# **NAVA** The **Abs**olute Standard

# MAX-iR<sup>™</sup> FTIR Gas Analyzer

Operating Manual Part Number 107-0131



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#### About this Manual

The MAX-iR is intended for use in non-hazardous, safe, or general-purpose classification areas. This operational manual provides instructions for setup and best practices in using the MAX-iR. By following the sections outlined below, you will cover all the basic installation, setup, and qualification procedures required to operate the MAX-iR.

#### Contact Information and Technical Support

Safe and reliable operation of this equipment is conditional on all installation, operation and maintenance procedures being carried out in accordance with the appropriate manuals, by personnel having appropriate qualifications, experience, and training. Failure to observe the requirements of the manual may result in the user being held responsible for the consequences and may invalidate any warranty.

For application or technical support:

- 1. Dial 1-800-532-4752
- 2. Select "option 2" for Unity Lab Services technical support.
- 3. For your instrument type, select "option 6" for Molecular, Vibrational Spectroscopy Based Spectrometers.
- Alternatively, you can e-mail for support to: us.techsupport.analyze@thermofisher.com

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## 1 MAX-iR Safety

This chapter identifies potentially hazardous conditions which may be present during normal operation of the MAX-iR. This system is intended for use in non-hazardous, safe, or general-purpose area classifications. The MAX-iR is not certified for use in a hazardous area.

## System Training and Support

Thermo Fisher Scientific offers both on-site and web-based training programs for companies interested in educating their employees on the MAX-iR operation. In addition, advanced maintenance, repair, and applications services are available through the MAX-Advantage Service & Support Contract.

To schedule a training session or set up a support contract, please contact Technical Support (see Contact Information and Technical Support).

## Equipment Intended Use

The equipment is intended for indoor use in an ordinary location. The equipment should be kept dry and should be operated only in a non-explosive and non-toxic environment.

The equipment is intended for the analysis of non-toxic, non-caustic and diluted combustible gases (gases below 25% of their lower explosive limit).

See the installation section of this manual for required operating temperature, power requirements, and other specific requirements for proper installation and operation of the equipment.

## Hazard Notices Used in this Manual

The equipment poses potential hazards during installation, operation, and service. In this manual you will find four levels of safety precautions and important notices that conform to ANSI Z535 and ISO 3864. These hazard notices identify the hazard, explain how to avoid the hazard, and identify probable consequences of not avoiding the hazard. These notations are provided primarily in the procedural sections and are intended to complement the ANSI and/or ISO safety labels physically located on the equipment.

## 

**Avoid hazard.** Danger notifications indicate a hazardous situation which, if not avoided, <u>will</u> result in serious injury or death. The hazard is imminent.

## 

**Avoid hazard**. Warning notifications indicate a hazardous situation which, if not avoided, <u>could</u> result in serious injury or death. The hazard is possible.

## 

**Avoid hazard.** Caution notifications indicate a hazardous situation which, if not avoided, could result in a moderate or minor injury and/or equipment damage.

Notice notifications provide information to follow to avoid damaging system hardware or losing data.

## Symbols Used on the Equipment

	On (Power) IEC 60417, No 5007
$\bigcirc$	Off (Supply) IEC 60417, No 5008
	Protective Earth Terminal IEC 60417, No 5019
$\blacksquare$	Fuse IEC 60417, No 5016
	General waring, refer to manual for further instructions ISO 7010, W001
4	Warning, risk of electric shock ISO 7010, W012
	Warning, hot surface. ISO 7010, W0017
<b>(</b> E	Equipment is compliant with requirements for the European Union. See Declaration of Conformity for further details on Directives and Standards used for compliance.
UK CA	Equipment is compliant with requirements for Great Britain. See Declaration of Conformity for further details on Directives and Standards used for compliance.
X	The equipment should not be discarded as unsorted waste but must be sent to separate collection facilities for recovery and recycling.

## General Safety Precautions

This section lists some of the hazards that could be encountered with the equipment. More specific hazards are listed throughout the manual in the relevant sections.

## 

**Read the Manual before Operation:** All operators should read and understand this manual before using the equipment. It is essential for all personnel to understand the operation procedures and how to avoid potential hazards associated with the use of the equipment.

## 

**Only trained and experienced service persons should perform maintenance and repairs.** Contact Max Analytical for service and/or training.

## 

**Do not substitute parts or modify equipment.** Do not install substitute parts or perform any modifications to the hardware that have not been authorized by Max Analytical.

## 

**Use the proper power cord.** Only use a detachable power cord that is rated for the voltage and current specified on the equipment nameplate. The power cord should have a minimum cross-sectional area of 0.75 mm<sup>2</sup> (18AWG). The power cord should be certified by an appropriately qualified agency such as UL, VDE, or Semko.

## 

**Explosion Hazard**: The equipment will expose sample gas to heated surfaces and is intended for the analysis of non- flammable gas mixtures only. The concentration of any flammable gases in the sample stream should be less than 25% of the lower explosive limit (LEL). Failure to comply may result in injury or death.

## 

**Inhalation Hazard**: Be sure that any sample exhaust ports are properly connected to a safe vent location to prevent exposure to potentially dangerous gas mixtures. Inhalation of certain gases may cause headache, dizziness, nausea, bodily irritation, irregular heartbeat, or death.

## 

**Shock Hazard**: The system enclosure contains high voltage. The system must be de-energized during all maintenance and service operations. Failure to comply could result in injury or death.

## 

**Compressed Gas Hazard:** The equipment requires nitrogen for purge and calibration gas cylinders for analysis. Check for leaks before turning on any gas supply and wear safety glasses to prevent injury. Failure to comply could result in injury.

