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A0314 Small Sample Introduction Module 2 (SSIM2) User Manual



Picarro Inc. 3105 Patrick Henry Drive Santa Clara, CA 95054, USA Phone: +1 408 962 3944 www.picarro.com Document Number 40037 Revision I Copyright © 2024 Picarro, Inc. All rights reserved.

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1. Introduction

This manual is written for operators, service technicians and maintenance technicians who install, operate, and maintain the A0314 Small Sample Introduction Module 2 (SSIM2). For repairs, or service, contact Picarro Customer Support or your local Picarro-authorized and certified representatives.

1.1 Intended Use

The Picarro A0314 Small Sample Introduction Module 2 (SSIM2) transforms certain Picarro continuously-sampling analyzers into instruments capable of measuring small, discrete gas samples that would be hard to measure in traditional "continuous flow" mode. The SSIM2 is an excellent solution for soil, headspace, plant, and other studies that provide gas samples in limited volumes or high concentrations.

The SSIM2 is designed to work primarily with Picarro isotopic carbon instruments. Under some circumstances, the SSIM2 is compatible with non-isotopic concentration analyzers also. For further information, on this compatibility, see APPENDIX A –Adapting Greenhouse Gas Analyzers for SSIM2 Use.

The SSIM2 automatically prepares and introduces the gas sample(s) to the Picarro analyzer and reports the results, performing the requested number of replicate analyses of each sample. See the schematic in Figure 1.

While the SSIM2 is not strictly the same as its predecessor, the SSIM, this manual uses SSIM2 and SSIM interchangeably to refer to the current SSIM2 build.

1.2 Other SSIM2 Features

The SSIM2 can be paired with the Picarro 16-Port Distribution Manifold (A0311) to enable it to automatically measure up to eight discrete samples.

The SSIM2 is designed primarily for isotopic ratio measurements, though it can be calibrated to provide accurate concentration measurements. The slight adjustment required to provide accurate concentrations stems from a small dilution caused by the tubing between the SSIM and instrument cavity, which cannot be fully evacuated of zero air before sample analysis, imposing roughly a 5% dilution of the sample concentration value. While the concentration value will read slightly low, the delta value for the isotopes should not be affected, as the diluent gas is zero air or N2.

For further information on dilution, refer to APPENDIX C –Dilution and Dilution Factors: Considerations and Calculations or to Picarro Application Note, Measuring Small Volume Gas Concentrations with the SSIM linked here: AN038. The SSIM2 uses a vacuum pump, zero air or N2, and a series of five valves to control the movement and evacuation of sample, calibrant, and zero air, to the CRDS or vacuum port. A full description of the flow diagram and valving can be found in APPENDIX B –Flow Diagram and Valve Sequences.



Figure 1: A0314 SSIM2 Schematic

1.3 HOW TO READ THIS MANUAL

We strongly recommend that users read through at least sections 1 to 5 as soon as they receive this manual to prepare for assembly or for an in-person install. Section 1: Introduction, gives a high-level overview, while section 2: Safety provides information on safety considerations associated with the SSIM2. Section 3: Unpacking lays out the contents of the shipping boxes, while section 4: Pre-Installation Requirements discusses materials like cylinders and regulators that are essential to operation of the system. Likewise, section 5: Syringe Sample Delivery Requirements discusses how to source and assemble syringe materials to ensure good repeatable injections. Without the materials discussed in these sections, users will not be able to get their SSIM2 up and running. Note that some materials, like specialty regulators, can take weeks or months to procure.

When you are ready to assemble the system, proceed to either to section 6.1: SSIM2 Setup with CRDS Analyzer Only, or section 6.2: SSIM2 Setup with CRDS Analyzer and A0311 16-Port Distribution Manifold as appropriate.

Section 7: Coordinators will briefly explain the different coordinator programs used to communicate with the SSIM2 (and A0311). Some users will want to proceed to section 13: Running the SSIM Leak Check to check that their SSIM2 is ready to be used.

Proceed to section 8: Operation: Measurement – SSIM2 and Analyzer or skip to section 9: Operation: Measurement – SSIM2 and 16-Port Manifold and Analyzer as appropriate, for instructions on operation of these peripherals. We recommend you practice these steps with samples filled from room air before continuing to research samples. Section 10: GUI Appearance During SSIM Runs provides guidance on what your injections should look like, and section 11: Outputted Files discusses the format and contents of the data and log files outputted by the SSIM2 Coordinator.

Users looking to better understand operation and accuracy of the SSIM2 should read the remaining sections 12: Calibration, and 14: Best Practices.

Users wishing to identify the cause of a problem should consult section 15: Troubleshooting.

The appendices also contain a great deal of useful information, pulled from the main text to avoid crowding. APPENDIX B –Flow Diagram and Valve Sequences discusses the overall operation of the SSIM2 in detail explaining the purpose of various valve states, while APPENDIX C –Dilution and Dilution Factors: Considerations and Calculations gives guidance on how to account for, or leverage, dilution in your samples. APPENDIX A –Adapting Greenhouse Gas Analyzers for SSIM2 Use will be relevant to concentration analyzer users (e.g. G2508), and APPENDIX D –Software Installation to those who purchased the SSIM2 separately from their analyzer, or who have to reinstall the software.

1.4 SSIM Specifications

Table 1: A0314 Specifications

Parameter	Specification
Minimum Sample Volume Per Measurement	20 mL or less, directly into the SSIM2* 23 mL through the 16-Port Manifold
Injection Time	Injection Time 10 or 15 minutes (Corresponds to 7- or 12-minute measurement time)
Connections	1/8" Swagelok
Temperature Range	See details for relevant paired instrument
Ambient Humidity Range	<85% R.H. non-condensing
Maximum Altitude	See details for relevant paired instrument
Dimensions	SSIM2: 8.5" w x 4" h x 9" d (21.6 x 10.2 x 22.9 cm) Pump: 7.5" w x 4" h x 11" d (19 x 10.2 x 28 cm)
Weight	SSIM2: 6.25 lbs (2.8 kg) Pump: 14.3 lbs (6.5 kg)
Power Requirements	SSIM2 powered through the USB 2.0 port of the analyzer. <3 watts additional power draw through analyzer. Pump: 150 watts startup; up to 150 W during operation
Gas Requirements	Zero air as carrier gas. ** Standards in zero air at appropriate concentrations**
Liquid Ingress Protection	None
Software	Controlled by the Picarro Analyzer Software Module

*Smaller sample sizes are possible using the SSIM dilution mechanism so long as the initial sample is high enough in concentration to meet the sample concentration requirements when diluted.

**N2 can be used as a carrier, diluent, and matrix gas if the CRDS instrument comes configured with an N2 mode.

1.5 Acronyms

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

Table 2: Acronyms, Formulas, Units, and Symbols

Acronym	Definition
" (as in 1/4")	Inches
%0	per mil
°C	Degrees Celsius
μL	Microliter
μg	Microgram
A0311	SKU for 16-Port Distribution Manifold, or Multiplexer Valve
A0314	SKU for SSIM2
CH4	Methane
cm	centimeters
CO2	Carbon Dioxide
CRDS	Cavity Ring-Down Spectroscopy
DAS	Data Acquisition System (the Analyzer)
GUI	Graphical User Interface
H2O	Water
НВ	Hotbox
mm	millimeters
ppb	Parts Per Billion
ppm	Parts Per Million
SKU	Stock Keeping Unit
SSIM	Small Sample Introduction Module (synonymous with SSIM2, as used in this manual)
SSIM2	Small Sample Introduction Module 2
WB	Warm box
ZA	Zero Air

1.6 Text Conventions

- Italic text identifies screen names and emphasizes important text, or certain features.
- Bold text is for actions to take (such as clicking on a UI button), cautions, statements, and text you should type or select in screens.
- Bold and Italicized text indicates a cross-reference link to another section within the manual. It is also used to reference a separate document or to emphasize textual content that requires special attention.

2. Safety

2.1 CE Certification

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

2.2 Warning Symbols

The following icons are used throughout this manual to emphasize important information in the text. These icons indicate dangers to either the operator or to the analyzer and peripherals, and other important information.

Table 3: Warning/Information Icons

<u>.</u>	Consult the user manual for important information (When you see this symbol placed at hazard points on equipment, consult the user manual).
NOTE	NOTE is important information that you should be aware of before proceeding.
	CAUTION alerts you of a potential danger to equipment or to the user.
WARNING	WARNING indicates an imminent danger to the user.
	REMINDER is a helpful hint to procedures listed in the text.

2.3 General Safety



Using the SSIM2 in a manner not specified by Picarro may result in damage to the unit and render it unsafe to operate.



The SSIM2 is for indoor use only and has an ingress protection rating of IPx0. It is NOT protected against exposure to water including dripping, spraying, splashing or immersion.



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



The SSIM2 contains no user serviceable components except for the Septum within the injection assembly (when performing syringe injections). Do not attempt any other repairs. Instead, report all problems to Picarro Customer SupportIPx or your local distributor. Please contact Picarro if you have any questions regarding the safe operation of this equipment.



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.

3. Unpacking

3.1 Shipping, Handling and Storage

- Picarro equipment may be transported in non-pressurized aircraft.
- Do not store boxes outside in the rain or in extreme heat or cold.
- Handle Picarro equipment with care. Do not drop or shake boxes.
- Do not stack boxes more than five high.

3.2 Inspect the Shipping Box

Picarro products are inspected and tested before leaving the factory. The shipping boxes provide proven safety from most dropping, crushing or spiking events.

If the equipment arrives damaged, photograph the damage, and contact Picarro (email pictures if possible) for consultation on the best course of action.



Save the original shipping materials for re-use when storing or shipping the unit.

3.3 Unpack the Shipping Boxes

Unpack the shipping boxes. They contain the following:

Table 4: Box 1: SSIM2 and Components

ltem (Qty)	Description
SSIM2 (1)	A0314 Small Sample Introduction Module 2
USB Cable (1)	A-B Connectors, 3' Long (for power and communications from Analyzer to SSIM2)
USB Cable (1)	A-B connectors 6' long (alternative length for power and communications from Analyzer to SSIM2)
Memory Stick (1)	USB, 2 GB
Swagelok Nut (6)	For 1/8" Swagelok, 316 SS
Swagelok Ferrule (6)	1 Front and 1 Back Ferrule for 1/8" Swagelok
Cable, Valves (1)	DB15 Female/Male, 2.5' long (for connection to 16-Port A0311)
Brass Plugs (8)	1/8" Swagelok for 16-Port A0311
Tubing/Fittings (1)	Kit for SSIM 2.0 with 16-Port Bundle only

Table 5: Box 2: Pump and Accessories

Item (Qty)	Description
Vacuum Pump (1)	Vacuubrand pump: Provides vacuum to SSIM2
Vacuum Hose (1)	Hose to connect the pump to the SSIM2. 27" long
AC Power Cable (1)	A power cable with connectors appropriate to your country is provided. Ensure that A2000 pump has been set to correct local voltage (120V/240V) on side of pump before operation.
Pump Manual (1)	Detailed instructions for pump.

Item (Qty)	Description
Zero Air Kit (1) (Optional)	Available at the Picarro Store: Picarro A0925 Zero Air Kit (includes items below)
CGA-590 Regulator (1)	0-10 PSIG (0-0.7 Bar, gauge) delivery pressure regulator for zero air tank (not compatible with N2 gas only, which requires CGA-580).
Toggle Valve (1)	On/off valve; to be added to regulator to allow simple shut off of zero air, while retaining consistent delivery pressure.
1/8" SS Tubing	10' of 1/8" outer diameter stainless steel tubing.
Adjustable wrench (1)	Small adjustable for connecting toggle valve to regulator.
Assorted fittings	Ferrule and nut sets, 1/8" to ¼" adaptor for zero air line from regulator to back of SSIM2.
Teflon tape (1)	¹ ⁄ ₄ " wide Teflon tape for sealing toggle valve to regulator.

Table 6: Box 3: A0925 Zero Air Kit (if purchased)
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Table 7: Box 4: A0311	16-port Manifold	(if purchased)
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Item (Qty)	Description
A0311 16-Port Manifold (1)	Refer to the manual, 16-Port Manifold User Manual, Including A0311, A0311-S, A0310, P/N 40-0038 for parts requirements.
Tubing connectors, 1/8" SS (3)	A set of three tubing connectors will ship either with the A0311, the A0314, or in the instrument box, depending on space considerations and shipment details.

4. Pre-Installation Requirements

Prior to setting up the SSIM2, the user will need the following items.

- A pressurized cylinder of dry, calibrated CO2 and CH4-free Ultra High Purity Zero Air (or N2 if N2 mode is enabled) complete with a pressure regulator so that gas can be supplied at ≥ 1 psi (0.07 bar) and < 5 psi (~0.5 bar). It should have < 1 ppm CO2 and < 5 ppb CH4 and < 10 ppm H2O.
- Various lengths of 1/8" tubing (stainless steel recommended) with 1/8" Swagelok connections on each for connecting calibration tanks.
- One or more cylinders of reference material for the gas species being measured, e.g., CO2, CH4, N2O, characterized for isotopic delta value as applicable. Must be controlled with a dual stage pressure regulator so that gas can be supplied at ≥ 1 psi (0.07 bar) and < 5 psi (~0.35 bar). Picarro typically uses a pressure of 2-3 psi. Cylinders should not exceed the concentration range for the relevant species of gas and instrument, unless they are being diluted.
- Sample container(s) such as Mylar or aluminum foil bags, syringes (Figure 2), or other fixed containers which can be attached to the system via 1/8" Swagelok fittings and which have manual valves so the samples can be isolated from the system during purging.
- A syringe with a needle and manual valve can be used with a septum by fitting the sample port with a septum adapter. See section 5.1 Hardware Requirements.

Depending on the revision of the SSIM2 the customer possesses, the 1/8" inlet fitting may or may not include a frit screen to filter out large particles. If you are unsure whether your SSIM2 has a frit, shine a flashlight into the inlet fitting.



If so, be aware that the syringe needle should not be pushed too far in, in such a way as to damage this screen.

If a screen is not present, and is desired, customers may purchase this frit screen from Valco Instruments, part number 10FR2-10 (Pack of 10).

NOTE

Sample bags and syringes are equally common configurations. (See section 5, Syringe Sample Delivery Requirements for more information on using syringe configurations.)

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Figure 2: Sample Bag and Syringes Connected via Manual Valve



Manual valves on the sample bags/containers or syringes are a requirement so the sample can be isolated during purge.

- Appropriate wrenches (7/16, 1/2, 9/16, and 11/16 inches) for making gas connections.
- The basic gas analyzer setup (CRDS analyzer and external vacuum pump as shown in Figure 3) should be completed. Setup information can be found in the manual of the CRDS analyzer.



