Σcnxn

4. **Curve fit:** Specifies to use non-linear least squares to fit an arbitrary function to data.

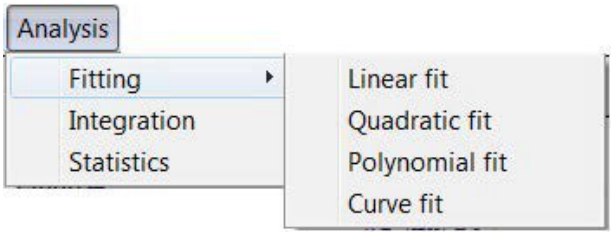


Figure 105: Analysis Menu

Integration calculates area under the curve using the composite trapezoidal rule.

Statistics calculates mean, standard deviation, and peak to peak for data in the current view.

After applying any of the above Analysis options, the results, statistics, or fitting function with coefficients are displayed in the lower portion of the Correlation Plot window (Figure 106).

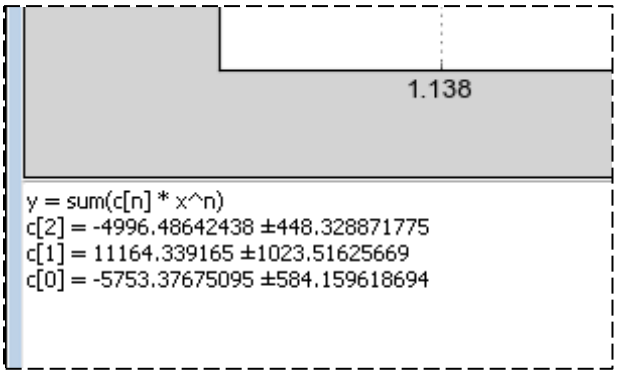


Figure 106: Results of Quadratic Fitting

APPENDIX C – Introduction to CRDS Technology

Picarro analyzers use time-based, optical absorption spectroscopy of the target gases to determine concentration in a sample. They are based on wavelength-scanned cavity ring-down spectroscopy (WS-CRDS), a technology in which light travels many times through the sample, creating a very long effective path length for the light to interact with the target gas, thus enabling excellent detection sensitivity in a compact and rugged instrument.

The Picarro analyzer is comprised of two modules:

- The analyzer contains the spectrometer, sample chamber, and a computer with a hard drive to store and analyze data. The single analyzer module controls the operation of the system and converts spectroscopic measurements into gas concentration data.
- The External Vacuum Pump draws the sample gas through the instrument.

C.1 Cavity Ring-Down Spectroscopy (CRDS)

Nearly every small gas-phase molecule (e.g., CO_2, H_2O, H_2S, NH_3) uniquely absorbs specific wavelengths of near-infrared light. The strength of the light absorption is related to the concentration of a molecule in a sample and the distance that light travels through the sample, called the path length.

Conventional infrared spectrometers are typically only sensitive enough to detect trace gases at levels in the part-per-million. Cavity Ring-Down Spectroscopy (CRDS), on the other hand, is one thousand to one million more times sensitive.

The increased sensitivity of CRDS is due to the design of the sample cavity and the time-based measurement. In the cavity, a series of mirrors reflects the infrared light through the sample, increasing the path length. For a Picarro cavity of only 25 cm in length, the effective path length of the cavity can be over 20 kilometers.

In Picarro analyzers, light from a single-frequency laser enters a cavity where three mirrors reflect the laser light as seen in Figure 111. The light enters through the mirror closest to the laser, bounces off the angled mirror in the lower right corner of the cavity, travels to the hemispherical mirror at the top of the cavity, bounces toward the mirror in the lower left corner of the cavity, and then returns to the first mirror. This motion becomes a continuous traveling light wave, which is represented by the dark orange path in Figure 111.