## 

**Burn Hazard**: The equipment contains heated components inside the enclosure and hot fittings on the back panel. Disconnect power and allow the equipment to cool before servicing and avoid touching the fittings on the back of the equipment. Failure to comply could result in injury.

## 

**Equipment Damage and Ergonomic Hazard:** The MAX-iR weighs approximately 75 lbs (34 kg), exceeding the recommended lifting weight (RLW) for one person. Improperly lifting the instrument may result in back injuries or the system being dropped or damaged. To avoid injury and equipment damage, exercise the proper safety precautions and always use at least two people to lift the equipment.

## 

**Follow Appropriate Procedures for Safe Handling of Chemicals:** When handling/using chemicals for preparation or use within the equipment, all applicable local and national laboratory safety practices must be followed. This would include, but is not limited to, following general laboratory and chemical handling safety practices, use of all relevant engineering controls such as ventilation hoods, and appropriate selection and use of Personal Protective Equipment (PPE). Failure to adhere to laboratory safety practices could lead to injury or death.

# 2 MAX-iR Overview

## MAX-iR FTIR Gas Analyzer

The MAX-iR is a Fourier-Transform Infrared (FTIR) based gas analyzer with a wide dynamic range, capable of measuring impurities in bulk gas from ppt to percent levels. The MAX-iR analyzer measures gases by absorption spectroscopy and for a given temperature and pressure, a compound's absorption is constant, meaning the FTIR calibration curve is transferable from instrument-to-instrument and should be valid for the life of the instrument.



The MAX-iR was specifically designed to perform with minimal operator requirements and is composed of three main sections: (1) an FTIR *spectrometer* using moisture impervious ZnSe optics and a solid-state (VCSEL) laser for timing, (2) a temperature-regulated 0.456L multiple pass *gas cell* with 9.86m path length which can operate under pressures from 1 to 5 atmospheres, and (3) an infrared *detector*.

The MAX-iR does not require liquid nitrogen to cool any of the three detector versions available (DTGS, MCT, or InAs) depending upon the application.





StarBoost is a patented, signal-enhancement technology that dramatically increases sensitivity, linearity and dynamic range over narrow spectral bands of interest. This technology allows for single digit ppbv detection of hazardous air pollutants (HAPs) in real-time.

The StarBoost hardware enhancement utilizes an optimized detector and optical filter to achieve very low-level detection limits for compounds like ethylene oxide, formaldehyde or BTEX. The technology is an optional supplement to the base MAX-iR for trace detection, CEM, and fugitive emissions applications. This technology enhancement follows the same Quality Assurance (QA) protocol outlined in standard extractive FTIR test methods, including US EPA Method 320 and ASTM D-6348.

The software can also incorporate an Auto-reference algorithm that eliminates baseline drift, when very high signal-to-noise data are being acquired and analyzed.

## Part Numbers and Configurations

#### TABLE 1. MAX-IR CONFIGURATIONS

Product Description	Part Number	Detector	StarBoost	Pressure Transducer	Windows	Std. O- Rings
MAX-iR, DTGS, Low Pressure, 120V	101-0343	DTGS	None	1atm	KBr (MgF2)	Viton
MAX-iR, DTGS, Low Pressure, 240V	101-0447	DTGS	None	1atm	KBr (MgF <sub>2</sub> )	Viton
MAX-iR, DTGS, High Pressure, 120V	101-0344	DTGS	None	5atm	KBr (MgF <sub>2</sub> )	Viton
MAX-iR, DTGS, High Pressure, 240V	101-0448	DTGS	None	5atm	KBr (MgF2)	Viton
MAX-iR SB, MCT, LP3400, Gas Purity, 120V	101-0416	МСТ	Long Pass Filter (3400cm <sup>-1</sup> )	1atm	$CaF_2$	Metal
MAX-iR SB, MCT, LP3400, Gas Purity, 240V	101-0450	МСТ	Long Pass Filter (3400cm <sup>-1</sup> )	1atm	$CaF_2$	Metal
MAX-iR SB, MCT, LP3400, Low Pressure, 120V	101-0429	МСТ	Long Pass Filter (3400cm <sup>-1</sup> )	1atm	CaF <sub>2</sub>	Viton
MAX-iR SB, MCT, LP3400, Low Pressure, 240V	101-0451	МСТ	Long Pass Filter (3400cm <sup>-1</sup> )	1atm	CaF <sub>2</sub>	Viton

## Overview of MAX Acquisition Software



The MAX Acquisition software is used to configure an Acquisition Method specific to the site's application needs. It provides all the End User controls for data acquisition tasks including starting, pausing, or stopping a data acquisition routine, displaying any potential alarm states as well as run-time concentration values from a single user interface. Once configured, the Acquisition Method has the capability to automatically control the operation of the MAX-iR as well as any other instrumentation and equipment defined within the selected configuration. Software can also be set-up to directly interface with a plant's DCS or PLC or a laboratory LIMs system if the plant uses MODBUS communication. For Analog communication, a FIM (Factory Integration Module) is required to interface with the plant's data system. The FIM can be purchased from MAX Analytical Technologies as an accessory.

While the end user can create and make changes to the Acquisition Method, this service is also provided by Max Analytical Technologies who can develop a custom method fit for purpose. Please contact the Max Application team at +1 860-386-6878 or call your local Thermo Fisher sales representative.

# 3 MAX-iR Facility Requirements & Installation

This chapter describes how to prepare a site for installation as well as procedures for uncrating and initial setup of the MAX-iR. Included in this chapter are guidelines for selecting sample and calibration gas lines and filter materials.