Figure 3: Basic Carbon Analyzer Setup

 Note If using an A2000 vacuum pump, set its 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 6).



Figure 4: Vacuum Pump Voltage Selection

• If using the A0311 16-Port Distribution Manifold, refer to its manual (PN 40-0038) while following the rest of this manual. The 16-Port Distribution Manifold automates the sampling of up to 8 samples at a time. Picarro recommends placing the A0311 immediately above the CRDS instrument, and below the SSIM (see Figure 23).

Prior to booting the instrument, the Valve Sequencer must be set to the OFF position on the analyzer. This is required when using the SSIM2 and 16-port manifold. This is accomplished by changing the Valve Sequencer MPV option in the Port Manager tab of the Setup Tool (Figure 4) in the Utilities folder on the desktop.



Any changes to this configuration must be enacted while the Picarro host software (green GUI) is stopped from "Stop Instrument" > "Stop Instrument but leave driver running" in the Diagnostics folder on the desktop.

Restart the instrument software from the Desktop using "Start Instrument." It may be necessary to also to reboot the analyzer if the instrument does not recognize the valve after these steps. Consult the A0311 manual, P/N 40-0038 for more information.

	1		1	C	1		-		
Data Logger	Port Manager	Data Delivery	GUI Pr	operties	Command Interface	Data Streaming	Electric	cal Interfa	ce
		Seria	al/So	ocket	Port Manager				
	Dat	Data Streaming			OFF v				
	Val	ve Sequencer	MPV	OFF		~			
	Cor	nmand Interfa	ace	COM1		~			
						•			

Figure 5: Setup Tool Port Manager



If the Valve Sequencer is not properly enabled, an error message will appear in the coordinator window (highlighted below in Figure 5). This same message appears if the 16-Port Distribution Manifold is not turned on or is improperly connected.

CRDS Coo	ordinator											
Control												
						New output file						
Filename	CFFDS2053	SSIM_201301	10_183646.cs	v								
Run Num	Sample Bag	Date/Time	Timestamo	Delta Mean	Delta Std	12CO2 Mean	12002 Std	13CO2 Mean	13CO2 Std	H2O Mean	H2O Std	Valve Posi
- Carriellin	- bumpic bug	Date/fille	Timestamp	Deres Hickin	Dena Sta	12002110011	12002.010	15002110011	10002.010	Theo Predit	1120 510	Ververros
<												>
						Log						
FSM thread	starts											
Meas buffe: Meas buffe:	r set r cleared											
Error Mult:	i-port valve	NOT enable	d correctly.									
Set soleno:	id valve mas	ik to 0										
Maximum in: Done!	let valve ch	lange: 500.0	0									
FSM thread	finished											
												\sim

Figure 6: Coordinator Multi-port Valve Error Message

5. Syringe Sample Delivery Requirements

This section provides details on hardware and other considerations for sample delivery using a syringe.



Figure 7: Example Syringe Setup

5.1 Hardware Requirements

Syringes

The syringe must have a twist lock valve or stop-cock and a Luer lock. These can be obtained from several manufacturers. Following are some typical examples:

- 1. Complete Syringe Assembly with Internal Twist Lock Valve and Luer Lock (available from Valco):
 - https://www.vici.com/syr/magnum.php
 - Select Valco PN 060044 50 mL with Luer lock
 - View Valco Catalog for details



Figure 8: Valco Magnum 50 mL Syringe with Luer Lock and Internal Valve

- 1. Syringe Assembly (Figure 8) with Luer Lock and separate Stop Cock Valve (manufactured by SGE):
 - SGE SG009660 Syringe or Standard 60 mL plastic syringe from common online retailers, e.g. 14-955-461 from Fisher Scientific
 - Masterflex one-way valve from Cole-Parmer, PN EW-30600-00



Figure 9: SGE 50 mL Syringe with Luer Lock and External Stop-Cock Valve



Figure 10: Standard 60 mL Plastic Syringe with Luer Lock and External Stop-Cock Valve

Syringe Needles

Picarro strongly recommends a side-port needle to avoid injection blockage by septum material. 21G and larger needles will also resist breakage better than smaller (higher gauge number) syringes. We recommend, e.g.:

• Hamilton metal hub side port needle, Part number 772907, available from Fisher Scientific, Part Number 14-815-486



Figure 11: Luer Lock Side-port Needle

Septum Adapter Assembly

Septum assemblies are required for delivering samples via syringe. The Septum assembly (Figure 6) needs to adapt to a 1/8" SSIM or A0311 sample port. Picarro recommends the following:

- Swagelok 1/4"to 1/8" Straight Tube Adapter; PN SS-400-R-2
- Swagelok 1/8" Nut Set; PN SS-200-NFSET
- Injection Port Septa: Picarro PN C0352

A0311 users will require 8 sets of the above parts.



Figure 12: Septum Adapter Parts

- 1. Screw the 1/8" Nut and ferrules of the nut set onto the SAMPLE port of the SSIM.
- **2.** Slide the adapter tube through the nut set and into the fitting until it stops (Figure 12).
- 3. Tighten the 7/16" wrench ¾ turn per Swagelok recommended technique to compress the ferrules onto the adapter tube. For instructions, refer to the Swagelok Tube Fittings section of the Installer's Pocket Guide for Swagelok® Tube Fittings.



Figure 13: Assembling 1/4" to 1/8" Adapter

4. Remove the 1/4" nut and any ferrules from the assembly.

5. With the ferrules removed, insert a septum into the recess of the 1/4" male nut, then reinstall the nut back on the adaptor and finger tighten. Do not overtighten, as this can cause the septum to deform.



Figure 14: Completed Adapter Assembly with Septum Installed

Septa

Use 1/4" Injection Port Septa: Picarro PN C0352.



Figure 15: Septa Picarro PN C0352

5.2 Injection Considerations

Insert the needle roughly 0.5" (12.7 mm) into the septum fitting.

Samples Containing Large Particles

Use a frit screen for large particle capture. To install, push the frit into the inlet port with a section of 1/8" tubing. If a frit screen is not present, but is desired, customers may buy frit screens from Valco Instruments, part number 10FR2-10 (pack of 10).



Figure 16: Frit Screen Examples

Injection Technique When a Frit is Present



Depending on the version of the SSIM2 the customer possesses, the inlet 1/8" fitting may or may not include a frit screen to filter out large particles. If so, be aware that the syringe should not be pushed in too far, in such a way as to damage the screen which could allow contamination of the inlet circuit. Insert the needle no further than 0.5" (12.7 mm).

If you are unsure if a frit is present in the SSIM (or an A0311) sample port, visually inspect by removing the septum assembly and using light, inspect the port opening for the presence of a frit.

Frit Replacement

A frit screen may occasionally become blocked with particles and need replacement.

To remove, pry it out using a needle or fine tweezers, inspect the area where it was seated for residual particles and clean if necessary. Install a new frit using a section of 1/8" SST tubing.

Sealing Luer Fittings

Users should consider using either vacuum grease like Apiezon M/N or Dow Corning Vacuum Grease (preferred), or 1/4" wide Teflon tape to seal Syringe and needle Luer connection points, which may not otherwise always seal consistently.



Figure 17: Silicone-free vacuum grease and Teflon Tape

6. SSIM2 Hardware Setup and Installation

Follow the steps described in this section to make the proper gas and electrical connections. All gas connections should be made with 1/8" Swagelok. There are two configurations – one with, and one without the 16-Port Distribution Manifold. This section includes installation information for both configurations.

Based on one's configuration, refer to one of the sections listed below:

- 6.1, SSIM2 Setup with CRDS Analyzer Only
- 6.2, SSIM2 Setup with CRDS Analyzer and A0311 16-Port Distribution Manifold



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



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.



When the SSIM2 and the analyzer is being integrated to an external system, the safety of that system is the responsibility of the assembler of that system.



It is imperative that all gas connections be free of leaks to achieve proper measurement of a sample and ensure performance of the system. For more details on ensuring leak-free connections, see section 13: Running the SSIM Leak Check. All gas connections should be made with 1/8" stainless steel tubing and Swagelok connectors.



It is imperative that the SSIM, analyzer and other peripherals have adequate ventilation and/or cooling to maintain the ambient temperature below 35 °C when operating. Failure to provide adequate airflow, especially clearance at the front and rear panels, to ensure proper airflow and/or cooling to the equipment will result in overheating of the analyzer causing a shutdown and potential damage. There should be 4" (10cm) of clearance in the front and back of the equipment.

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

6.1 SSIM2 Setup with CRDS Analyzer Only



Figure 18: A0314 Positioning to Minimize Sample Line Dead Space



Figure 19: Typical SSIM2 Benchtop Setup

Features available with SSIM2 Alone:

- Automation of sampling: No. Each sample must be manually injected or connected, and manually advanced.
- Dilution: Yes.
- Calibration check: Yes.
- Automatic repeats of sample or standard: Yes.
- Continuous Loop: Yes.

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Figure 20: A0314 to Analyzer Connections

If the SSIM2 is used alone with the analyzer, refer to Figure 17 and Figure 19 and follow the setup steps below.

- 1. Before starting to connect components, make sure all the Pre-Installation Requirements have been met, and that the instrument is turned on and reporting gas concentrations for at least an hour. Ensure that isotopic values are stable, not trending upwards.
- **2.** Ensuring the zero air is NOT YET connected to the back of the SSIM, position SSIM2 near the analyzer's inlet connection (see Figure 17).
- **3.** Connect the USB A-B cable from the USB B port on the back of the SSIM to any open USB A port on the back of the instrument.
- **4.** Connect the beige-gray Valve cable, observing the pin configurations. In some cases, it may be necessary to remove the two small silver standoff threads from one side of the cable.
- 5. Use the short C-shaped stainless steel tube to connect from the SAMPLE OUTLET port of the SSIM2 to the analyzer's gas INLET port. The ¼" adaptor side attaches to the instrument inlet. At this time, air will flow from the open ZERO AIR in port on the SSIM, through a bypass loop, out the SAMPLE OUTLET port, and to the instrument INLET.
- 6. Connect the external vacuum pump to the VACUUM port on the SSIM2 with the supplied vacuum line (Figure 19). Ensuring the pump is set to the correct local voltage (120 vs 240 V) using the voltage selector switch as described in section 4: Pre-Installation Requirements. Connect the pump to line power and turn on.
- 7. With the regulator on the zero air tank tightened in place, open the zero air cylinder valve. Adjust the regulator delivery pressure so that it provides 2-3 psi (0.14-0.21 bar) on the delivery pressure gauge.
- **8.** Attach the carrier gas line to the ZERO AIR connection at the SSIM2 back panel. Within a few seconds, the user should begin to see gas concentrations dropping as the carrier gas flows to the instrument.
- 9. Wait until gas concentraions are nearly zero (broadly H2O < 100 ppm; CO2 < 2 ppm; CH4 < 10 ppb, etc) and then attach a sample bag or container containing expendable sample to the SAMPLE port on the front of the SSIM2 using a small length of 1/8" tubing.

If delivering the sample with a syringe, attach a septum adapter to the SAMPLE port following the guidance in section 5: Syringe Sample Delivery Requirements. Do not yet insert the syringe sample needle into the septum.

10. If using calibration gas, attach the calibration gas standard supply to the CAL input of the SSIM2 (front left side of the SSIM2). Set the supply gas pressure at between 2-3 psi (0.07-0.14 bar).Locate the Read SSIM Pressure program on the Desktop and double click it. (After it is open, you can minimize but do not close the window).

A window (Figure 20) will appear which will find the SSIM2 chamber pressure sensor at a port. Once the Read SSIM Pressure program is on, SSIM2 Pressure can be monitored on the main GUI by selecting SSIM2 Pressure on the pull-down menu, allowing it to be logged in the UserData.dat files.

If at any time the software is restarted, the "Read SSIM Pressure" program needs to be closed and restarted.

If "Read SSIM Pressure" does not launch properly, it may be necessary to either point the shortcut correctly or reinstall the driver. For instructions on these steps, please see APPENDIX D –Software Installation.

🥺 Select Read Ext Sensor
Config file specified at command line: C:\Picarro\G2000\AddOns\SSIM\ReadExtSenso▲ r.ini ReadExtSensor application started. Testing COM1
Testing COM2
Testing COM3
Testing COM4
Testing COM5
Testing COM6
Testing COM7
Testing COM8
Testing COM9
Testing COM10
External sensor found at COM10
-

Figure 21: Read External Sensor (SSIM2 Pressure)

11. Proceed to section 8, Operation: Measurement – SSIM2 and Analyzer.



Sample containers and syringes require a manual valve to isolate them during the purging of the SSIM2. Without an isolation valve, the sample will be lost during the SSIM purge step.

6.2 SSIM2 Setup with CRDS Analyzer and A0311 16-Port Distribution Manifold



Figure 22: Component Positioning for Shortest Gas Line Lengths

Picarro recommends placing the A0311 16-port distribution module on top of the CRDS analyzer, and the SSIM2 on top of the A0311 at the middle of the back edge. Use the supplied connections to minimize dead volumes. For the next steps, refer to Figure 23.



Figure 23: Typical SSIM2 Benchtop Setup with A0311 Valve

Features available with SSIM2 and 16-Port:

- Automation of sampling: Yes. Up to 8 samples can be run in a row without user intervention between samples.
- Dilution: Yes (recommendation: at least 3 ccs sample volume).
- Calibration check: Yes.
- Automatic repeats of sample or standard: Yes.
- Continuous Loop: No. See section 14.2 for an explanation.



Note that the gas line lengths shown below in Figure 23 are represented for simplicity and clarity, not as recommended line lengths.



Figure 24: SSIM2 to 16-Port Distribution Manifold to CRDS Analyzer Setup





Figure 25: Sample Bag Connected to 16-Port Manifold via Manual Valve



Use an adjustable platform such as a lab jack to support sample syringes when injecting into an A0311 16-Port Manifold port.



Figure 26: Sample Syringes Connected to 16-Port Manifold via Manual Valve

When the SSIM2 is used with the 16-Port Distribution Manifold and the analyzer, the following hardware setup steps are required.

- 1. Make sure all the Pre-Installation Requirements have been met.
- 2. Connect line power to the A0311 and ensure the rear power switch is set to on (|).
- **3.** Connect the hand pad to the A0311 Manifold and ensure the display lights up red to show a position. If necessary, use the home button on the hand pad to return the manifold to position 1. If the hand pad display does not come on with the A0311 plugged in and turned on, follow the troubleshooting steps in the A0311 manual, P/N 40-0038.
- **4.** Attach the supplied serial communications cable from the COM MPV connector on the Distribution Manifold to the COM 2 port on the CRDS Analyzer.
- 5. Turn on the instrument pump and then instrument.
- 6. When the instrument green GUI loads, select Show/Hide Valve Sequencer from the Tools menu. The Valve Sequencer window will show up. If does not show up, hit Alt-Tab to bring it to the front.