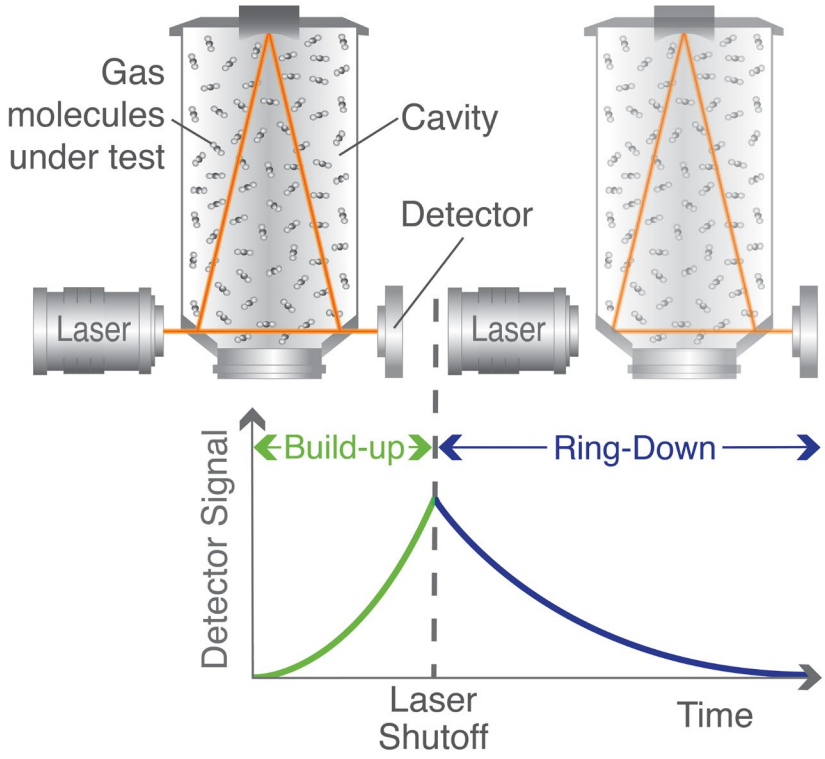


Figure 107: Schematic of Picarro CRDS Analyzer Cavity

When the laser is on, the cavity quickly fills with laser light. A small amount of the laser light is transmitted through the mirror closest to the photodetector, which turns the incident light into a signal that is directly proportional to the light intensity in the cavity.

When the photodetector signal reaches a threshold level (in a few tens of microseconds), the laser is turned off. The light contained within the cavity continues to bounce between the mirrors (about 40,000 times). Since the mirrors have slightly less than 100% reflectivity (99.999%), the light inside the cavity steadily leaks out of the cavity. The intensity of the light reaching the detector decreases, falling exponentially until it reaches zero. This decay, or “ring-down,” is measured in real time by the photodetector.

C.2 Relating Ring-Down Time to Absorption Intensity

The time it takes to ring-down is inversely related to the total optical loss in the cavity, including the strength of molecular absorption at a given wavelength of light. For an empty cavity, the time it takes for the intensity to decrease by a given percent is determined solely by the reflectivity of the mirrors. A cavity containing gas that absorbs light will have a shorter ring-down time than an empty cavity. As

the light circulates in a cavity with a gas sample, the molecular absorption by the gas results in a decrease of the light intensity.

Determining absorption intensity at a specific wavelength requires comparing the ring-down time of an empty cavity to the ring-down time of a cavity that contains gas (Figure 112). A cavity can be empty if it contains no gas; it will also appear empty if the molecules of the sample inside the cavity do not interact with the specific wavelength of light.

Picarro instruments gather measurements from an “empty” cavity by switching the light to wavelengths that are not absorbed by the target molecules. The analyzer subsequently measures ring-down times at wavelengths that are absorbed by the target gas. The analyzer automatically and continuously compares these two types of ring-down times, and the software uses those comparisons to calculate absorption intensities.