## 

Do not attempt to install, commission, maintain or use the MAX-iR FTIR unless you have been trained or are an experienced instrument technician.

## 

The MAX-iR is not ATEX certified and is not suitable for installation in hazardous areas.

### MAX-iR Site Requirements

#### **Facilities Requirements**

 TABLE 2. MAX-IR FACILITIES REQUIREMENTS

Component	Requirement	Cords/Tubing	Fittings/Connection
Power (NA 120V)	120 VAC, 50/60Hz, 3.7A	10A North American Power	IEC 320-C13 to
		Cord, 5-ft (1.5-meter)	NEMA 5-15 Plug
Power (Europe)	208-240VAC, 50/60Hz, 2A	10A Euro Power Cord, 1.5-meter (5-ft)	IEC 320-C13 to Euro CEE7/7 Plug
Purge Gas	Nitrogen, N3.0 or Better, 20psig	¼" High Purity HDPE	¼" Swagelok (¼" fitting Provided)
Calibration Gas Requirements	Calibration gas in a balance of N2, 20psig	¼" High Purity HDPE	¼" Swagelok
Zero Gas Requirements	Nitrogen, N4.0 or Better, 20psig	¼" High Purity HDPE	¼" Swagelok
Computer Interface Connections	Ethernet Communication to Computer	CAT5E/6 Patch Cord	RJ45 Connector
	Serial Communications to Computer	USB Type A-B Cord, 3-ft (1-meter)	USB Type B Connector

#### **Environmental Requirements**

The system is suitable for indoor use in a dry location only. The equipment is cooled by an internal ventilation fan, so leave at least a 6-inch (15-cm) clearance around the FTIR to allow suitable airflow through the enclosure.

Component	Requirement
Operating	20 to 30°C
Temperature Range	68 to 86°F
Humidity	10-90% relative humidity, non-condensing
Warm up time	Typically, 1 hours from 20°C to 191°C
Ingress Protection	The system is designed to meet IP20
Overvoltage Category	Category II - Equipment with plug and socket connector or fixed connection supplied from the Table 4. Gas Sampling Requirements electrical system of a building.
Mains supply voltage fluctuations	±5%

TABLE 3. MAX-IR ENVIRONMENTAL REQUIREMENTS

#### Sample and Exhaust Requirements

TABLE 5. MAX-IR GAS AND EXHAUST REQUIREMENTS

Component	Requirement
Sample Gas Temperature	35°C, 150°C or 191°C are standard
Sample In Gas Line	For monitoring heated sources such as combustion stacks or engines, a dual core heated ¼" sample line with ¼" HDPE calibration line is required; customer supplied. Low temperature (35C) non-condensing samples require ¼" HDPE.
Sample Gas Flow Rate	Sample 1 to 5 LPM (20 psig).
Purge Gas Flow Rate	0.2 to 0.5 LPM (200 to 500 sccm). In cases where detection limits on the order of ppm are desired, nitrogen purge can be applied and then sealed off.
Purge Gas Condition	UHP grade (N3.0), oil and particulate free, non-condensing, filtered to 0.1 $\mu$ m
Exhaust Gas Vent	Connect the outlet of the MAX-iR to a separate atmospheric vent, free from back-pressure.

#### IT Requirements

#### System Control

The MAX-iR is controlled by connecting the FTIR to a computer (which is running the MAX Acquisition software) via a standard Ethernet connection. This connection is set within Windows to the IPv4 address 192.168.254.11, which will directly connect to the MAX-iR. In addition, a USB serial interface is needed between the operational computer and the MAX-iR in order to monitor the gas cell temperature and pressure.

#### Max Analytical Remote Support

The MAX-iR FTIR can be monitored and controlled remotely through the commercially installed remote desktop software, such as TeamViewer. To engage remote Technical Support, the facility must provide temporary Internet access, and this generally requires IT support from the customer side to grant access.

#### Workspace Installation Requirements

Make sure that the unit placement allows for proper ventilation to prevent any accumulation of gases within the enclosure and maintain proper internal operating temperatures including airflow through the vents on the side of the analyzer.

TABLE 6. MAX-IR WORKSPACE DIMENSIONS

MAX-iR	Dimension (W x D x H)	Min. Clearance (Front, Rear, Left/Right)	Weight (est.)
US Measurements	19.0 x 25.7 x 8.75 in	6in, 12in, 6in	75 lbs.
European Measurements	482.7 x 654 x 222.3 mm	152mm, 304mm, 152mm	34 kg

## 

*Lifting Hazard:* The weight of the MAX-iR is approximately 75lbs (34kg). Do not attempt to lift the unit alone as severe damage to muscles and ligaments could occur.

## Installation Drawings and Figures





#### MAX-iR Rear View



### MAX-iR Side View



MAX-iR Top View



## Unpacking the MAX-iR

The MAX-iR is carefully packed to reach its destination in excellent condition. When the instrument is received, inspect the packaging for any defects and check any shock and tilt indicators to be certain that damage has not occurred during shipment. If you find any damage, please notify Technical Support immediately (see Contact Information and Technical Support). You must obtain a Return Material Authorization (RMA) number from Thermo Fisher Scientific before shipping any component back to the factory.

Save the original packing material as this will be required to return the system to Thermo Fisher Scientific if a return is necessary. The use of unsuitable packing material during shipping will void the instrument warranty.

## 

*Equipment Damage:* Allow 24 hours for the instrument to reach room temperature before unpacking. Unpacking the MAX-iR when it is cold may result in damaging condensation on the electronic components and/or optics.