E Ext	ternal Valve Sequence	r					
File	Action						
	Start Sequencer	1					
	Go To First Step						
	Reset All Valves	E	Extern	al Valve S	Sequencer		
	Hide Sequencer Inte	erface					
	Current Step #	Remaining Time	e (min)	Current Valve State	Current Valve Code	Current Rot. Valve Code	
	0	0			0	0	

Figure 27: External Valve Sequencer Tool

- **7.** Confirm that the Current Rot. Valve Code cell in the upper right hand corner is green. If it is not, follow the steps in the A0311 manual, PN 40-0038.
- 8. The instrument will take about 25 minutes to reach its temperature set point. Once it is reporting measurements, it may take another 30 minutes for the delta values to stabilize. Wait until values are stable, not trending upwards.
- **9.** Ensuring the zero air is NOT YET connected to the back of the SSIM, position SSIM2 along the back edge of the A0311, roughly in the middle (see Figure 21).
- **10.** Connect the USB A-B cable from the USB B port on the back of the SSIM to any open USB A port on the back of the instrument.

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- **11.** Connect the beige-gray Valve cable between the SSIM and instrument, observing the pin configurations. In some cases, it may be necessary to remove the two small silver standoff threads from one side of the cable.
- **12.** Connect the external vacuum pump to the VACUUM port on the SSIM2 with the supplied vacuum line (Figure 23). Ensure the pump is set to the correct local voltage (120 vs 240 V) using the voltage selector switch as described in section 4: Pre-Installation Requirements. Connect the pump to line power and turn on.
- **13.** Connect the SAMPLE OUTLET from the back of the A0311 to the SAMPLE inlet on the front of the SSIM using the long dog-legged piece of tubing. In some cases, this may require adding an extra bend to the tubing, or adjusting one of the existing bends slightly.
- 14. Use the long C-shaped stainless steel tube to connect from the SAMPLE OUTLET port of the SSIM to the analyzer's gas INLET port. The ¼" adaptor side attaches to the inlet. At this time, air will flow from the open ZERO AIR in port on the SSIM, through a bypass loop, out the SAMPLE OUTLET port, and to the instrument INLET port. Air will not yet circulate through the A0311 manifold.
- **15.** With the regulator on the zero air tank tightened in place, open the zero air cylinder valve. Adjust the regulator delivery pressure so that it provides 2-3 psi (0.14-0.21 bar) on the delivery pressure gauge.
- **16.** Attach the carrier gas line to the ZERO AIR connection at the SSIM2 back panel. Within a few seconds, the user should begin to see gas concentrations dropping as the carrier gas flows to the instrument.
- **17.** If not already completed, attach brass plugs on all odd-numbered sample positions (e.g.: 1,3, ...15).
- Wait until gas concentraions are nearly zero (broadly H2O < 100 ppm; CO2 < 2 ppm; CH4 < 10 ppb, etc) and then begin to attach the sample bags or container to the even-numbered SAMPLE ports on the front of the A0311 using a small length of 1/8" tubing (e.g.: 2, 4, ... 16)

If delivering the sample with a syringe, attach a septum adapter to all SAMPLE ports. Do not yet insert the syringe sample needle into the septum. First read section 5.2, Injection Considerations.

- **19.** If using, attach the calibration gas standard supply to the CAL input of the SSIM2 (front side of the SSIM2). Set the supply gas pressure at between 2-3 psi (0.07-0.14 bar).
- **20.** Locate the Read SSIM Pressure program on the Desktop and double click it.

A window will appear (Figure 27) which will find the SSIM2 chamber pressure sensor at a port. Once the Read SSIM Pressure program is on, SSIM2 Pressure can be monitored on the main GUI by selecting SSIM2 Pressure on the pull-down menu, allowing it to be logged in the UserData.dat files.

If "Read SSIM Pressure" does not launch properly, it may be necessary to either point the shortcut correctly or reinstall the driver. For instructions on these steps, please see APPENDIX D –Software Installation.

21. Proceed to section 9, Operation: Measurement – SSIM2 and 16-Port Manifold and Analyzer.



You may minimize the Select Read SSIM Pressure window, but do not close it.



If at any time the software is restarted, the "Read SSIM Pressure" program needs to be closed and restarted.



For full details about the 16-Port Distribution Manifold, see the User Manual (P/N 40-0038) for this accessory.



Sample containers and syringes require a manual valve to isolate them during the purging of the SSIM2. Without an isolation valve, the sample will be lost during the SSIM purge step.



All ODD-NUMBERED ports on the Distribution Manifold must be capped with the provided 1/8" Swagelok brass caps. These odd-numbered ports are used in the SSIM's purge operation.

IF SAMPLES ARE CONNECTED TO ODD-NUMBERED PORTS, THEY WILL BE EXHAUSTED THROUGH THE VACUUM PUMP AND WILL BE LOST. Sample containers or syringes must have manual valves to isolate them during the SSIM2 purge operation.

Select Read Ext Sensor	⊐×
Config file specified at command line: C:\Picarro\G2000\AddOns\SSIM\ReadExtSens r.ini ReadExtSensor application started. Testing COM1	30
Testing COM2	
Testing COM3	
Testing COM4	
Testing COM5	
Testing COM6	
Testing COM7	
Testing COM8	
Testing COM9	
Testing COM10	
External sensor found at COM10	
	-

Figure 28: Read External Sensor (SSIM2 Pressure)

7. Coordinators

Coordinators are programs which work alongside the Picarro host software (green GUI) to coordinate the operation of peripheral and interfacing devices, typically to allow users to run discrete samples. Coordinators send signals to the external devices, coordinate the timing of actions, run averages on host software data, visually mark the host data that contributed to a sample in red, and then display the calculated discrete averaged data measurements as individual lines within the coordinator window. These values are saved automatically to a CSV file, which is noted in the upper left corner of the coordinator window.

The coordinator program is launched from a Coordinator Launcher icon on the desktop. This executable brings up a small window, allowing the user to select from the available coordinators installed on the instrument appropriate for their peripherals. The SSIM has its own yellow "SSIM Coordinator Launcher" icon, which may come with any of the following coordinators, depending on the configuration purchased by the user.

7.1 SSIM Gxxxx Coordinator

The main coordinator program used for ~95% of use cases. This coordinator runs discrete gas samples. It allows certain customizations by the user including (but not limited to): 16-port operation vs standalone SSIM operation; diluted vs non-diluted and working tank calibration check vs none. See sections 8 and 9 for a description of this coordinator with and without the 16-port manifold, respectively.

7.2 SSIM Coordinator w/ Double Injection

(Name may vary). A coordinator provided when requested, based on the main coordinator, allowing users to provide two back-to-back samples to overcome the slight concentration dilution effect associated with the standard coordinator. See Table 13: Overview of Injection Sequence – Double Inject (DI) for a description of this coordinator.

7.3 SSIM Ready Test

A test of the readiness of the SSIM. Typically performed at the factory as part of the final test of the peripheral, it can also be run by the user if they suspect an issue with the function of the valves, or the connection to the instrument. See Appendix D.3.

7.4 SSIM Leak Test

A test designed to determine whether the valves within the SSIM are leak-tight, and functional. Leaks are checked variously by vacuum or zero air pressure. A description of this coordinator may be found in section 13: Running the SSIM Leak Check.

8. Operation: Measurement – SSIM2 and Analyzer

If using the SSIM2 alone with the analyzer, follow the steps below for measurements:

1. With the SSIM Pressure reading as recommended in section 6.1, double click the "Coordinator Launcher" program on the desktop.

A screen will appear (Figure 28), allowing the user to choose the SSIM G2xxx Coordinator. Choose the G2xxx coordinator, and then click Launch to continue.

Picarro Coordina	_		×						
Picarro Coordi	nator	Launc	her						
Select Coordinator SSIM G2201-i V									
SSIM G2201-i SSIM Ready Test SSIM Leak Test									
Copyright Picarro	Copyright Picarro, Inc. 1999-2011								

Figure 29: Picarro Coordinator Launcher – Coordinator Selections

2. Upon clicking Launch, the Select Reference Gas screen will appear. Select the appropriate reference gas being used. (Hitting OK when no gas is being used will not affect the run.)

Reference gases can be added, removed, or changed by editing the ReferenceGases.ini file in C:\Picarro\G2000\AddOns\SSIM2. This certified value will be populated in another column in the Coordinator window alongside the measured value for the calibration standard gas each time the cal gas is run.

Reference Gas	Reference Gas G2131-i1	•
	Reference Gas G2131-i1	
Press 'OK' after	Reference Gas G2131-i2	
	Reference Gas G2131-i3	
		OK

Figure 30: Reference Gas Selection (model number will vary by instrument)

3. After clicking OK, on the "Select Reference Gas" screen, the "User Editable Parameters" screen (Figure 30) will appear. Enter the appropriate values based on the descriptions below.

User Editable Parameters	×
Multi-Port Valve: 1=Use 16PortDistributionManifold; 2=Don't Use 16PortDistributionManifold	2
If using Multi-Port Valve: Number of Sample Ports (between 1 and 8)	1
Number of Repeats per Sample (between 0 and 5)	1
Number of Repeats of Standard (between 0 and 5)	0
Standard Mode: 1=Between Each Sample Port; 2=Beginning and End	2
Measurement Mode: 1=One Time; 2=Continuous Loop	2
Measurement Speed: 1=Standard; 2=Fast	2
Sample Loading: 1=Manual; 2=Automatic; 3=Syringe	3
Sample Dilution: 1=No Dilution; 2=Dilute Sample with ZA	1
	OK

Figure 31: User Editable Parameters Window

User Editable Parameter Definitions

- Multi-Port Valve: Specify whether to use the 16 Port Distribution Manifold. Enter 1 if using a 16-Port Distribution Manifold. Enter 2 if NOT using a 16-Port Distribution Manifold (use this selection in this case). The 16-port is compatible with both dilution and sample repeats.
- If using Multi-Port Valve: Number of Sample Ports: Specify the number of sample ports of the 16-port distribution manifold the user will be measuring from. The number of samples can range from 1 to 8. When not using the 16 Port Distribution Manifold, leave this value set to "1".
- Number of Repeats per Sample: Specify the number of times the user wants to measure each sample. The number, n, can be as small as 0 (if only running calibration gases from the CAL port) and as great as 5. The user should have a little more than 20 mL * n of gas in a single sample vessel (e.g., for 5 repeats, the user should ideally have ~100-120 mL of gas total). Compatible with SSIM-only and SSIM-16-port.
- Number of Repeats of Standard: Specify the number of times the user wants to measure each standard. The number can be as small as 0 (if only running sample gases from the sample port) and as great as 5.
 Setting this to 0 will turn off the Standard Mode feature for the whole run. Compatible with SSIM-only and SSIM-16-port.

- Standard Mode: Enter 1 if wanting to measure standard between the measurement of each sample port, or 2 if wanting to measure the standard just in the beginning and at the end. Most users select 2.
- Measurement Mode: Enter 1 if samples will be measured one time, or 2 if they will be measured in a continuous loop (CRDS will continue to measure until the user ends the program). 16-port users should enter 1.
- Measurement Speed: Enter 1 if wanting standard measurement (12 minutes per measurement), or 2 if wanting fast measurement (8 minutes per measurement). The times do not include the 3-minute purge and pump cycle to clean the SSIM2 and analyzer between measurements.
- Sample Loading: 1 is intended for bag samples that will equilibrate pressure easily into the SSIM sample volume. 2 is intended for use with the 16-port valve principally, as the program will not perform purge and evacuation steps between samples. 3 is intended for use with a syringe, as the user may have to actively push the syringe slightly to adequately force sample air into the SSIM sample volume.
- Sample Dilution: Enter 1 if no dilution is to be used, or 2 if the injected sample is to be diluted with zero air. Compatible with SSIM-only and SSIM-16-port. The dilution feature will only work if a small volume of gas is used (rec: >3 ccs for 16-port) and cannot be used in conjunction with multiple sample repeats. See APPENDIX C –Dilution and Dilution Factors: Considerations and Calculations.
- 4. Once you have finished making your selections, click OK to continue. The CRDS Coordinator window (Figure 31) will appear. Follow the instructions the coordinator provides to PLEASE HOOK UP ALL SAMPLE BAGS OR SYRINGES WITH VALVE CLOSED AND SELECT "RESUME" UNDER "CONTROL" TO CONTINUE.



Ensure the manual valve (connected to the sample bag or syringe) is closed or the sample will be lost! The system pumps out the gas lines all the way up to the manual valve.

CRDS Coo	ordinator												- 🗆	×
<u>C</u> ontrol	Control													
Filename:	Filename: CFIDS2348_SSIM_20221004_153704.csv													
New Output File														
Run Num	Sample Bag	Date/Time	Timestamp	HR De	HR	HP	HP	Delta 13CO	Delta 13CO	HR 12CH4	HR 12CH4	HR 13CH4	HR 13CH4	HP 12
1	1	10/04/22 1	166489838	-29.030	11.1	99	0.000	-21.905	0.243	0.719	0.005	0.008	0.000	-0.00
2	1	10/04/22 1	166490030	-6.237	4.512	99	0.000	-21.654	0.251	1.729	0.006	0.020	0.000	-0.00
3	1	10/04/22 1	166490137	-6.050	5.442	99	0.000	-21.712	0.293	1.798	0.006	0.020	0.000	-0.00
4	1	10/04/22 1	166490220	-4.422	4.269	99	0.000	-21.702	0.261	1.730	0.006	0.020	0.000	-0.00
<	< \rightarrow >										>			
(Restart wi	th sample)						i	Log						^
<pre>(Restart with sample) Evacuating the SSIM Maximum inlet valve change: 500.00 Ready for the next measurement State Al starts State Al starts</pre>														
PLEASE HOOK	UP ALL SAM	PLE BAGS OR	SYRINGES WI	TH VALVE	CLOSEI	DAND	SELECT	"RESUME" UI	NDER "CONTRO	DL" TO CONTI	WE			*

Figure 32: Coordinator Window



The upper portion of the coordinator window shows the various parameters measured during analysis and is identical to the data that is saved in the CSV file.

The bottom portion of the coordinator window displays various messages about the state of the system. Prompts to the user are also noted there in capital letters (as shown above in Figure 31).