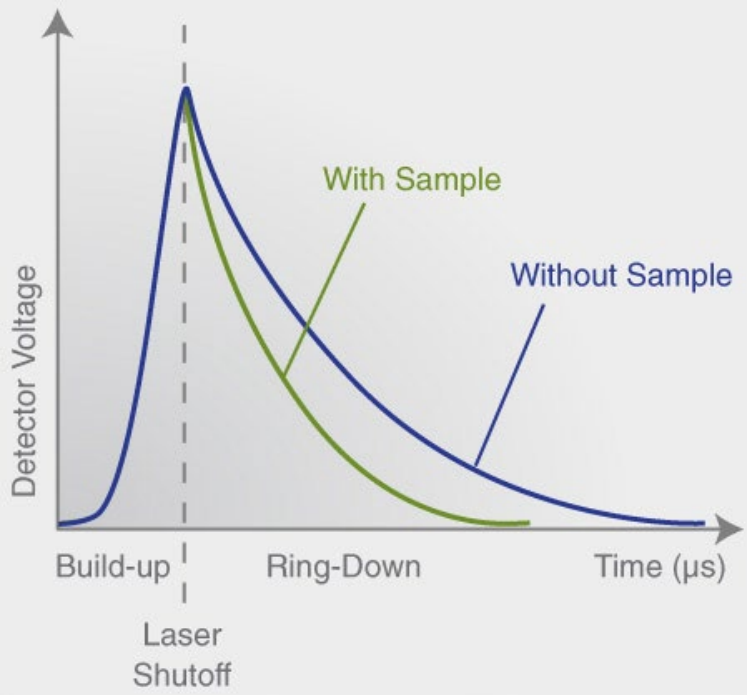


Figure 108: Light Intensity as Function of Time in CRDS System

C.3 Converting Absorption Intensity to Concentration

Plotting the absorbance at each measured wavelength generates an optical spectrum. This spectrum contains absorbance peaks that are unique to each molecule in the sample. The height of a particular absorption peak is proportional to the concentration of a molecule that generated the signal.

The height of the peak is calculated by subtracting the maximal absorbance from the baseline absorbance. Figure 73 shows a plot of ideal optical spectra with a clean, uniform baseline on either side of the absorption peak.