## Storage

If you must store the MAX-iR before installation, ensure that the instrument is stored in its original packing in an area that is both humidity-controlled and temperature-controlled to the following conditions:

Condition	Requirements
Temperature	+4 to +38°C (39 to 100°F)
Humidity	20-80% non-condensing
Packaging	Original packaging, must stay closed

TABLE 7. LONG TERM STORAGE REQUIREMENTS

## 

*Equipment Damage:* Storing the MAX-iR in an environment outside of these specifications may cause equipment damage which is not covered under warranty.

## Hardware Installation

The MAX-iR is designed to be installed in a climate controlled, sheltered location only and can be mounted in a standard 19.5-inch rack or placed on a suitable table or shelf. When installing the MAX-iR in a rack, it is recommended to use a shelf to support the weight while using four rack screws to secure the MAX-iR in the rack. Clearance of at least 6 inches should be maintained on the sides of the enclosure and clearance of at least 12 inches should be maintained at the back to provide suitable ventilation.

Use the two handles on the front and the handle on the rear to lift carefully into the installation position.





*Lifting Hazard:* The weight of the MAX-iR is approximately 75lbs (34kg). Do not attempt to lift the unit alone as severe damage to muscles and ligaments could occur.

## Power and Gas Connections

#### **Power Connections**

Using the power cable provided, connect the MAX-iR to a suitable power outlet. Be sure to use an outlet with the voltage required for the MAX-iR as stated on the product label on the rear panel. (See Facilities Requirements).

The power cords provided are rated for 10A service and have appropriate safety certifications for the local region. Be sure any replacement cord has the same or higher current rating and appropriate local safety certifications. For regions other than North America and Europe you must check the rating on the label before applying power.



#### Gas Stream Connections

The figure below describes the gas connections that must be made to the MAX-iR. All connections are  $\chi''$  Swagelok.

If the MAX-iR is not purchased with an ASC-10 Automated Sampling Console, then the user must install a 1.0, 5.0 or 10.0 LPM flow controller (rotameter or mass flow controller) on the *Sample Inlet* port to control the flow rate going through the MAX-iR gas cell, which are typically in the range of 1-5 SLPM.

A 1.0 LPM flow controller (rotameter or mass flow controller) is recommended to control the N<sub>2</sub> gas flow rate going to the MAX-iR optics through the *Purge In* port. The recommended N<sub>2</sub> purge gas flow rate is 0.2 - 0.5 SLPM at the maximum N<sub>2</sub> gas supply pressure is 20 PSIG. If the application does not require low level (ppbv) detection limits, the purge ports can be sealed after running a N<sub>2</sub> purge.

Connect a line to the *Sample Out* port and channel the flow to an appropriate exhaust vent. The line should be short as possible, to avoid any back pressure on the system, and should be installed so the flow is channeled downwards, to avoid any moisture condensation buildup within the line. The exhaust line is typically 3/8" HDPE and 10–30ft in length.



## 

**Equipment Damage:** To avoid damage to the MAX-iR electronics due to moisture condensation, wait at least 1 hour after powering up the system before connecting the nitrogen purge to the instrument. Wait until the gas cell is at temperature until connecting sample gas to the Sample Inlet.

## 

**Inhalation Hazard:** If the MAX-iR is to be installed in a shelter that does not have an active air flow replacement mechanism, then you must also connect an exhaust gas line from the  $N_2$  Purge Outlet port to an appropriate exhaust vent to avoid the buildup of  $N_2$  gas within the room (if N2 purge is being employed).

## Computer Setup

For customers setting up a computer for the first time, complete the network configuration and software installation instructions outlined below. If the computer was provided and/or configured by Thermo Fisher Scientific, proceed directly to Getting Started with MAX-Acquisition.

#### I/O Connections

The diagram below shows the Ethernet and USB connection locations on the back of the MAX-iR. Connect the ethernet cable provided with the analyzer from the LAN port on the back of the FTIR to an Ethernet port on the control computer. This ethernet network must remain isolated and should not be connected to a local area network. Connect the USB cable provided with the analyzer from the USB port on the back of the FTIR to one of the USB ports on the control computer.



#### Network Configuration

After the ethernet and serial cables are connected to the control PC, configure the PC's Network Connections according to the table below.

TABLE 8. MAX-IR NETWORK CONFIGURATION

Component	IPv4 Address	Subnet Mask
Ethernet on PC to MAX-iR	192.168.254.11	255.255.255.0

# 4 Software Installation and Setup

This chapter reviews the different types of files used in the Max Analytical software package and how they are incorporated into gas analysis methods.

### Installing MAX Analytical Software on the Control PC

#### License Key

Two USB-bound license keys are provided with the purchase of one MAX-iR. Each key includes a copy of the software package and the standard MAX files required for analyzing data. To install the software, the key MUST be inserted into the USB port of the PC connected to the instrument. The license limits the use of the full software package to one user on one computer at a time. All software should be installed in a Windows Pro 10 (or higher) Operating System.

#### Software Installation

- 1. Download the two installers to the Control PC
  - MAX Analytical Installer
  - o MAX Analytical Quant Library Installer

#### 2. Run the MAX Analytical Installer

- Make sure the License USB Key is installed on the Control PC
- Open the *MAX Analytical Installer* by double clicking on the EXE File.
- When prompted for the license key, press the *Refresh* button to upload the license information from the USB to the PC. Then press the *Next* button

icense Agreement		ΛÌ
Please review the license terms before installing MAX Ana 3.13.1.	lytical Analytical Te	echno
If you have a USB license key, please insert it into one of select Refresh'. The license file on the key should automa manually browse for the license file.	your computer's USB port stically be selected. You m	and ay also
C: ProgramData/MAX Analytical/Feature.ic	Brov	wse fresh

• Follow the prompts to finish installing the MAX-Acquisition software

#### 3. Run the MAX Analytical Quant Library Installer

- Open the MAX Analytical Quant Library Installer by double clicking on the EXE File.
- When prompted for the license key, press the *Refresh* button to upload the license information from the USB to the PC. Then press the *Next* button
- o Follow the prompts to finish installing the MAX-Acquisition software

## Getting Started with MAX-Acquisition

- 1. Launch the MAX-Acquisition software from the desktop icon  $(\stackrel{1}{\bowtie})$ .
  - o Make sure that the MAX-iR is powered up and is detected by the software
  - Press the *Select* button for the *Instrument Configuration* set up on the *Getting Started* pop up panel.