5. The SSIM will proceed with a series of pumping and evacuation steps, varying between ValveMasks 8 (evacuating the SSIM sample volume) and 5 (flowing ZA through the SSIM sample volume). At the end of this process, follow the instructions to "PLEASE OPEN ALL THE SAMPLE BAG OR SYRINGE VALVES AND SELECT "RESUME" UNDER "CONTROL" TO CONTINUE ..." (Figure 32).

```
Log
State A3 starts...
Set solenoid valve mask to 8
PLEASE OPEN ALL THE SAMPLE BAG OR SYRINGE VALVES AND SELECT "RESUME" UNDER "CONTROL" TO CONTINUE...
```

Figure 33: User Prompt to Open Sample Valve(s)

6. The Coordinator will advance through an additional set of valve changes, and automatically advance to the next step, opening the SSIM cavity directly to the sample line. (Syringe users watching carefully may be able to detect a slight inward movement of the syringe plunger during this step, roughly 1 mL.) Follow the instructions to inject the sample by squeezing the bag, or syringe plunger until you feel resistance. At this point, we recommend closing the on/off toggle valve (this is not called out in the Coordinator window) if the user is running single repeats per sample and wants to minimize sample dilution.



Figure 34: Prompt to Inject Syringe Contents

- The analysis of the sample will begin (duration of measurement is 12 or 8 minutes per position, depending on the measurement option chosen standard or fast).
- 8. While the samples are running, confirm that peaks are stable and flat, and that the SSIM Pressure drops slowly as shown in Figure 34 below (absolute values will depend on the altitude/ambient pressure of the lab space).
- **9.** The Coordinator will continue to prompt the user for samples injections until the Coordinator program is terminated or until the number of samples specified by the user is complete.

The gas concentration and isotope ratio data will look similar to Figure 34 below where three similar samples were run one after the other. Each time a sample is finished, the latter portion of the peak will be highlighted in red, and a new line will be populated into the Coordinator's upper window. If a sample does not have adequate signal (typically due to an accidental purge step sample loss, an inadequately low concentration sample, or a user error), the peak will not be highlighted in red, and will not populate a line in the upper Coordinator window.



It is normal to have alternating "Pressure High/Pressure Low" warnings in the GUI Status Log since the analyzer is constantly adjusting the pressure during the discontinuous gas flow that occurs because of the SSIM2 purging and gas delivery steps. If these warnings persist and are accompanied by a persistent "System Alarm" indicator, this could indicate a problem and it is advisable to contact Picarro Support.



If the user ever desires to close the Coordinator, the red "X" can be used to simply close the window which will terminate the program.

Allow the program to terminate itself (it may take one minute depending on the state of the SSIM2 and analyzer). The Coordinator, if allowed to close itself properly, will return the SSIM2 and analyzer to a safe state.)

Note that the GUI shown in Figure 34 below is for a G2201-i analyzer, which measures iCH4 and iCO2. Depending on the type of CRDS analyzer being used, the look of the main GUI will vary slightly.



Figure 35: GUI for a G2201-i Analyzer

9. Operation: Measurement – SSIM2 and 16-Port Manifold and Analyzer

If the SSIM2 is used with the 16-Port Distribution Manifold and the analyzer, follow the steps below for measurements:

- **1.** With the SSIM Pressure reading as recommended in section 6.2, double click the "Coordinator Launcher" program on the desktop.
- **2.** A screen will appear (Figure 35), allowing the user to choose the SSIM G2xxx Coordinator. Choose the G2xxx coordinator, and then click Launch to continue.

Picarro Coordina	_		×						
Picarro Coordi	nator	Launc	her						
Select Coordinator SSIM G2201-i V									
	SSIM SSIM SSIM	G2201-i Ready Tes Leak Test	st						
Copyright Picarro, Inc. 1999-2011									

Figure 36: Picarro Coordinator Launcher – Coordinator Selections

3. Upon clicking Launch, the Select Reference Gas screen will appear. Select the appropriate reference gas being used. (Hitting OK when no gas is being used will not affect the run.)

Reference gases can be added, removed, or changed by editing the ReferenceGases.ini file in C:\Picarro\G2000\AddOns\SSIM2. This certified value will be populated in another column in the Coordinator window alongside the measured value for the calibration standard gas each time the cal gas is run.

Select Reference	Gas	×
Reference Gas	Reference Gas G2131-i1	•
	Reference Gas G2131-i1	
Press 'OK' after	s Reference Gas G2131-i2 Reference Gas G2131-i3	
		OK

Figure 37: Reference Gas Selection

4. Once the user clicks OK on the Select Reference Gas screen, the User Editable Parameters screen (Figure 37) will appear. Enter the appropriate values based on the descriptions below.

User Editable Parameters	×
Multi-Port Valve: 1=Use 16PortDistributionManifold; 2=Don't Use 16PortDistributionManifold	1
If using Multi-Port Valve: Number of Sample Ports (between 1 and 8)	8
Number of Repeats per Sample (between 0 and 5)	1
Number of Repeats of Standard (between 0 and 5)	0
Standard Mode: 1=Between Each Sample Port; 2=Beginning and End	2
Measurement Mode: 1=One Time; 2=Continuous Loop	1
Measurement Speed: 1=Standard; 2=Fast	1
Sample Loading: 1=Manual; 2=Automatic; 3=Syringe	2
Sample Dilution: 1=No Dilution; 2=Dilute Sample with ZA	1
	OK

Figure 38: User Editable Parameters Window

User Editable Parameter Definitions

- Multi-Port Valve: Specify whether to use the 16 Port Distribution Manifold. Enter 1 if using a 16-Port Distribution Manifold. Enter 2 if NOT using a 16-Port Distribution Manifold (use this selection in this case). The 16-port is compatible with both dilution and sample repeats.
- If using Multi-Port Valve: Number of Sample Ports: Specify the number of sample ports of the 16-port distribution manifold the user will be measuring from. The number of samples can range from 1 to 8. When not using the 16 Port Distribution Manifold, leave this value set to "1".
- Number of Repeats per Sample: Specify the number of times the user wants to measure each sample. The number, n, can be as small as 0 (if only running calibration gases from the CAL port) and as great as 5. The user should have a little more than 20 mL * n of gas in a single sample vessel (e.g., for 5 repeats, the user should ideally have ~100-120 mL of gas total). Compatible with SSIM-only and SSIM-16-port.
- Number of Repeats of Standard: Specify the number of times the user wants to measure each standard. The number can be as small as 0 (if only running sample gases from the sample port) and as great as 5. Setting this to 0 will turn off the Standard Mode feature for the whole run. Compatible with SSIM-only and SSIM-16-port.

- Standard Mode: Enter 1 if wanting to measure standard between the measurement of each sample port, or 2 if wanting to measure the standard just in the beginning and at the end. Most users select 2.
- Measurement Mode: Enter 1 if samples will be measured one time, or 2 if they will be measured in a continuous loop (CRDS will continue to measure until the user ends the program). 16-port users should enter 1.
- Measurement Speed: Enter 1 if wanting standard measurement (12 minutes per measurement), or 2 if wanting fast measurement (8 minutes per measurement). The times do not include the 3-minute purge and pump cycle to clean the SSIM2 and analyzer between measurements.
- Sample Loading: 1 is intended for bag samples that will equilibrate pressure easily into the SSIM sample volume. 2 is intended for use with the 16-port valve principally, as the program will not perform purge and evacuation steps between samples. 3 is intended for use with a syringe, as the user may have to actively push the syringe slightly to adequately force sample air into the SSIM sample volume.
- Sample Dilution: Enter 1 if no dilution is to be used, or 2 if the injected sample is to be diluted with zero air. Compatible with SSIM-only and SSIM-16-port. The dilution feature will only work if a small volume of gas is used (rec: >3 ccs for 16-port) and cannot be used in conjunction with multiple sample repeats. See APPENDIX C –Dilution and Dilution Factors: Considerations and Calculations.
- Once finished, click OK to continue. The CRDS Coordinator window, as shown in Figure 38, will appear. Follow the instructions the coordinator provides to PLEASE HOOK UP ALL SAMPLE BAGS OR SYRINGES WITH VALVE CLOSED AND SELECT "RESUME" UNDER "CONTROL" TO CONTINUE.



Ensure the manual valve (connected to the sample bag or syringe) is closed or the sample will be lost! The system pumps out the gas lines all the way up to the manual valve.

Control Filename: CFIDS3248_SSIM_20221004_153704.csv New Output File Run Num Sample Bag Date/Time Timestamp HR De., HR., HP., HP., Delta 13CO., Delta 13CO., HR 12CH4., HR 13CH4., HR 13CH4., HR 1 1 10/04/22 1., 16649033., -29.030 11.1., 99., 0.000 -21.905 0.243 0.719 0.005 0.008 0.000 -0. 2 1 10/04/22 1., 16649033., -6.327 4.512 99., 0.000 -21.654 0.251 1.729 0.006 0.020 0.000 -0. 3 1 10/04/22 1., 166490137., -6.050 5.442 99., 0.000 -21.702 0.261 1.730 0.006 0.020 0.000 -0. 4 1 10/04/22 1., 166490220., -4.422 4.269 99., 0.000 -21.702 0.261 1.730 0.006 0.020 0.000 -0. (Restart with sample) Evacuating the SSIM Maximum inlet valve change: 500.00 Ready for the next measurement State Al starts	CODE C															
Control Filename: CFIDS2348_SSIM_20221004_153704.esv New Output File Run Num Sample Bag Date/Time Timestamp HR De HR HP Deta 13CO HR 12CH4 HR 13CH4	CRDS Coo	ordinator												- U	~	
Filename: CFIDS2348_SSIM_20221004_153704.csv New Output File Run Num Sample Bag Date/Time Timestamp HR De HR HR ID/04/22 1 HR Be HR HR De HR HR 10/04/22 1 HR 13CH4 HR	<u>C</u> ontrol															
New Output File Run Num Sample Bag Date/Time Timestamp HR De HR HP Pl Deta 13CO Deta 13CO HR 12CH4 HR 13CH4	Filename: CFIDS2348_SSIM_20221004_153704.csv															
Run Num Sample Bag Date/Time Timestamp HR De HR HP Delta 13CO Delta 13CO HR 12CH4 HR 13CH4 HI 100000	New Output File															
1 1 10/04/22 1 166489838 -29.030 11.1 99 0.000 -21.905 0.243 0.719 0.005 0.008 0.000 -0. 2 1 10/04/22 1 166490030 -6.237 4.512 99 0.000 -21.654 0.251 1.729 0.006 0.020 0.000 -0. 3 1 10/04/22 1 166490137 -6.050 5.442 99 0.000 -21.712 0.293 1.798 0.006 0.020 0.000 -0. 4 1 10/04/22 1 166490220 -4.422 4.269 99 0.000 -21.702 0.261 1.730 0.006 0.020 0.000 -0. 4 1 10/04/22 1 166490220 -4.422 4.269 99 0.000 -21.702 0.261 1.730 0.006 0.020 0.000 -0. Log Log Log Ready for the next measurement State Al starts <td colspa<="" td=""><td>Run Num</td><td>Sample Bag</td><td>Date/Time</td><td>Timestamp</td><td>HR De</td><td>HR</td><td>HP</td><td>HP</td><td>Delta 13CO</td><td>Delta 13CO</td><td>HR 12CH4</td><td>HR 12CH4</td><td>HR 13CH4</td><td>HR 13CH4</td><td>HP 12</td></td>	<td>Run Num</td> <td>Sample Bag</td> <td>Date/Time</td> <td>Timestamp</td> <td>HR De</td> <td>HR</td> <td>HP</td> <td>HP</td> <td>Delta 13CO</td> <td>Delta 13CO</td> <td>HR 12CH4</td> <td>HR 12CH4</td> <td>HR 13CH4</td> <td>HR 13CH4</td> <td>HP 12</td>	Run Num	Sample Bag	Date/Time	Timestamp	HR De	HR	HP	HP	Delta 13CO	Delta 13CO	HR 12CH4	HR 12CH4	HR 13CH4	HR 13CH4	HP 12
2 1 10/04/22 1 166490030 -6.237 4.512 99 0.000 -21.654 0.251 1.729 0.006 0.020 0.000 -0. 3 1 10/04/22 1 166490137 -6.050 5.442 99 0.000 -21.712 0.293 1.798 0.006 0.020 0.000 -0. 4 1 10/04/22 1 166490220 -4.422 4.269 99 0.000 -21.702 0.261 1.730 0.006 0.020 0.000 -0. 4 1 10/04/22 1 166490220 -4.422 4.269 99 0.000 -21.702 0.261 1.730 0.006 0.020 0.000 -0. 4 1 10/04/22 1 166490220 -4.422 4.269 99 0.000 -21.702 0.261 1.730 0.006 0.020 0.000 -0. Log Log Log Log State Al stats State Al stats	1	1	10/04/22 1	166489838	-29.030	11.1	99	0.000	-21.905	0.243	0.719	0.005	0.008	0.000	-0.00	
3 1 10/04/22 1 166490137 -6.050 5.442 99 0.000 -21.712 0.293 1.798 0.006 0.020 0.000 -0. 4 1 10/04/22 1 166490220 -4.422 4.269 99 0.000 -21.702 0.261 1.730 0.006 0.020 0.000 -0. 166490220 -4.422 4.269 99 0.000 -21.702 0.261 1.730 0.006 0.020 0.000 -0. 166490220 -4.422 4.269 99 0.000 -21.702 0.261 1.730 0.006 0.020 0.000 -0.	2	1	10/04/22 1	166490030	-6.237	4.512	99	0.000	-21.654	0.251	1.729	0.006	0.020	0.000	-0.00	
4 1 10/04/22 1 166490220 -4.422 4.269 99 0.000 -21.702 0.261 1.730 0.006 0.020 0.000 -0.	3	1	10/04/22 1	166490137	-6.050	5.442	99	0.000	-21.712	0.293	1.798	0.006	0.020	0.000	-0.00	
K Log (Restart with sample) Evacuating the SSIM Maximum inlet valve change: 500.00 Ready for the next measurement State Al starts State Al starts	4	1	10/04/22 1	166490220	-4.422	4.269	99	0.000	-21.702	0.261	1.730	0.006	0.020	0.000	-0.00	
Log (Restart with sample) Evacuating the SSIM Maximum inlet valve change: 500.00 Ready for the next measurement State Al starts State Al starts	< \vec{b}{b} > >										>					
Evacuating the SSIM Maximum inlet valve change: 500.00 Ready for the next measurement State Al starts	(Pestart ui	th sample)							Log							
PLEASE HOOK UP ALL SAMPLE BAGS OR SYRINGES WITH VALVE CLOSED AND SELECT "RESUME" UNDER "CONTROL" TO CONTINUE	Evacuating Maximum inl Ready for t State Al st Set solenoi PLEASE HOOK	Log (Restart with sample) Evacuating the SSIM Maximum inlet valve change: 500.00 Ready for the next measurement State Al starts Set solenoid valve mask to 8 PLEASE HOOK UP ALL SAMPLE BAGS OR SYRINGES WITH VALVE CLOSED AND SELECT "RESUME" UNDER "CONTROL" TO CONTINUE											~			

Figure 39: CRDS Coordinator Window



The upper portion of the coordinator window shows the various parameters measured during analysis and is identical to the data that is saved in the CSV file.