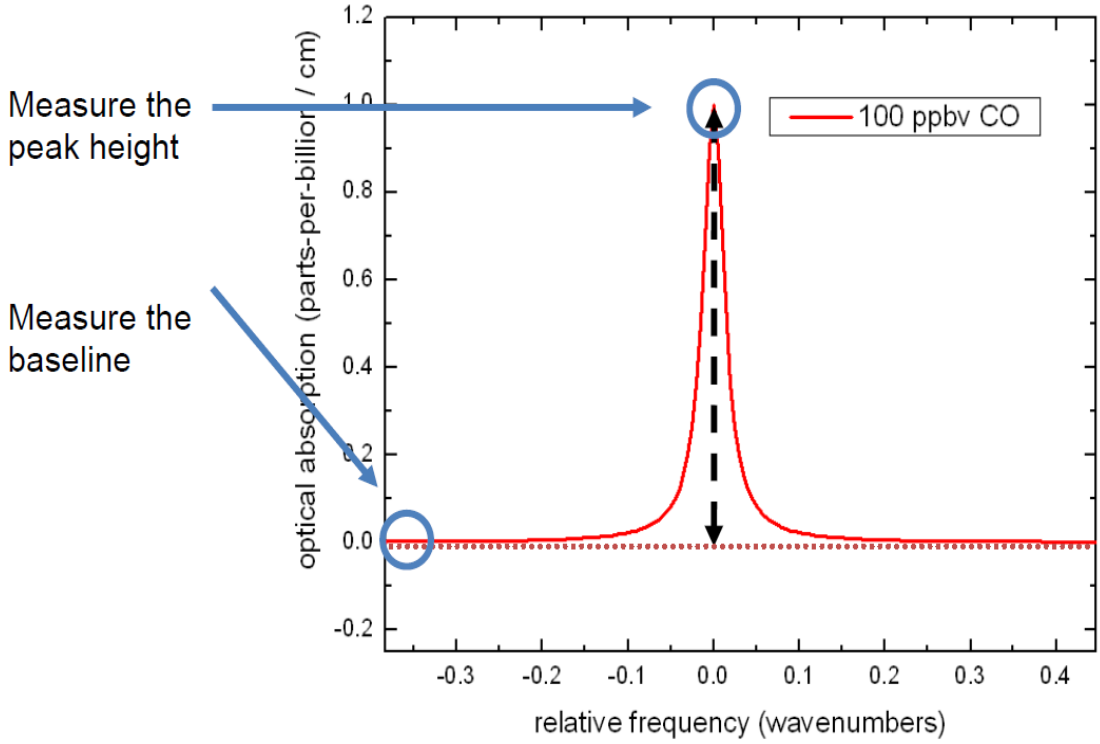


Figure 109: Absorption Spectral Curve

However, optical spectra often contain several absorption lines, nested closely together. A particular absorption peak may be visible between lines, but the absorption may not return to the baseline before it rises in response to another molecule.

Picarro analyzers calculate the baseline underneath a poorly resolved peak by modeling the absorption peaks from other surrounding molecules and subtracting contributions from neighboring peaks to the absorption intensity.

C.4 Spectral Precision and High Sensitivity Measurements

Picarro analyzers contain two features that provide high spectral precision:

- A proprietary wavelength monitor (WLM) that measures the absolute laser wavelength to a precision that is a few orders of magnitude narrower than the spectral linewidth: Picarro's patented WLM measures absolute laser wavelength to a precision more than 1,000 times narrower than the observed Doppler-broadened linewidth for small gas-phase molecules.

The instruments lock the laser to the WLM, and then the monitor tunes to wavelengths known to be maximally and minimally absorbed by the target molecule. The result is closely clustered absorption intensities, measured at wavelengths just before peak absorption, at peak absorption, and just after peak absorption, as the absorbance returns to the baseline.

- Precise temperature and pressure control in the sample cavity: Accurate absorption measurements at precisely known wavelengths account for little unless the temperature and pressure of the CRDS measurement cavity are known. The observed line intensity and shape depend on the temperature and pressure inside the sample cavity. Small temperature and pressure instabilities can result in large concentration errors due to fluctuating peak heights and baselines. To completely minimize instrument measurement drift, temperature and pressure must be actively stabilized to constant values.

For precise temperature control, the sample cavity is surrounded by layers of thermally insulating material to provide a high degree of passive thermal stability. The cavity is further actively stabilized by means of a solid-state heating system locked to the output of a thermal sensor. This enables the temperature of the cavity to be within 20 mK of the set temperature.

For precise pressure control, the cavity pressure is monitored using a high-linearity pressure transducer. The system computer uses this pressure data in a feedback loop to control proportional valves that adjust the inlet and outlet gas flow of the cavity.

APPENDIX D – Limited Warranty

Picarro, Inc. warrants its Products to be free from defects in material and workmanship and to perform in the manner and under the conditions specified in the Product specifications for twelve (12) months from shipment.

This warranty is the only warranty made by Picarro with respect to its Products and no person is authorized to bind Picarro for any obligations or liabilities beyond this warranty in connection with its Products. This warranty is made to the original Purchaser only, is non-transferable and may only be modified or amended by a written instrument signed by a duly authorized officer of Picarro. Sub-systems manufactured by other firms, but integrated into Picarro Products, are covered by the original manufacturer's warranty and Picarro makes no warranty, express or implied, regarding such sub-systems. Products or parts thereof which are replaced or repaired under this warranty are warranted only for the remaining, un-expired portion of the original warranty period applicable to the specific Product replaced or repaired.

WARRANTY DISCLAIMER

THE FOREGOING WARRANTY IS EXCLUSIVE AND IN LIEU OF ALL OTHER WARRANTIES WHETHER WRITTEN, ORAL, OR IMPLIED, AND SHALL BE THE PURCHASER'S SOLE REMEDY AND PICARRO'S SOLE LIABILITY IN CONTRACT OR OTHERWISE FOR THE PRODUCT. PICARRO EXPRESSLY DISCLAIMS ANY WARRANTY OF MERCHANTABILITY OR FITNESS FOR A PARTICULAR PURPOSE.