File Edit View Tools Help Methods	1 N d c	- 9 Q	🖈   ک 🕒 😡	None								- [	1 X
	Alarm Mo	nitor Alarm I	fistory									Cle	ar Alarms
	State		Hard	ware Alarm			Stat	te		Gas Ala	arm		Value
		😌 Getting	Started					-		×			
		The application of the second	ation has not been	configured. \	fou need to :	select which	instrument	configuratio	in you are				
		Instrumen	t Configuration						Select	-			
		Instrumen	nt Method:						Select	-			
	-								Continu	16			
	Concentration	n					_						
Actions													
Start Acquisition	Concerna												
Basada												 	

- 2. Select the Instrument Configuration.
  - A separate window will pop up with the list of default Product Configurations. Click to highlight the *MAX-iR* and press the *Select* button at the bottom.

😔 Product Configuration List Editor	-	×
C:\MAX Data\Acquisition\Instrument Met	hods	
1 🖍 🕅		
Method		
MAX-IR		
	Soloct	200
	Select	se

- The *Getting Started* pop up should now have *MAX-iR* listed next to *Instrument Configuration*.
- The Default method called *MAX-iR* will be listed next to *Instrument Method*.

😔 Getting Started	_		$\times$
The application has not been configured. You need to select which instrument co running.	onfiguratio	n you are	
Instrument Configuration: MAX-IR		Sele	ct
Instrument Method: MAX-IR		Sele	ct
		Cont	inue

3. In the Getting Started window, press Continue. These settings can be changed later.

Once the application is configured from the Getting Started window, follow the instructions for **Connecting to MAX-iR for the first time**.

## MAX-iR Hardware Connection

#### Connecting to MAX-iR for the first time

To connect to the MAX-iR for the first time, follow the instructions below.

- 1. Edit the MAX-iR Product Configuration.
  - From the main MAX Acquisition menu, Go to Edit > Product Configuration to open the Product Configuration List Editor.
  - Click to highlight the MAX-IR configuration, then click Edit (
- 2. Search for the MAX-iR spectrometer instance.
  - Click on the MAX FTIR spectrometer module in the Product Configuration window. Under Spectrometer Instance, click Search...

e Product Configuration - MAX-IR	-		×
<b>÷</b> × < ⇒			_
Info Scheduling Workflow MAX FTIR MAX FTIR			
Detector Type: DTGS ~			
Arm Speed: Default * cm/sec			
Detector Gain: 27.13 ×			
Path Length: 9.860 Meters			
Laser Frequencies			
Spectrometer Instance Instrument Name	S	earch	٥
This spectrometer instance can optionally be set. If unset, the system will search for the available spectrometers on t automatically connects to the first one found.	he networ	k and	
Setting the spectrometer instance binds the configuration to a specific spectrometer. This can speed up connecting but makes the configuration less reusable between multiple installations.	to the spe	ctrometer	,
Reset Check	ОК	Can	cel

 The software will search the spectrometer MAC address. Once found, click to highlight the MAC address.

Search Local Network		-	
			Refresh
Name	IP Address		In Use
MAC_00_02_2C_08_05_B7	192.168.254.12		

- Click OK to return to the Product Configuration editor.
- 3. Search for the pressure and temperature sensor COM port.
  - Click on the MAX FTIR pressure and temperature sensor module in the Product Configuration window. Next to COM Port, click the Search button.



Product Configuration - MAX-IR		-		<
🕂 💥 🗢 🔿				
Info Scheduling Workflow MAX	FTIR MAX FTIR			
✓ Use Pressure/Temperature Sensor				
Communication				
Connection Type: Serial Y				
COM Port: Search				
Baud Rate: 9600 Y	Data Bits: 8 ~			
Parity: None *	Stops Bits: 1 ~			
Devices				5
Device Sensor Type	Override			
Temperature CN142 Cell Heater ~	35.00 °C			
Pressure Keller Precise ~	5.000 Atm			
Cell Heater CN142 Cell Heater ~				
Reset Check		ОК	Cancel	

• Once the software detects the pressure and temperature sensor, a pop-up will identify COM port. Click OK to select the COM port.



- 4. Once the spectrometer and pressure and temperature sensors are detected, click OK to return to the main MAX-Acquisition window.
  - If the spectrometer and/or temperature and pressure sensors were not detected, proceed to Chapter 10 Troubleshooting.

#### Checking the MAX-iR Hardware Connection Status

The hardware connection status will appear in the lower left corner of the window. The status will say "Connecting" as the computer initiates communications with the hardware any time the software is launched or a new Acquisition Method or Product Configuration is selected. After a moment, the status should read "Idle" if the computer can connect to the MAX-iR. Definitions of all status indicators are listed below:

Status	Function
ldle	The software can connect to the hardware and is ready to acquire data.
Offline	There is a communication issue between the software and hardware.
Acquiring	The software is in runtime mode, collecting spectral data and storing it to the PC.
Paused	The data acquisition has been manually paused.
Error Recovery	Acquisition was interrupted by a hardware connectivity issue.
Waiting on Preconditions	One or more devices must reach a precondition (mainly a temperature setpoint). Acquisition will automatically begin once the precondition is met.