The bottom portion of the coordinator window displays various messages about the state of the system. Prompts to the user are also noted there in capital letters (as shown above in Figure 38).

- 6. The SSIM will proceed with a series of pumping and evacuation steps, varying between ValveMasks 8 (evacuating the SSIM sample volume) and 5 (flowing ZA through the SSIM sample volume) for each of the 16 positions on the 16-port manifold valve. (If a smaller number than 8 is used, for example 3 positions only, n*2 positions will be evacuated, i.e. 6 positions.) At the end of this process, follow the instructions to "PLEASE OPEN ALL THE SAMPLE BAG OR SYRINGE VALVES AND SELECT "RESUME" UNDER "CONTROL" TO CONTINUE ..." Open valves on ALL connected bags or syringes.
- 7. The Coordinator will advance through an additional set of valve changes, and automatically advance to the next step, opening the SSIM cavity directly to the sample line. The sample from the first sample port will expand into the sample chamber of the SSIM2. There, the sample will make its way to the analyzer, where measurements will be taken automatically. At this point, no further user input is necessary to analyze sample(s) from sample container(s). Duration of measurement is 12 or 8 minutes depending on the

measurement option chosen – standard or fast – with an additional ~3 minutes of purging and flushing steps per sample.

If the user selected more than one repeat per sample, repeats will be done sequentially in that same sample position before moving to the next sample position.

When the first sample is complete, the Coordinator will automatically advance the 16-port valve forward to the next position and continue repeating the analysis until the number of samples is complete. If the user wishes to run more than eight samples, they should close the coordinator, hook up eight new samples, and start the coordinator again with the same settings as before.



It is normal to have alternating "Pressure High/Pressure Low" warnings in the GUI Status Log since the analyzer is constantly adjusting the pressure during the discontinuous gas flow that occurs because of the SSIM2's purging and gas delivery steps. If these warnings persist and are accompanied by a persistent "System Alarm" indicator, this could indicate a problem and it is advisable to contact Picarro.



If the user ever desires to close the Coordinator, the red "X" can be clicked to close the window which will terminate the program. Allow the program to terminate itself (it could take one minute depending on the state of the SSIM2 and analyzer). The Coordinator, if allowed to close itself properly, will return the SSIM2 and analyzer to a safe state.

The gas concentration and isotope ratio data will look similar to Figure 39: GUI for a G2201-i Analyzer below where three similar samples were run one after the other. Each time a sample is finished, the latter portion of the peak will be highlighted in red, and a new line will be populated into the Coordinator's upper window. If a sample does not have adequate signal (typically due to an accidental purge step sample loss, an inadequately low concentration sample, or a user error), the peak will not be highlighted in red, and will not populate a line in the upper Coordinator window.



The GUI shown in Figure 39 below is for a G2201-i analyzer (measuring iCH4 and iCO2) without an A0311 valve. Depending on the type of CRDS analyzer and configuration being used, the look of the main GUI will vary slightly.



Figure 40: GUI for a G2201-i Analyzer

10. GUI Appearance During SSIM Runs

This section provides descriptions of the expected behavior of several key variables during a standard SSIM run. Runs with a 16-port manifold, dilution, or sample repeats will look slightly different, but will share many of the same characteristics.



Figure 41: GUI Appearance During SSIM Runs

10.1 Delta Values

Delta values during the illuminated red (sample) portions of the injection should be quite stable/flat. Between injections, when the concentration of the gas drops to nearly zero, the noise on the delta signal will be significantly elevated, with standard deviation in the 100s+ per mille. The mean of the delta value may be lower, near, or higher than the delta value of the sample itself, and this should not be a matter for concern.

10.2 Concentration

During the sampling step, concentration will rise and slowly asymptote, though if the user zooms in, the concentration may still change by 5 or 10 percent over the red-illuminated sample period. During the purging and evacuation steps, the concentration should be close to zero for a given gas, e.g., <10 ppm for CO2, <10 ppb for CH4.

10.3 SSIMPressure

During the initial pre-sample steps, the SSIM Pressure will vary between vacuum (ValveMask 8, evacuation) and slightly ambient (ValveMask 5, purge).

If the sample is passively pulled in by the vacuum at the injection step, the SSIM pressure will look like the example at 11:12 (Figure 40), with a peak value around or slightly below ambient pressure. If the injection is pushed into the chamber, and the on/off valve closed, it will look like the signal at 11:25 (high, as much as 1000 or more torr, depending on how firmly the user pushes the sample in). The pressure value should be stable and flat until the user clicks "resume" after the injection.

SSIM Pressure will drop quickly during the first few minutes of an injection, and then flatten out when the flow in the system slows significantly as the inlet pressure drops and the outlet valve nearly or fully closes down, keeping sample gas in the cavity.

10.4 CavityPressure

Cavity Pressure for the system should be quite stable during an SSIM run, with the exception of brief transient signals due to valve switching.

10.5 OutletValve

OutletValve controls the pressure of the instrument cavity and closes as the flow of the system decreases. During SSIM injections, gas first moves quickly to the cavity from the SSIM chamber, and then slows significantly, with the sample held in the chamber for several minutes as the instrument measures the values. Accordingly, OutletValve will typically start in the 30,000-45,000 range, and will dip rapidly to values in the low-mid 20,000 range (this may differ on some systems depending on valve characteristics and instrument model), and then flatline.

10.6 ValveMask

Follow guidance in APPENDIX B – Flow Diagram and Valve Sequences for the valve mask values you should see during the injections. We have tried to include descriptions of the most common valve sequences expected based on combinations of behaviors (standard, 16-port, dilution, etc.).

If you believe that your signals don't match the expected behavior for your system, consult the Troubleshooting section (15) for guidance on diagnosing and identifying system behavior.



Figure 42: Typical SSIM2 Sample Measurement Process

11. Outputted Files

The SSIM program outputs two types of files to the Picarro file system under either the folder C:\Picarro\IsotopicData or C:\IsotopicData. These files can be thought of as the saved contents of the upper and lower panes of the SSIM Coordinator window, respectively.

11.1 Data files

	A	В	С	D	E	F	G
1	Run Num	Sample Bag	Date/Time	Timestamp	HR Delta iCH4 Mean	HR Delta iCH4 Std	HP Delta iCH4 Mean
2	1	0	5/3/22 13:43	1651610379	-39.631	4.901	-42.865
3	2	0	5/3/22 13:57	1651611218	-39.034	5.563	-42.775
4	3	1	5/3/22 14:11	1651612057	-37.882	4.193	-41.092
5	4	1	5/3/22 14:25	1651612896	-37.336	4.847	-40.787
6	5	1	5/3/22 14:39	1651613734	-36.866	4.79	-40.736
7	6	1	5/3/22 14:53	1651614573	-38.182	5.357	-41.387
8	7	1	5/3/22 15:07	1651615413	-36.766	5.159	-40.458
9	8	0	5/3/22 15:21	1651616252	-38.555	5.057	-42.732
10	9	0	5/3/22 15:35	1651617091	-38.903	5.155	-42.983
11	10	1	5/3/22 15:49	1651617930	-36.962	4.826	-40.414
12	11	1	5/3/22 16:03	1651618769	-36.466	5.194	-40.306
13	12	1	5/3/22 16:17	1651619608	-36.714	5.054	-40.369
14	13	1	5/3/22 16:31	1651620446	-37.338	4.602	-41.015
15	14	1	5/3/22 16:45	1651621284	-36.108	5.051	-40.203
16	15	0	5/3/22 16:59	1651622122	-39.073	5.435	-43.614
17	16	0	5/3/22 17:13	1651622962	-39.201	5.623	-43.412

File name format: SN#####_SSIM_YYYYMMDD_hhmmss.csv

Figure 43: Example of SSIM Data File From G2201-i Instrument

These files are most easily opened in Excel, and contain a large number of columns, often as many as 30, for the variables as reported across multiple modes. For certain elements in this table, values will show up as "9999999", which signifies "NaN". This refers to the fact that a value cannot be reported for a given column because a particular mode is not in use. In the example below, a mean value for isotopic CH4 in the "High Precision" (HP) low concentration mode is not possible, because the instrument is running in the "High Range" (HR) high concentration mode.

E	F	G	Н
HR Delta iCH4 Mean	HR Delta iCH4 Std	HP Delta iCH4 Mean	HP Delta iCH4 Std
-48.951	0.257	9999999	0

Figure 44: Example of 9999999 Values in SSIM Data File

11.2 Column Meanings (select)

Run Num refers to the injection number in a given SSIM run, always rising monotonically from 1 with each new injection. This is not the same as position or sample number.

Sample Bag refers to the position. 0 refers to injections taken from the calibration port, and 1 from the sample port. For systems with the 16-port manifold, the value is reported between 1-8, corresponding to positions 2, 4, 6, 8, 10, 12, 14, and 16 on the manifold.

Date/Time is provided in format YY/MM/DD hh/mm

Timestamp is provided in Epoch time, which outputs a value in seconds elapsed since 00:00:00 on Jan 1, 1970, UTC.

Measurement values have units equivalent to the units read in the instrument GUI, e.g., delta values in per mille, and concentrations variously in ppb or ppm.

11.3 Log files

File name format: SN#####_SSIM_YYYYMMDD_ hhmmss.txt

Log files record the behavior of the SSIM (and 16-port manifold if used) during the SSIM Coordinator run. Consult section APPENDIX B –Flow Diagram and Valve Sequences for an in-depth explanation of the meaning of the log messages.

```
• • •
                              CFIDS2333_SSIM_20220315_213358.txt
FSM thread starts
Meas buffer set
Meas buffer cleared
Maximum inlet valve change: 500.00
Inlet valve gain1 = 80.00, gain2 = 1.00
Set solenoid valve mask to 0
State A1 starts...
Set solenoid valve mask to 8
PLEASE HOOK UP ALL SAMPLE BAGS OR SYRINGES WITH VALVE CLOSED AND SELECT "RESUME" UNDER "CONTROL" TO
CONTINUE...
State A2 starts...
Set solenoid valve mask to 10
Set solenoid valve mask to 26
State A3 starts...
Set solenoid valve mask to 8
PLEASE OPEN ALL THE SAMPLE BAG OR SYRINGE VALVES AND SELECT "RESUME" UNDER "CONTROL" TO CONTINUE...
State A4 starts...
Set solenoid valve mask to 8
Set solenoid valve mask to 5
Set solenoid valve mask to 8
Set solenoid valve mask to 5
State B starts...
Set solenoid valve mask to 8
Set solenoid valve mask to 8
```

Figure 45: Log file From G2201-i Instrument

12. Calibration

The user may choose between various options for calibrating their instrument.

- 1. Calibrating to the instrument directly from the tank. Connecting up to the back of the instrument provides the most appropriate calibration for an instrument that samples ambient air. The user may either adjust the slope and intercept of the instrument using the User Recal tool (see instrument manual), or may use the observed value to post-process raw data.
- 2. Calibrating through the SSIM using a syringe. This method most closely approximates the way samples are run as aliquots on the SSIM. A user may pull aliquots of air from a sampling line downstream of the calibration tank (ensure that the connection is leak-tight, and make sure to overflow and waste the standard twice before pulling a final sample), and run discrete standards as if they were samples following the advice in section 8: Operation: Measurement SSIM2 and Analyzer.
- **3.** Calibrating through the SSIM Sample port with a tank. The user may choose to run standards through the sample port using an on/off valve just upstream of the sample port following the advice in the diagram below. This is a fairly simple way to calibrate, which closely approximates the way a sample is run, and which simplifies the process of preparing calibration standard aliquots. Use the following editable user parameters for this configuration assuming a 16-port valve is not being used: 2,1,5,0,2,2,1,3,1.

For further instructions on calibration, refer to the Calibration section in your analyzer user manual.



Figure 46: Setup for Calibration via SSIM

13. Running the SSIM Leak Check

With time, the valves inside the SSIM can become leaky or stuck. The SSIM Leak Test checks for the functionality of these valves, looking for an upward leak from vacuum across a variety of valve configurations. This test can only be run with the SSIM connected directly to the analyzer, not with the A0311 manifold.

In order to begin the leak test, follow these steps:

- **1.** Confirm that the USB and Valves cables between the analyzer and SSIM and connected as they would be for normal SSIM operation.
- **2.** Ensure the SSIM sample tubing is connected to the analyzer inlet.
- 3. Ensure that the carrier gas is on and connected to the ZERO AIR port.
- **4.** Ensure that the vacuum line is connected between the pump and SSIM, and that the vacuum pump is on.
- **5.** Using the brass plugs provided as part of the SSIM kit, plug both the SAMPLE and CAL ports on the front of the SSIM.
- **6.** Ensure that the Read SSIM Pressure program is closed/not communicating through the USB. This will typically cause a communications conflict with the leak test.
- **7.** Click on the Coordinator Launcher from the Desktop, and select SSIM Leak Test.



Figure 47: Coordinator Launcher – SSIM Leak Test Selection

8. The Leak Test coordinator window will load (Figure 47), resembling the standard SSIM coordinators program window.

Once the program has confirmed communications are working, it will ask you to confirm that the SAMPLE and CAL ports are capped and then to resume the test.

CRDS Coordinator	PICARRO	Isotopic Nitrous	
Control	11011110		
Filename: JDDS5103 SSIM Test 20230103	211524 cav		
New Output File			
Comment RawData ValveResult			
Moving to:			
SSIM status:			
Connected			
Now will ca			
Moving to:			
	Log		
FSM thread starts			*
Meas buffer set			
SSIM status: ok from Arduino board			
Connected to com port: 6			
Successful with attempts to speak with A	rduino in SSIM via COM port		=
Now will calculate base pressure			-
Set solenoid value mask to 8			
PLEASE ATTACH CAPS TO SAMPLE AND CAL POR	TS AND SELECT "RESUME" UNDER "CONTROL"	TO CONTINUE	
<u>'</u>			T

Figure 48: Leak Test Coordinator – Communication Confirmation and Port Cap Attachment

9. From the upper left Control menu, select Resume to confirm and continue the test. Over the next roughly 15 minutes, the program will observe the SSIM cavity pressure, looking for increases in the pressure of various sample loops to assess the performance of valve 1, then 3, and then 5.