The Purchaser's exclusive remedy with respect to any defective Product shall be to have Picarro repair or replace such defective Product or credit the Purchaser's account, whichever Picarro may elect in its sole discretion. If it is found that any Product has been returned which is not defective, the Purchaser will be notified, and such Product returned at the Purchaser's expense. In addition, a charge for testing and examination may, at Picarro's sole discretion, be made on any Product so returned.

These remedies are available only if: **1)** Picarro is notified in writing by the Purchaser promptly upon discovery of a Product defect, and in any event within the warranty period; **2)** Picarro's examination of such Product discloses to Picarro's satisfaction that such defects actually exist and the Product has not been repaired, worked on, altered by persons not authorized by Picarro, subject to misuse, negligence or accident, or connected, installed, used or adjusted otherwise than in accordance with the instructions furnished by Picarro.

The following warranty conditions shall apply to all Picarro, Inc. products unless amended by a written instrument signed by a duly authorized officer of Picarro:

ADJUSTMENT – No electrical, mechanical, or optical adjustments to the product(s) are permitted.

PARTS AND LABOR - New or factory-built replacements for defective parts will be supplied for twelve (12) months from date of shipment of the product. Replacement parts are warranted for the remaining portion of the original warranty period. There will be no

charge for repair of products under warranty where the repair work is done by Picarro, Inc.

NOT COVERED BY THE WARRANTY – Damage to any optical surface from improper handling or cleaning procedures. This applies specifically to those items subjected to excess laser radiation, contaminated environments, extreme temperature, or abrasive cleaning. Damage due to ESD, abuse, misuse, improper installation or application, alteration, accident, negligence in use, improper storage, transportation, or handling. No warranty shall apply where the original equipment identifications have been removed, defaced, altered or where there is any evidence of alterations, adjustments, removal of protective outer enclosure, any attempt to repair the product by unauthorized personnel or with parts other than those provided by Picarro, Inc.

DAMAGE IN SHIPMENT - Your analyzer should be inspected and tested as soon as it is received. The product is packaged for safe delivery. If the product is damaged in any way, you should immediately file a claim with the carrier or, if insured separately, with the insurance company. Picarro, Inc. will not be responsible for damage sustained in shipment. All Picarro products are F.O.B. origin, shipped from the Picarro factory or Picarro distributor. The price of all Products, unless otherwise specifically stated, is Ex-Works, Sunnyvale, CA as defined by Incoterms, 2020. The cost of normal packaging for shipment is included in the invoiced price. Where Buyer specifies special packaging, a charge will be made to cover any extra expense.

CLAIMS ASSISTANCE - Call Picarro, Inc. Customer Service or your local distributor for assistance. Give our representative the full details of the problem. Helpful information or shipping instructions will be provided. If requested, estimates of the charges for non-warranty or other service work will be supplied before work begins.

RETURN PROCEDURE - Customers must obtain a Return Merchandise Authorization Number from Picarro, Inc. prior to returning units. Products being returned for repair must be shipped in their original shipping cartons to avoid damage.

About Picarro

Picarro is a leading provider of solutions to measure greenhouse gas (GHG) concentrations, trace gases, and stable isotopes across many scientific applications, along with the energy and utilities markets. Our patented Cavity Ring-Down Spectroscopy (CRDS) is at the heart of all Picarro instruments and solutions, enabling the detection of target molecules at part per billion or better resolution.

Product Support

Utilize Picarro support resources for product support. Join the Picarro community to ask questions and get answers, search the document library for datasheets and user manuals, download software, and purchase products and replacement parts.

Access to online User Manuals is available to all registered Picarro customers with login credentials. If you do not yet have an account, please email us at support@picarro.com to request access. Note must be a registered user and logged in to access the following resources:

- Picarro Document Library
- Picarro Community (Forums)
- Picarro Software Downloads
- Picarro Literature (Scientific Resources)
- Picarro Web Store

Contact Picarro for questions regarding specific applications and additional information.

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