 TABLE 9. HARDWARE CONNECTION STATUS INDICATORS

If the software cannot connect to the hardware, a pop-up will indicate that the *Acquisition Status* of the MAXiR is offline and failed to connect, and the User Interface will display 'Offline' status in the lower left corner.

😔 Acquisition Status	-		×
'MAX-IR' is offline.			
Failed to connect to: MAX FTIR			
		Clo	se

*Close* the pop-up panel and check that all Ethernet and USB connections are connected to the Control PC. Refer to **Chapter 10 Troubleshooting** for instructions.

## Installing Methods on the Control PC

#### Overview of Required Files

There are three types of files that make up the framework of method development for every application:

- 1. Product Configuration
- 2. Acquisition Method
- *3. Quant Method*

#### These files are application-specific.

Standard product configurations and methods are embedded in the MAX Analytical Quant Library installer. They are locally stored as Archives (ZIP) in *C:\MAX Data\Quant Library\Archives*.

For custom method development, please reach out to your local Thermo Fisher Scientific sales representative.

#### Product Configuration

The *Product Configuration* outlines the hardware components connected to the computer. For the MAX-iR it establishes connections to spectrometer and temperature/pressure controller. Additional devices may include the Data Recorder and Modbus Slave Publishing.

Method *Scheduling* (optional) is set up within the *Product Configuration Editor*. Any *Acquisition Method* can be scheduled to run daily, weekly, monthly, or while the system is Idle.

In this table, the user can also choose which methods are displayed on the control panel in *Monitor View*.

#### Acquisition Method

The Acquisition Method is where the FTIR setpoints and parameters are specified. It also contains the *Workflow*, which defines a programmed sampling sequence with worksteps and timing. A Workflow can be set up for performing Daily QA checks as well as for routine gas monitoring.

#### Quant Method

The *Quant Method* contains the MAX-iR calibration files (*Reference Profiles*) and analysis parameters for each compound. Optional Gas Alarms and Algebraics are setup in the *Quant Method*.

#### Measurement Standards (Optional)

*Measurement Standards* define thresholds that can be shared between quant methods. They are used to quickly alter a group of alarm ranges to meet different quality metrics. You can reference these *Measurement Standards* when creating alarms. These standards are critical for modifying alarms during the replacement of CTS and Calibration gas cylinders.

Measurement standards are accessed from the top toolbar at Edit > Measurement Standards.

The user can review or modify the *Linked Standard* and the list of criteria for individual gas standards. Upper and lower thresholds as well as non-detect (ND) limits can be specified by the user.

#### Installing Methods using the Archive Extraction Tool

If custom methods were provided by Thermo Fisher Scientific in the form of an Archive (ZIP) file, follow the instructions below to extract the files onto the control PC and load the methods in MAX Acquisition.

## NOTICE

**Do NOT extract the Archive file in Windows File Explorer.** Leave it in the original format as a '\*.zip' and follow the instructions below to extract the files in the Max Analytical software. The Max Analytical software requires this format to properly upload all the information and files.

- 1. Load the (\*.zip) file that contains the custom method(s).
  - In the main viewing panel go to the top toolbar and select *Tools > Extract Archive*.
    - MAX Acquisition 4.0 MAX-IR

       File
       Edit
       View
       Tools
       Help

       Methods
       Add Sample to Method...

       MAX-iR (
       Reporting...

       [1cm-1] [
       Archive Data...

       MAX-iR (
       Extract Archive...

       [1cm-1] [
       Options...
  - o A window will open titled Archive Extraction Options.

#### 2. Select the appropriate extraction options.

- Press the top *Browse* button to open Windows File Explorer.
- Navigate to the save location of the Archive file (\*.zip).



3. Select the file and click Open to return to the Archive Extraction Options window.

## NOTICE

The default save location for the extracted files is C:\MAX Data. It is not recommended to change the *Extract To* file path.

- 4. Check the boxes as they appear in the figure below. This will extract all potential Max Analytical files contained within the archive folder.
  - Please note that the required checked boxes may be different if only certain files are needed, or if existing files need to be overwritten.

😔 Archive Extraction Options	_	
Archived: Extract To: C:\MAX Data Options Overwrite Existing Files I Open when complete		Browse Browse
Extract  Data Set  Quant Method  Measurement Standards  Reference Profiles  Acquisition Method  Product Configuration		
List	ОК	Cancel

- 5. Click OK at the bottom of the Archive Extraction Options window.
  - A pop-up panel will list the files that were *Extracted* or *Skipped*. It also states the total number of files extracted. Select *Close* to return to the main screen.

😔 Archive Results	_		×
Issue			
Extracted 29 files			~
Quant Library\MAX-Bev 2.0 Quant Library [35C]\methods			
Impurities in Carbon Dioxide 2021-11-15.pqm			
Standards			
ISBT.mslist			
Quant Library\MAX-Bev 2.0 Quant Library [35C]			
Acetaldehyde [75-07-0] [35C] [5atm] [4cm-1].pgrf			
Acetone [67-64-1] [35C] [1atm] [4cm-1].pgrf			~
<			>
Copy to Clipboard Sa	ve As	Clo	se

• If multiple Acquisition Methods were extracted, please continue to the next section for instructions on selecting a method from the list of available methods.

# 5 MAX-Acquisition Software Overview and Features

This chapter will cover the functions of MAX-Acquisition and the tools needed for general operation.