Control Menu	ı – Selec	t Resume	
Filename: JDDS5103_SSIM Test_20230103_	211524.csv		
New Output File			
Comment	RawData	ValveResult	*
Will collect data for 6 minutes	MeasPress MeasTime		
Measured slope: 0.0006 torr/sec			
Leak check passed spec: 0.04 torr/sec			
Passed leak check at Ambeint pressure			
Moving to: StateA4		VS passed leak test	4 111
		Ion	-
1672781202.113, 1672781202.261, 16727812 1672781203.448, 1672781203.596, 16727812 1672781204.779, 1672781204.927, 16727812 Measured slope: 0.0006 torr/sec Leak check passed spec: 0.04 torr/sec Passed leak check at Ambeint pressure V5 passed leak test Moving to: StateA4	02.408, 167 03.743, 167 05.078, 167	72781202.555, 1672781202.71, 1672781202.854, 1672781203.002, 1672781203.149, 1672781203.3, 72781203.891, 1672781204.038, 1672781204.19, 1672781204.342, 1672781204.485, 1672781204.632, 72781205.226, 167	*
Set solenoid valve mask to 50 PLEASE REMOVE CAPS FROM SAMPLE AND CAL E	ORTS AND SE	ELECT "RESUME" UNDER "CONTROL" TO CONTINUE	-

Figure 49: Coordinator Running SSIM Leak Test

10. When prompted, remove caps from the CAL and SAMPLE ports, and click Resume from the Control menu. This will allow the leak test script to assess leaks from ambient across V4 and finally V2. The test will take roughly 20 more minutes to run. If any components fail, the test will state which component has failed in the upper and lower portions of the window during the test, as seen below in Figure 49.

CRDS Coordinator		- 0	×
<u>C</u> ontrol			
Filename: CFIDS2315 SSIM Test 2023	20321 230644.csv		
	-		
New Output File			
Comment	RawData	ValveResult	
Will collect data for 6 minutes			
	Mascherrure - [-0.860706 -0.022706 -0.020787 -0.016406 -0.005001 0.006427 0.016808 0.025615 0.020200		
	Meastime = [104/904215.918, 104/904210.005, 104/904210.212, 104/904210.30, 104/904210.507, 104/904210		
Measured slope: 0.0607 torr/sec			
Leak check failed spec: 0.04 torr/sec			
Failed leak check at Base pressure			
Now will check to see if V1 or V3 is leaking			
Opening valve: Valve 2			
	Log		
1647904224.469, 1647904224.617, 164	7904224.764, 1647904224.912, 1647904225.059, 1647904225.207, 1647904225.354, 1647904	225.501,	
1647904225.649, 1647904225.796, 164	7904225.944, 1647904226.091, 1647904226.239, 1647904226.386, 1647904226.534, 1647904	226.681,	
1647904226.828, 1647904226.976, 164	//904227.123, 1647904227.27, 1647904227.418, 1647904227.566, 1647904227.713, 16479042 7804229 45 1647904227.27, 1647904227.418, 1647904227.566, 1647904227.713, 16479042	27.861, 1647904228	3.008,
1647904229.482. 1647904229.629. 164	7904229.777. 1647904229.924. 1647904230.072. 1647904230.219. 1647904230.367. 1647904	230.514.	
1647904230.662, 1647904230.809, 164	.7904230.957, 1647904231.104, 1647904231.252, 1647904231.399, 1647904231.546, 1647904	231.694,	
1647904231.841, 1647904231.989, 164	7904232.136, 1647904232.284, 1647904232.431, 1647904232.578, 1647904232.726, 1647904	232.873, 164790423	33.02,
1647904233.168, 1647904233.316, 164	7904233.463, 1647904233.61, 1647904233.758, 1647904233.905, 1647904234.053, 16479042	34.2, 1647904234.3	348,
1647904234.495, 1647904234.642, 164	7904234.79, 1647904234.938, 1647904235.085, 1647904235.233, 1647904235.379, 16479042	35.527, 1647904238	5.675,
1647904235.822, 1647904235.97, 1647	904236.117, 1647904236.264, 1647904236.412, 1647904236.56, 1647904236.707, 164790423 7904237 444 1647904237 591 1647904237 729 1647904237 986 1647904238 024 1647904	6.854, 1647904237.	.002,
1647904238.329. 1647904238.476. 164	7904238 624. 1647904238 771. 1647904238 919. 1647904239.066. 1647904239.214. 1647904	239.361.	
1647904239.508, 1647904239.656, 164	7904239.803, 1647904239.951, 1647904240.098, 1647904240.246, 1647904240.393, 1647904	240.541,	
1647904240.688, 1647904240.835, 164	7904240.983, 1647904241.13, 1647904241.278, 1647904241.425, 1647904241.573, 16479042	41.72, 1647904241	.868,
1647904242.015, 1647904242.162, 164	7904242.31, 1647904242.457, 1647904242.605, 1647904242.752, 1647904242.9, 164790424		
Measured slope: 0.0607 torr/sec			
Failed leak check at Base pressure	ec		
Now will check to see if V1 or V3 i	s leaking		
Opening valve: Valve 2	-		
Set solenoid valve mask to 2	Т		

Figure 50: Complete Test – Showing Passing Result

CRDS Coordinator		- 🗆 X
Control		
Filename: CFIDS2315 SSIM Test 20220322 000620	. CSV	
New Output File		
Comment	RawData ValveRi	lesult
Measured slope: 0.0597 torr/sec		
Leak check failed spec: 0.04 torr/sec		
Failed leak check at Base pressure		
	V3 faile	ed leak test
Moving to: StateDone		
Closed all valves		
Last state: StateBasePLeakCheck		
Done!		
	Log	
Measured slope: 0.0597 torr/sec	SSIM Test X	
Leak check failed spec: 0.04 torr/sec		
Failed leak check at Base pressure		
V3 failed leak test Moving to: StateDone	SSIM Test is now complete	
Set solenoid valve mask to 0		
Closed all valves		
Last state: StateBasePLeakCheck	ОК	
Done:		

Figure 51: Complete Test – Showing Failing Result on Valve 3

- **11.** If the test shows no leaks, remove the caps from the SAMPLE and CAL ports, and set back up the SSIM for sampling as appropriate.
- **12.** If the test shows any leaks, contact support@picarro.com. Leaks within the SSIM are fairly simple to address if the user possesses replacement face-seal O-rings. Picarro Support can provide these parts, and guidance on how to replace them.
- **13.** If the test shows no internal leaks in the SSIM, but a leak is still suspected based on SSIM performance (downward sloped sample peaks, typically), refer to section 15, Troubleshooting for information on diagnosing a possible leak in the sample line between the SSIM and CRDS.

14. Best Practices

14.1 Leak Tightness

It is critical that there be no leaks in the plumbing connections associated with the SSIM2 and analyzer. It is possible to use the analyzer itself as a diagnostic to find leaks. The purge (zero air) should be nearly dry, as should the calibration standards.

The primary tool available to the user is the Leak Check described in section 13: Running the SSIM Leak Check. This check diagnoses leaks in the valves of the SSIM, where small leaks can lead to significant biasing of sample values. Other leaks can be diagnosed by peak shape as discussed below and can be addressed by tightening (but not overtightening) or replacing leaking fittings, especially the 1/8" fittings between the SSIM and instrument.

14.2 Use Case Examples

I have 100 mL of sample. Should I use SSIM2?

In this case, you have two alternatives:

- 1. Run the gas directly to the instrument inlet. Isotopic analyzers, and concentration analyzers modified for low flow typically draw about 25-40 sccm. So, 100 mL of sample run directly into the analyzer could produce as much as ~4 minutes of data, more than adequate to allow the sample delta value and concentration to stabilize. This approach will provide the most accurate concentration estimate, but will not provide a calculated set of Coordinator values for the sample, which the user will have to calculate offline using the data files.
- 2. Use the SSIM: In contrast, the user may use the SSIM and provide five discrete injections over roughly 45 minutes. This method will be less accurate on absolute concentration, but will provide replicate values that improve the precision by decreasing the sample-to-sample uncertainty.

I have less than 20 mL of sample. Will I get reliable results on the SSIM using dilution?

This depends upon the concentration of the gas used. If diluting the concentration by a factor of X, the concentration of the gas should ideally be at least X times the lower allowable concentration of the instrument. For an instrument with a 380 ppm lower level (e.g., for CO2), a sample of 5 ccs should have a concentration of at least 1520 ppm. If the diluted concentration falls below the lower limit of the instrument, the noise of the signal may become larger, and in some cases the delta value may be biased.

I have pure samples. How much sample do I need to dilute my sample in these cases?

SSIM2 can handle pure CO2 samples if the user has a well calibrated syringe capable of pulling a recommended 10 μ L sample size (0.45 μ moles, 20 μ g of CO2). Another option, which would allow replicate sampling, is for the user to dilute the sample into a sample bag (e.g., Tedlar or Cali5-Bond aluminum foil), targeting a value within the concentration range of the instrument, and then connecting that sample bag up to the SSIM sample port.

I have concentrated samples. Can I select dilution and more than one repeat per sample for either SSIM alone or SSIM+16-port?

Not automatically, no. The method for dilution relies on a fixed sample volume available to the SSIM in the user's bag or syringe, e.g.: 2 mL of total gas at 20,000 ppm CO2. Likewise, the repeat per sample option relies on a single sample container with enough gas to be run 20 mL x # repeats and does not require that the user close and reopen the valve between each repeat. Combining these two methods makes it impossible to draw in a small aliquot without pulling in a full 20 mL at a time.

Can the SSIM+16-port support multiple repeats per sample, and is this done automatically?

Yes, the SSIM+16-port handles the repeats automatically as long as there are at least 23 mL * # of repeats.

Can the 16-port handle more than 8 samples at a time, and can I select "Continuous Loop"

Technically yes, but the program is not currently written in a way to support pausing after 8 samples and encouraging the user to hook up 8 new samples. As such, "Continuous Loop" mode will just revisit the samples currently hooked up. This can work for some exceptional use cases (microcosm incubation studies where small sample removal is desired over long periods of time) but is not practical for most users. It is best to run in "One Time" mode and after the 8 positions are complete, hook up 8 new samples, and start the coordinator again.

14.3 Pump Lifetime

The A2000 vacuum pump diaphragms have a rated lifetime of 15,000 hours (1.7 years) of continuous operation. We recommend keeping a rough estimate of the running hours of the pump and replacing the diaphragms appropriately (see Picarro's Environmental Video Gallery for instructions). An aging pump will have the same symptom as a plumbing leak – the Coordinator program may time out. One way to monitor if the pump is functioning well is to track the SSIM2 Pressure on the GUI to determine if it can evacuate the sample chamber to 20 torr reliably.

15. Troubleshooting

15.1 Why did my sample get pulled in from my syringe or bag before the sampling step?

This typically happens if a user has either forgotten to include an on/off valve between the sample vessel and the SSIM injection port, or if the user has opened the sample valve too early in the process.

The sample valve should only be opened when the program reaches its second prompt, "OPEN VALVES," instead of "PLEASE HOOK UP ALL SAMPLE BAGS OR SYRINGES WITH VALVE CLOSED AND SELECT "RESUME" UNDER CONTROL TO CONTINUE." If the user opens the valve too early, the contents will be evacuated during the SSIM purge steps. It will also happen if the user does not include a valve between the sample/bag and the SSIM.

15.2 Why does my syringe plunger bounce back out when I push it in?

This is usually the behavior of a syringe whose needle is "cored" by septum material, preventing gas from being pushed out to the SSIM. Inspect the needle tip, replace the needle if needed, and consider purchasing a side-port needle, as described in section 5: Syringe Sample Delivery Requirements.



Figure 52: Syringe Needle Tip Showing Stuck "Cored" Septum Material

15.3 Why does my syringe plunger get pushed out during the run?

This is an uncommon issue typically relating to a leak across Valve 2 or 5, and should not happen during a standard run, even with dilution. If this occurs, run the SSIM Leak Check, and call technical support to help assist with a solution.

15.4 Why is my 16-port valve not recognized?

If the valve control cables are not appropriately attached (typically to COM2 on the back of the analyzer), or if the Setup Tool is not correctly configured to recognize that port, this may cause errors in the Coordinator program. If this occurs, consult the user manual for the Distribution Manifold or contact Picarro. To ensure a reliable electrical connection, engage the locking screws on the valve control cables at both the instrument and SSIM ends.

15.5 Why are my concentrations different from what I calculated or expected?

Concentration values depend on a few factors like dead volume and regulator pressure. These topics are discussed in length in APPENDIX C –Dilution and Dilution Factors: Considerations and Calculations.
15.6 Why do my peaks drop (or rise) significantly during a run?



Figure 53: Leak in Inlet Line Between SSIM and CRDS

There are at least two reasons why the slope of a SSIM injection might drop or rise during the injection: an inlet line leak, and a SSIM Valve 1 leak. They can be differentiated by the following metrics.

1. A leak in the inlet line between the SSIM out and instrument inlet (see Figure 52 above) is the result of an inward leak of air from ambient. The slope of this peak might trend either up or down, but will typically trend downward as sample concentrations for most instruments are often above ambient. The delta values for isotopic instruments will likely change during this leak unless the ambient and sample delta values are the same (this occurred, but is not visible in the image above due to Y axis scaling of the d15N and d18O values). This sort of leak results from a poor connection, and is possible because the inlet line drops well below ambient pressure while the sample is pulled into the instrument. This sort of leak will not be detected by the SSIM Leak Test coordinator, which cannot assess leaks in any lines outside the SSIM itself (as it cannot control the behavior of gas entering or exiting the SSIM).

2. A cross-port leak on SSIM Valve 1 allows zero air (or N2) from the carrier gas flow to bleed into the SSIM sample chamber or the line to the CRDS. This leak can be diagnosed by the fact that the trend in concentration is always downward, while the delta value remains relatively unaffected. It can also be confirmed by running the SSIM Leak Test coordinator (see section 13, Running the SSIM Leak Check).



Figure 54: SSIM Valve 1 Cross-port Leak

15.7 Why won't my SSIM Pressure approach zero between samples?

See Figure 54 for an example. This is typically due to a pump that is either off or failing to create an adequate vacuum. Check that the pump is on, that the vacuum line is tight at the back of the SSIM and the inlet of the SSIM pump, and if needed, replace the pump diaphragms. Replacement pump diaphragms can be purchased at store.picarro.com by searching for "pump diaphragms" and choosing the model appropriate to the user's setup, typically the A2000 Vacuubrand pump (silver).