#### Software Display Views

There are three viewing modes in MAX Acquisition: Monitor View, Detailed View, and Diagnostic View.

TABLE 10. MAX-ACQUISITION DISPLAY OPTIONS

View	Function
Monitor View	A simplified display that allows for starting/stopping data acquisition, monitoring alarms, and viewing historical reports.
Detailed View	Displays the real-time instrumental settings, the concentration results for each gas in the method, and the sample spectrum.
Diagnostic View	Used for performing routine, diagnostic checks on the MAX-iR. Allows the user to set the laser frequency and monitor the resolution and SNR.

The mode can be changed by clicking *View* on the top tool bar and selecting one of the three options from the dropdown menu. The current viewing mode is denoted with a checkmark.

File Edit View Tools Help Sample 20 MAX-iR Ca Monitor View Diagnostic View Diagnostic View Data Filters Show Run Description Show Spectrum File Details Prefix: Average: Show Error Logging Edit	😂 MAX A	cquisit	ion 4.0 - MAX-IR	
Sample 20 MAX-iR Ca Monitor View E To Detailed View ect Diagnostic View Data Filters Data Filters Show Run Description Work Step Prefix: Average: Show Error Logging Edit	File Edit	View	Tools Help	
	Sample 20 MAX-iR Ca MAX-iR Ca Work Step Prefix: Average:	~	Monitor View Detailed View Diagnostic View Data Filters Show Run Description Show Spectrum File Details Show Data Table Show Error Logging	e To ect

#### Monitor View

*Monitor View* enables the user to readily check the MAX-iR hardware health. It also displays any application-specific gas alarms and has controls for starting and stopping data acquisition.

SMAX Acquisition 4.0 - MAX-IR						
File Edit View Tools Help						
Methods	💺 🖑 🗔 🔻 🍳 📿 😥 😢 🎋 🗍 💯 None					
MAX-iR Calibration [1cm-1] [191C] [1atm]	Alarm Monitor Alarm History		Clear Alarms			
MAX-iB Calibration	State Hardware Alarm	State Gas Alarm	Value			
O[1cm-1] [35C] [1atm]	Hardware Health Alarm	CTS Direct Check				
	Available Disk Space	_				
Combustion Method	MAX FTIR Health					
Acquisition						
Acquisition						
Method						
Control	Alarm Panel					
Panel	Alditi Falici					
	000					
	Concentration - CTS Direct Check					
Actions						
		Runtime				
Start Acquisition		Concentration				
Reports	-0.05					
		00.00.00 00.00.00 00.00.00 00.00.00	00:00:00			

Acquisition Method Control Panel

The *Acquisition Method Control Panel* lists the available Acquisition Methods for the active Product Configuration. Each method can be run instantaneously or paused by clicking on its respective button.

Additionally, the operator can begin collecting data by pressing the "Start Acquisition" button in the *Actions* panel on the lower left of the window. When acquiring data, this same button will turn green and say, "Stop Acquisition." Clicking this button will stop the run. If the scheduling tool is implemented, this button will say "Start Scheduler" and "Stop Scheduler."

The *Reports* button on the bottom left allows the user to view historical reports in an HTML format. All raw spectra are stored indefinitely on the computer harddrive for validation.

#### Alarm Panel

The *Alarm Panel* section has two tabs, the *Alarm Monitor* and *Alarm History*. The *Alarm Monitor* tab displays the hardware health statuses and gas alarms. The *Alarm History* panel is a log of all alarms that occurred within a current run, as well as their timestamps and current alarm state.

User defined critical alarms may be programmed to latch so that when they trip, an operator must click the "Clear Alarms" button.

Alarm M	Ionitor Alarm History	/			Clear Alar
State		Hardware Alarm	State	Gas Alarm	Value
•	Hardware Health Alarm			CTS Direct Check	
•	Available Disk Space				
	MAX FTIR Health				

#### Runtime Concentration

The bottom panel in Monitor View displays a real-time Concentration plot of the actively selected gas component. This plot updates during acquisition.

If there are gas alarms in the active method, the runtime profile plot will track the item selected from the Gas Alarm list.



#### Detailed View

Detailed View displays all acquisition controls and spectral information and is intended for advanced users. This viewing mode is arranged into five main panels: *Runtime UI, Gas List, Concentration Profile, R<sup>2</sup> Spectral Analysis,* and the *Spectrum Display*. The figure below is an example of *Detailed View*.



#### Runtime UI Panel

The *Runtime UI* displays metrics and controls relevant to the active run. The user can start, stop, and pause data acquisition from the *Runtime UI*. This panel also shows the current instrumental conditions. For the MAXiR, the Runtime UI will display the following tabs: *Info, Workflow*, and *MAX FTIR*. Additional tabs may be visible if subcomponents are added to the system.

TABLE 11. RUNTIME UI TOOLS AND ICONS

TAB / ICON	Name	Function
	Start Acquisition	Initiates data collection. Begins a new run if started from the "Idle" state. Resumes acquisition if a run is paused.
	Pause Acquisition	Pauses data acquisition during an active run.
0	Stop Acquisition	Stops data acquisition and ends a run.
	Previous/Next Steps	Changes the current work step. Can manually advance to the next step in the sequence or backtrack to repeat a previous step.
	Info	Displays FTIR spectral file name, timestamp, pressure, temperature, and Quantification Method options.
<b>1</b> -2 3 <b>✓</b>	Workflow	Displays the active Work Step and file prefix of the pending spectrum. Allows the user to edit the file prefix and spectral averaging.
Q •	MAX FTIR	Displays the real-time gas cell temperature, pressure, and signal. Displays the detector temperature (StarBoost only). A progress bar shows the number of scans until the next spectrum is published.