Figure 55: SSIM Pressure Failing to Approach Zero Between Samples

15.8 Why does my SSIM Pressure value show up as a value between 0 and 1, rather than the expected 0 – ~1000 torr?

This occasionally happens when a value in the SSIM pressure reading code is set for internal testing at the Picarro factory and is not returned to the value appropriate for the GUI. Support can assist with remedying this, or the user can navigate to the following file:

C:\picarro\G2000\AddOns\SSIM\ReadExtSensor

and change "queryCommand = u8" to instead read "queryCommand =u7".

APPENDIX A – Adapting Greenhouse Gas Analyzers for SSIM2 Use

A.1 Introduction

The inlet orifice on most Picarro analyzers is used to create near-constant volume flow in a simple flow path without the need for additional sensors and controllers. If the SSIM2 module will be used with analyzers that are used for measuring greenhouse gases (such as the G2301, G2401, and G2508), this orifice may need to be changed to slow the flow to the analyzer.

The internal volume of the SSIM2 requires that sample be routed to the instrument at a slower flow rate than many greenhouse gas analyzers are tuned to. The following orifice replacement instructions guide the user on how to swap in a lower-flow critical orifice in the instrument flow path to reduce the instrument flow from ~250-350 sccm to <50 sccm.



Before making a change to a different orifice, check with Picarro Support to ensure that such a change will not alter the flow characteristics of the instrument in a way that could destabilize instrument performance. The typical replacement orifice is A-7-NY, P/N S3169, which can be ordered from support@picarro.com.

A.2 Orifice Change Instructions

Tools Needed

For Orifice Replacement:

- A-7-NY replacement orifice in ¹/₄" tube (P/N S3169)
- 2 mm hex (Allen) wrench
- 2x 9/16" wrench
- 5/8" wrench
- 11/16" wrench
- 7 mm or small adjustable wrench

For Leak Check:

- A cylinder of dry gas
- Snoop™ or equivalent leak check solution

Orifice Change Steps

1. Remove the cover of the analyzer cover using the 2mm hex driver to remove the six small screws. Place the screws in an appropriate container to avoid losing them.



Figure 56: Cover Removal

- 2. Remove the lid and note the location of the hot box (the larger of the two silver boxes which sits to the right rear of the instrument when seen from the front of the instrument).
- **3.** Using either a 7 mm or small adjustable wrench, back off the two nuts on the hot box lid about a turn or two leaving the nuts on the screw just enough to loosen and lift the lid.



Figure 57: Opening Hot Box Cover

4. Remove the small foam piece at the inlet and the larger foam piece covering the filter and orifice (Figure 57). This will expose the bulkhead nut (which must be loosened for filter and orifice removal), the particulate filter, and orifice).





Figure 58: Foam Piece Removal

- **5.** Loosen the bulkhead nut using a 5/8" wrench (Figure 58). This nut retains the inlet particulate filter foam cover (B). Back the nut off far enough so the foam and metal cover can be removed. This will expose the orifice downstream of the filter (Figure 58).
- **6.** Using a 9/16" and 11/16' wrenches, loosen the filter input nut (Figure 58).



Figure 59: Loosening Bulkhead Nut and Filter Input Connection

7. Place the 11/16" wrench on the flats of the particulate filter inlet and the 9/16" wrench on the inlet nut of the orifice (Figure 59), and loosen the nut until you can remove the particulate filter (Figure 60).



Figure 60: Loosening Orifice Inlet Nut from Filter Outlet

8. Place the 11/16" wrench on the flats of the particulate filter inlet and the 9/16" wrench on the inlet nut of the orifice (Figure 60), and loosen the nut until you can remove the particulate filter.



Figure 61: Filter Removed



Carefully note the location of the nylon orifice within the current stainless-steel tube and ensure the replacement orifice is oriented in the same direction (Figure 61). This ensures correct flow characteristics and flow rate.



In the next step, be careful to "back" the wrench on the valve side so you do not loosen the fitting from the valve block body.

9. Use two 9/16" wrenches to disconnect the orifice from the inlet valve block. Remove the orifice.



Figure 62: Orifice Location and Orientation

- **10.** Install the new orifice (Figure 62) in place of the old, with the nylon orifice in the same orientation within the tubing assemble as the original orifice tubing.
- **11.** Reassemble the particulate filter to the orifice inlet. Ensure the flow direction arrow on the filter points away from the analyzer rear panel.
- **12.** Leave the foam pieces to the side, and Hot Box lid open so leak testing can be performed (next section).



Figure 63: Orifice and Filter Installation

Leak Test

- 1. With the instrument still turned off, and absorbent cloth or paper under all relevant fittings, connect a tank of dry gas to the analyzer inlet and set the pressure to 2-3 PSIG (Figure 63).
- **2.** Apply Snoop[™] or an equivalent leak test solution to each fitting that was broken, watching for any bubbles to form.
- **3.** If no bubbles form, the system is ready to be used. Wipe away all excess soap solution, close and tighten the Hot Box lid, replace the two foam pieces, and replace the analyzer cover.



Figure 64: Leak Test After Reassembly

APPENDIX B – Flow Diagram and Valve Sequences

B.1 SSIM Flow Diagram

The purpose of the SSIM is to make it possible to spend more time analyzing a clean discrete sample on a Picarro CRDS. It does so by preparing a consistent volume (20 ccs) of gas, variously purging, and evacuating the lines upstream and downstream of this sample volume of any residual gas from prior samples, and then slowly allowing the gas to flow passively to the CRDS.

The SSIM has two points of connection to the Picarro CRDS analyzer—a USB A-B cable for power and communications, and a 15-pin valve cable. This section discusses the purpose and function of the valves powered by this valve cable.

The CRDS analyzer controls five valves within the SSIM using the valve cable. These valves control the flow of carrier, calibration, and sample gas to the CRDS or vacuum line. The schematic in Figure 64 below shows the flow diagram of the SSIM. 3-way valves are noted as black circles with either blue pathways (normally open) or dashed-red pathways (normally closed). Overlapping blue and dashedred lines indicate the common port of the 3-way valve. A black circle with only a dashed-red pathway shows a normally closed on/off valve.



Figure 65: Flow Diagram with Related Components

Broadly, the valves within the SSIM are configured to provide a constant flow of either zero air, sample gas, or calibration gas to the CRDS while the other positions are stopped. During operation, the SSIM switches every few seconds or minutes between a variety of states to evacuate and backflush the sample volume, allow sample air or calibration air into the sample volume, and then passively pull the sample or calibration air from the sample volume.

Before we describe the flow pathways fully, we must define a few critical terms.

B.2 Terminology

Valve: For the discussion in this section, "Valve" refers to a solenoid valve in either an on/off configuration, or a 3-way configuration. The state of the solenoid changes when a current is applied to the valve.

3-way Valve (or Solenoid): A solenoid valve with three ports, for which a shared port has a common pathway from either a normally open or normally closed position depending on whether the valve is energized (on) or de-energized (off), respectively.

Valve State: Whether a valve is energized (powered, receiving a current of electricity) or de-energized (off, receiving no current of electricity).

Common: The port on a 3-way valve that is common to the flow path whether one or the other of the two optional paths, "normally open" or "normally closed", is selected.

Normally Open: the position or pathway a valve defaults to when it is deenergized (when it is off). In a 3-way valve, the common position accepts gas from the "normally open" position when it is de-energized. This term can also be applied to on/off valves if they default to open when off, however this is a fairly uncommon choice, since it is usually safer for valves to default to a closed position (no gas flow) when a system loses power.

Normally Closed: The position or pathway a valve defaults to when it is energized (on). In a 3-way valve, the common position accepts gas from the "normally closed" position when it is energized. Most on/off solenoid valves are configured as "normally closed" because it makes most sense for them to default to a closed state when power to a system fails.

Valve Number: The arbitrary value from 1 to 5 assigned to a particular valve in the SSIM.

Valve Code: The computed binary representation of a given valve n when the valve is energized, where Valve Code = 2(n-1). For Valve 1 when energized, the Valve Code would be 2(1-1) = 20 = 1. For Valve 5, when energized, the Valve Code = 2(5-1) = 24 = 16. A de-energized valve has a Valve Code of 0.

Valve Mask: A single value, here a binary "bitmask," representing the state of all valves in the system, where each valve value is added to the total only if that valve is energized. Valve Mask follows the form: sum (ValveCode 1 ... ValveCode 5). This format helps to simplify the reporting of multiple valve states in data files, since it requires only one column rather than many (here 5). By proof, the integer represented by a bitmask can only ever describe one state of the system. I.e.: a value of 31 (1 + 2 + 4 + 8 + 16) can only ever describe the state where valves 1, 2, 3, 4, and 5 are all energized. No other combination of valve values can ever add up to the same integer sum, simplifying interpretation by an individual or computer. An example of the Valve Mask of the SSIM is 17. This is the sum of the values 1 and 16 uniquely, suggesting that Valve 1 (1) and Valve 5 (16) are energized, while all other valves are de-energized.

Valve Number	Valve Code
1	= 2(1-1) = 1
2	= 2(2-1) = 2
3	= 2(3-1) = 4
4	= 2(4-1) = 8
5	= 2(5-1) = 16

Table 8: Valve Number and Associated Valve Code

Example:

Consider the default unpowered state of the SSIM when it is first turned on with zero air connected to the back, and the sample outline connected to the CRDS. The default normally open (non-energized) state can be represented by the blue lines in Figure 64 above. In this state, the following flow occurs:

- 1. Zero air routes through a tee and to V3, where it is routed to the CRDS.
- **2.** The sample line is stoppered at V2.
- 3. The calibration tank line is stoppered at V5.
- **4.** Despite the connection at V2 to the 20 ml sample volume, the sample does not flow to the CRDS because it is stoppered at V3.
- **5.** The vacuum line is stoppered at V4. V4 is an on/off valve, so when it is not energized, it is closed. This has the effect of not pulling a vacuum in the 20 mL sample volume.

B.3 Valve Mask Sequences Associated with Various Coordinators

The following tables describe the displayed ValveMask values and associated valve states during an SSIM sampling sequence (variously 1, 2, or 8 samples).

Valve Mask	Energized Valves	Time (sec)	Description	
8	4	20	Vacuum pumps down the SSIM Chamber through V2 up to V3	
5	1, 3	20	ZA (Zero Air) gas flows through the SSIM Chamber to the Analyzer	
8	4	20	Vacuum pumps down the SSIM Chamber through V2 up to V3	
5	1, 3	60	ZA gas flows through the SSIM Chamber to the Analyzer	
8	4	20+	Vacuum pumps down the SSIM Chamber through V2 up to V3	
6	2, 3	8	Valve 2 opens to allow Sample to flow into the SSIM Chamber while the analyzer creates a vacuum up to Valve 2	
4	3	420 or 720	The Analyzer begins to pull on the Sample in the SIM Chamber	

Table 9: Overview of Injection Sequence – Sample

Table 10:	Overview	of Injection	Sequence -	Calibration
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Valve Mask	Energized Valves	Time (sec)	Description	
8	4	20	Vacuum pumps down the SSIM Chamber through V2 up to V3	
5	1, 3	20	ZA gas flows through the SSIM Chamber to the Analyzer	
8	4	20	Vacuum pumps down the SSIM Chamber through V2 up to V3	
5	1, 3	60	ZA gas flows through the SSIM Chamber to the Analyzer	
8	4	20+	Vacuum pumps down the SSIM Chamber through V2 up to V3	
22	2, 3, 5	8	Valves 2 and 5 open to allow Standard to flow into the SSIM Chamber while the analyzer creates a vacuum up to Valve 2	

Valve	Energized	Time	Description
Mask	Valves	(sec)	
4	3	420 or 720	The Analyzer begins to pull on the Standard in the SSIM Chamber

The SSIM2 can also be paired with a 16-port distribution manifold (A0311). When paired with a 16 port, it is possible to analyze 8 discrete samples in sequence. The Valve Mask below is the same during the cycle, though the A0311 valve will move position along with the SSIM to evacuate the odd-numbered sample ports between the eight samples in the even-numbered ports.

Valve Mask	Energized Valves	MPV Port	Time (sec)	Description
8	4	Odd	20	Vacuum pumps down the SSIM Chamber through V2 up to V3
5	1, 3	Odd	20	ZA gas flows through the SSIM Chamber to the Analyzer
8	4	Odd	20	Vacuum pumps down the SSIM Chamber through V2 up to V3
5	1, 3	Odd	60	ZA gas flows through the SSIM Chamber to the Analyzer
8	4	Odd	20+	Vacuum pumps down the SSIM Chamber through V2 up to V3
6	2, 3	Even	8	Valve 2 opens to allow Sample to flow into the SSIM Chamber while the analyzer creates a vacuum up to Valve 2
4	3	Even	420 or 720	Analyzer pulls sample through V2 and V3, slowly creating a vacuum in the chamber with time

 Table 11: Overview of Injection Sequence – with 16-port manifold

During a sequence with dilution, one additional step is performed briefly before the sample is sent to the CRDS. After the sample is pulled into the sample volume, and after the user selects "resume," the valve mask is briefly changed to 1 to allow zero air into the SSIM sample volume. After this, the sample is pulled into the instrument as usual.

Valve Mask	Energized Valves	Time (sec)	Description	
8	4	20	Vacuum pumps down the SSIM Chamber through V2 up to V3	
5	1, 3	20	ZA gas flows through the SSIM Chamber to the Analyzer	
8	4	20	Vacuum pumps down the SSIM Chamber through V2 up to V3	
5	1, 3	60	ZA gas flows through the SSIM Chamber to the Analyzer	
8	4	20+	Vacuum pumps down the SSIM Chamber through V2 up to V3	
6	2, 3	8	Valve 2 opens to allow Sample to flow into the SSIM Chamber while the analyzer creates a vacuum up to Valve 2.	
1	1	3	ZA flows into the SSIM Chamber and through to V3, filling up the remaining volume to the pressure of the regulator.	
4	3	420 or 720	Analyzer pulls sample through V2 and V3, slowly creating a vacuum in the chamber with time	

Table 12: Overview of Injection Sequence – Dilution

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The Double Inject (DI) mode allows for more accurate concentration results. The final 6 and 4 Valve Mask steps are repeated without pump down (8) and sweepouts (5), allowing sample to flow back into the sample volume and sampling lines while the analyzer is pulling in the first injection, with the effect that the dilution of the sample is reduced.

Valve Mask	Energized Valves	Time (sec)	Description	
8	4	20	Vacuum pumps down the SSIM Chamber through V2 up to V3.	
5	1, 3	20	ZA gas flows through the SSIM Chamber to the Analyzer.	
8	4	20	Vacuum pumps down the SSIM Chamber through V2 up to V3.	
5	1, 3	60	ZA gas flows through the SSIM Chamber to the Analyzer.	
8	4	20+	Vacuum pumps down the SSIM Chamber through V2 up to V3.	
6	2, 3	8	Valve 2 opens to allow Sample to flow into the SSIM Chamber while the analyzer creates a vacuum up to Valve 2.	
4	3	180+	Analyzer pulls sample through V2 and V3, slowly creating a vacuum in the chamber with time.	
6	2, 3	8	Valve 2 opens to allow Sample to flow into the SSIM Chamber while the analyzer creates a vacuum up to Valve 2.	
4	3	420 or 720	Analyzer pulls sample through V2 and V3, slowly creating a vacuum in the chamber with time. This time, the sample is less dilute because it is being diluted by gas that is ~95% sample, rather than zero air.	

Table 13: Overview of Injection Sequence – Double Inject (DI)

APPENDIX C – Dilution and Dilution Factors: Considerations and Calculations

Dilution of sample concentration is an important consideration for SSIM users. Intentional sample dilution using the "Sample Dilution" option in the SSIM Coordinator requires a few method considerations to ensure accurate dilution factors. Similarly, the unintentional slight dilution of the sample concentration by system tubing dead volumes requires some planning ahead for users intending to characterize the concentration of their gas accurately. This section aims to discuss both forms of dilution in a variety of contexts.

C.1 Coordinator Sample Dilution

Best practices: Syringe Choice

Diluting high concentration samples must be done with small sample syringes filled only with the amount of sample needed for the dilution procedure. If the user has a 20 mL syringe filled with a high concentration gas and desires a 20 times dilution (target sample volume: 1 mL), all of the available 20 mL of gas will be pulled into the SSIM sample volume when the sampling step begins, preventing the user from diluting the sample. To avoid this happening, choose instead a small-volume syringe which can be used to provide a reasonably accurate volume of gas. 1 to 5 mL syringes are typically best.

Dilution with Sample Repeats?

As discussed in a prior section, dilution is not practicable using the Coordinator's "sample repeats" feature. When running diluted samples, run with sample repeats set to the default value of 1. This is not practicable because the user would have to control the aliquoting of e.g. 1 mL of gas repeatedly from a larger volume syringe, keeping up with the automatic behavior of the Coordinator as it runs repeats. This is not currently supported.

Sample Dilution From the 16-Port

Sample dilution is supported with the 16-port valve, but the user should be aware that the amount of gas required for the dilution may be slightly higher than expected due to the volume of lines between the sample port and the SSIM. Picarro recommends increasing the volume of gas 50-100% at a 16-port sample port to achieve a dilution. For example, if a 20-times dilution is desired, the user may want to try 1.5-2 mL of gas at a given port, rather than the 1 mL required for the SSIM alone.

C.2 Calculating a Dilution Factor

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Calculating the actual dilution associated with the dilution mode in the SSIM coordinator is not quite as simple as dividing the provided sample volume (e.g., 5 ccs) by 20 ccs. The ambient pressure, zero air cylinder's delivery pressure (in gauge pressure units above ambient), and dead volumes may all affect this calculation. These equations (provided here in PSI and torr units only) represent the best effort at standardizing the dilution factor associated with a small sample. Some recommendations are also provided below for determining empirical setup-specific relationships for back-calculating concentration.

The dilution factor can be calculated using the following formula where the pressurecylinder is the delivery pressure in gauge pressure (above ambient) as read on the delivery side gauge, the samplevolume is the volume of sample provided to the SSIM (typically <20 ccs here), the chambervolume is the volume of the chamber, 20 ccs, and the pressureambient is the ambient atmospheric pressure of the laboratory in torr.



Figure 66: Injection Sequence – Dilution

For example: If a user is at sea level (~760 torr) and injects 5 mL of sample gas from a syringe and is using a regulator with a delivery pressure of 3.5 PSIG, the dilution factor is not 4 (20/5), but 4.95 due to the delivery pressure of the gas. This ratio will be closer to the estimated ratio when a lower pressure of gas is used. Picarro recommends a typical gauge pressure of 2-3 PSIG to avoid issues with accuracy in the 0-2 PSIG range.



Figure 67: Injection Sequence – Dilution: Example

C.3 Determining a Setup-specific, or Empirical Correction Factor

If the equation above does not accurately capture the dilution effect on a user's configuration, factors like the accuracy of the regulator pressure gauge or the

dimensions of the sample container may contribute to this effect. Picarro provides the following guidance on improving this equation and/or creating an empirical relationship.

- **1.** Make sure to use the provided C-shaped 1/8" tube between the SSIM and instrument to reduce any dilution effects downstream of the sample volume.
- 2. Check the accuracy of the delivery pressure value (pressuredelivery) used with an accurate pressure gauge. A regulator gauge is seldom as accurate as a dedicated pressure sensor.
- **3.** Similarly, whenever possible, use a regulator with an on/off toggle valve. If the delivery pressure setting is consistent from use to use because the delivery pressure adjustment knob isn't spun in and out each time, the dilution effect will be more consistent.
- 4. Check for any dead volume considerations relating to the interface used for the syringe or bag. It may be necessary to adjust the chambervolume value up slightly if an extra 1 or 2 ccs of volume exists between the sample vessel and the chamber.
- 5. Determining an empirical relationship. Using a consistent delivery pressure from the zero air tank, take a known gas, and run back to back samples starting at 1 cc, and moving up to 20 ccs. The exact relationship and dilution factor for a given sample volume should be calculable from a fit to this empirical relationship if the hardware is not changed between uses.

C.4 Dilution During Undiluted Single-Injection

Though single-injection undiluted samples will register as close to their true concentration, users should be aware that a small amount of dilution is brought about by the zero air in the sample lines between SSIM V3 and the cavity that arrives at the cavity before the sample. This leads to an unavoidable dilution on order 5%. This effect can be minimized using the double-injection technique when the associated coordinator is present.

C.5 Dilution During Undiluted Dual-Injection

The dual-injection method uses twice the volume of gas run in immediate succession without an intervening evacuation step, to ensure that the gas that precedes the second sample (the slightly diluted first sample) is close to the concentration of the second sample.

For further information on dilution effects with single and dual injection coordinators, refer to the Picarro Application Note, Measuring Small Volume Gas Concentrations with the SSIM linked here: AN038.

APPENDIX D – Software Installation

D.1 Coordinator Program Installation

Typically, the coordinator for the SSIM is already installed and can be launched from the Coordinator Launcher icon located on the desktop. Under certain circumstances, the user may have to install the coordinator. Follow the instructions below if the coordinator is not installed (there are no SSIM-related shortcuts on the Desktop).

The Installer is available on the provided USB Flash drive, or it can be requested from Picarro Customer Support.

 Double click on the file setup_SSIM2.exe in order to begin the installation process. The Picarro SSIM2 AddOn Installer window (Figure 67) will appear. Click Next.

You will be prompted to select a destination for the installed files (Figure 68). It is recommended that the user maintains the default entries.



Figure 68: Picarro SSIM2 Add On Installer

🖟 Setup - Picarro SSIM AddOn Installer
Select Destination Location Where should Picarro SSIM AddOn Installer be installed?
Setup will install Picarro SSIM AddOn Installer into the following folder.
To continue, click Next. If you would like to select a different folder, click Browse.
C:\Picarro\G2000 Browse
At least 1.5 MB of free disk space is required.
< <u>B</u> ack <u>N</u> ext > Cancel

Figure 69: Picarro SSIM2 Add On Installer Path for Installation

- 2. Upon clicking Next, you will be prompted to select the type of CRDS analyzer. The drop down menu includes several options (with the below options not being comprehensive):
 - G2101-i: Measures isotopic CO2 (discontinued)
 - G2132-i: Measures isotopic CH4
 - G2201-i: Measures isotopic CO2 and CH4

Select Components	
Which components should be install	ed?
Select the components you want to install. Click Next when you are rea	install; clear the components you do not want to dy to continue.
G2101-i	~
G2101-i	
G2132-i	
G2201-i	
	< Back Next > Cancel

Figure 70: Picarro SSIM2 Add On Installer Component Selection

3. After selecting the correct instrument model and clicking Next, a window will appear asking for a folder in which to place the program's shortcuts. It is recommended that the user maintains the default entries.

🕫 Setup - Picarro SSIM AddOn Installer
Select Start Menu Folder Where should Setup place the program's shortcuts?
Setup will create the program's shortcuts in the following Start Menu folder.
To continue, click Next. If you would like to select a different folder, click Browse.
Picarro SSIM Software Browse
< <u>Back</u> <u>N</u> ext > Cancel

Figure 71: Picarro SSIM2 Add-On Installer – Shortcut Path

4. Upon clicking Next, a review window will appear that outlines the details of all previous selections that had been made during the installation process. Click Install after reviewing your choices, or click Back to make any changes.

1🖥 Setup - Picarro SSIM AddOn Installer
Ready to Install Setup is now ready to begin installing Picarro SSIM AddOn Installer on your computer.
Click Install to continue with the installation, or click Back if you want to review or change any settings.
Destination location: C:\Picarro\G2000
Setup type: G2101-i
Selected components: Isotopic CO2 Isotopic CO2 with CH4 correction
Start Menu folder: Picarro SSIM Software
< <u>B</u> ack Install Cancel

Figure 72: Picarro SSIM2 Add On Installer – Verification and Install

5. When the installation is complete, the following window will appear. Click Finish to end. Several icons will appear on the desktop following the completion of installation.



Figure 73: Picarro SSIM2 Add On Installer – Installation Completion

D.2 Arduino Driver Installation

The SSIM software installation adds a shortcut to a Read SSIM Pressure script. The pressure sensor is being controlled by the Arduino board (the USB cable connection of the SSIM). To use that connection, proper drivers are required by the system.

- 1. Download the Arduino software from: https://www.arduino.cc/en/software
- 2. Install it with default settings on the Analyzer.

After this step, the Read SSIM Pressure should now find the Arduino board on one of the COM ports and will start reporting the SSIM Pressure in the main GUI and the results data files. Please contact support@picarro.com if you have any questions about this step.

D.3 Ready Test

Some users will wish to perform a ready check on the instrument to confirm gas is flowing properly from the SSIM to the instrument. For the ready check, the pump should be on and connected to the SSIM. Zero air should be connected to the SSIM also. The Ready Test program will use a reference gas attached to the CAL port to ensure the instrument is ready to make measurements. It is best not to use

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an expensive calibration standard for this test so as to save gas—a simple tank containing the target gas species should be enough.

1. Locate the Coordinator Launcher program on the desktop and double click it. A screen will appear (Figure 73), allowing the user to choose from various programs, including "Ready Test." Choose the Ready Test mode, then click Launch to continue.

Picarro Coordina	_		\times			
Picarro Coordi	nator	Launc	her			
Select Coordinator	SSIM	G2201-i	~			
	SSIM SSIM SSIM	G2201-i Ready Te Leak Test	st			
Copyright Picarro, Inc. 1999-2011						

Figure 74: Picarro Coordinator Launcher – Ready Test Selection



The above image was taken from a G2201-I analyzer. Depending on the CRDS instrument being used, the drop-down menu may vary.

Upon clicking "Launch," the User Editable Parameters screen (Figure 74) will appear. The time indicated is the time after which the program will shut down if the appropriate instrument conditions have not been met. It is not recommended to change the default time. Click OK.

User Editable Parameters		
Maximum test duration (minutes)	10.0	
		ОК

Figure 75: Maximum Ready Test Time

3. Upon clicking OK, the CRDS Coordinator window will appear (Figure 75).

A file is automatically started each time the Coordinator is started. Various messages about the state of the system are displayed in the bottom window and prompts to the user are also noted there in capital letters.

The upper portion of the coordinator window shows the various parameters measured during analysis and is identical to the data that is saved in the CSV file.

4. The Ready Test program will run until the analyzer has met the necessary conditions that determine stability or it will shut down after ten minutes. Every thirty seconds that it is running, an update will be printed.

Following the installation of the Coordinator program and running the Ready Test, it is time to begin analysis by launching the Coordinator program. Based on one's hardware configuration, refer to one of the sections listed below:

- 8, Operation: Measurement SSIM2 and Analyzer
- 9, Operation: Measurement SSIM2 and 16-Port Manifold and Analyzer

CRDS Coordinator											
Control											
New output file											
Filename	CFFD52053_SSIM_20130109_224030.csv										
Date/Time	Delta Mean	Delta Std	12CO2 Mean	12CO2 Std	c12_pzt_st	c13_pzt_st	adjust_87	adjust_88	Cavity Pre	Cavity Te	Warm Box
01/09/13 14	-1539.489	0.000	1.007	0.000	144.573	160.456	0.0000e+000	0.0000e+000	140.006	45.001	45.000
01/09/13 14	-1125.715	638.956	8.399	13.558	145.260	215.746	2.8686e-005	0.0000e+000	140.015	45.001	44.999
01/09/13 14	-60.995	13.394	151.346	48.180	142.039	265.501	5.3808e-005	1.2146e-005	139.998	45.000	44.999
01/09/13 14	-48.425	1.815	259.346	19.757	130.315	248.894	-7.1959e-006	5.5821e-007	139.992	45.000	44.998
01/09/13 14	-45.687	2.195	311.323	10.933	178.362	186.202	-7.1513e-006	2.7478e-005	139.993	45.000	44.998
01/09/13 14	-45.518	1.680	340.756	6.558	145.345	156.785	-6.0042e-007	-2.6103e-005	140.005	44.999	44.997
01/09/13 14	-44,482	2.099	357.947	3.545	133.076	161.731	7.9056e-006	-1.2780e-006	140.000	44.999	44.997
01/09/13 14	-45.379	1.425	367.849	2.192	132.620	215.152	1.1578e-005	2.9469e-005	139.996	44.999	44.996
01/09/13 14	-45.663	1.558	373.687	1.049	135.450	350.492	-2.3619e-005	-5.2260e-005	139.997	44.998	44.996
01/09/13 14	-44.799	2.064	377.267	0.831	156.469	188.411	4.9906e-006	2.6009e-005	139.999	44.998	44.995
Log											
Set solenoid	i valve mas.	k to 20									<u>^</u>
Set solenoid	i vaive mas.	x to 22									
Set solenoid	i vaive mas	k to 20									
Set solenoid valve mask to 22											
30 second update											
Evacuating the cavity											
Set solenoid	d valve mas	k to 0									
Done!											_
FSM thread f	finished										~

Figure 76: CRDS Coordinator Window

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
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- Picarro Web Store

Contact Picarro for questions regarding specific applications and additional information.

US 1	Fechnical Support:	Inter	national Technical Support:	Customer Service:		
Email:	support@picarro.com	<u>Email:</u>	support@picarro.com	<u>Email:</u>	support@picarro.com	
Phone:	+1 408 962 3991	Phone:	+31 85 888 1650	Phone:	+1 408 962 3992	