The Gas List tabulates the analytical results of the current run for all the compounds in the Quant Method.

- The results update after each spectrum is collected.
- Each compound is listed in the *Gas ID* column and sorted alphabetically.
- The *Value* column displays the concentration results.
- The units and significant figures can be modified in the Quant Method.
- the SD column publishes the standard deviation of the concentration.
- The colorful squares convey the gas color in the *Concentration Overlay*.
- The actively selected gas is highlighted in blue.

+	M 🖪 🐟 🗖			
	Gas Id	Value	SD	
	1,1-Difluoroethylene [35C] [			
	Acetic Acid [35C] [64-19-7]			
	Acetylene [35C] [74-86-2]			
	Ammonia [35C] [7664-41-7]			
	Carbon Dioxide [35C] [124-:			
	Carbon monoxide [35C] [63			
	Chlorotrifluoroethylene [350			
	Ethane [35C] [74-84-0]			
	Ethylene [35C] [74-85-1]			
	Ethylene Oxide [35C] [75-21			
	Methane [35C] [74-82-8]			
	Nitric oxide [35C] [10102-43			
	Nitrogen Dioxide [35C] [101			
	Nitrous oxide [35C] [10024-			T
	R116 Hexafluoroethane [35			
	Tetrafluoromethane [35C] [7			
	Toluene [35C] [108-88-3]			
	Trifluoromethane [35C] [75-			
	Water [35C] [7732-18-5]			

Data quality indicators for each compound are displayed in the first column. An asterisk next to the ratings indicates a suspected quality issue with the gas analysis.

Good

Near Detection Limit

Moderate

\*00Below Detection Limit

#### Concentration Profile Plot

The plot at the top of the screen displays the Concentration profile over time for the selected Gas ID.

To display a plot that includes every gas, click on the *Concentration Overlay* icon (A) in the top tool bar.

On the graph, the bold line represents the values of the gas selected in the gas list, and the lighter lines represent the other individual gas measurements. The color legend for each component is on the right side of the gas list.



#### R<sup>2</sup> Spectral Analysis

The plot in the middle displays the  $R^2$  over time for the selected Gas ID. It demonstrates the fit of the gas reference spectrum to the sample spectrum.

#### Spectrum Display

Displays the raw infrared absorbance spectrum. The dropdown menu on the toolbar provides the user with the following spectrum display options:

- Sample
- Single Reconstruction
- Subtraction
- SBeam
- IGram
- Residual
- Regression Reconstruction

#### **Diagnostic View**

Diagnostic View is described in detail in Chapter 6 MAX-iR Diagnostics.

## Display and Plotting Tools

The following table describes the tools needed to manipulate the displays in *Monitor View, Detailed View, and Diagnostic View*. The function of each tool is also listed.

For most of these tools and display options, the plot the user wants to edit must be selected. Select the desired plot by clicking on its panel. The actively selected plot will have a blue banner. For example, in the image below, the Concentration plot is selected:



TABLE 12. GENERAL REFERENCE LIST FOR PLOTTING AND DISPLAY VIEW ICONS

ICON	Description	Function
	Move Selection Cursor	Click to move the Spectrum Selection Slider across Concentration Panel.
Ŵ	Pan View	Click and drag on any plot to pan the viewing region.
	Drag Zoom	Click and drag the cursor on any plot to zoom to the selected region. Click and drag along the x- or y-axis in the grey area outside of the plot to zoom in one direction while the other is held constant.
€	Zoom In	Located in the drop-down menu of the <i>Drag Zoom</i> . Click on the screen to zoom in.
Ø	Zoom Out	Located in the drop-down menu of the <i>Drag Zoom</i> . Click on the screen to zoom out.
Ŷ	Track Values	When selected, click & drag across data on any of the plots to display more detailed results for each point.
Ø	Hide / Show Legend	Will hide or show the legend for the highlighted / selected display panel.
<del>ار</del> ک	Reset Pan/Zoom	Reset the selected plot to full scale.
<del>(#)</del>	Set Viewing Area Numerically	Manually enter the display range of the x- or y-axis on the selected plot.
<del>نې</del>	Find Sample Spectrum Cursor	Resets the Sample Spectrum Locator (green hashed trace) to the center of the viewing region on the concentration plot.
	Show All Gases in Spectrum View	Reference spectra for all Gas ID's will be overlaid on <i>Spectrum Display</i> plot.
	Detailed Analysis	Displays concentration plot, R <sup>2</sup> analysis, and the FTIR sample spectrum and quantification regions for spectroscopists and advanced users.
Ą	Concentration Overlay	Displays a concentration plot with all gases overlayed.
2	Data Filter	Add custom data filters for viewing results based on designated parameters.

#### Changing the Displayed Sample Spectrum

Spectrum Selection Slider is a scroll bar that can be dragged to coarsely scroll through the spectral dataset. It can also be fine-tuned using the (+) and (-) buttons to the right of the slider. See the Red boxes below showing the slider location for the Monitor and Detailed views. When a new point is added to the active screen the locator will go to the end of the dataset. If you have a rapid running analysis this function will not be useful since it will continue to jump to the end. Considering pausing the data collection if you need to investigate a previous spectrum or point.



Sample Spectrum Locator (see the red arrows above) is the hashed green trace on the concentration and R<sup>2</sup> plots. It appears once data has been collected. Like the Spectrum Selection Slider, this line can be dragged to scroll through the dataset. Select the Move Selection Cursor () tool, to drag the green trace to the spectrum of choice. The Sample plot displays the spectrum at the same point in time as the green trace.

## Selecting an Acquisition Method

If the active Product Configuration is linked to multiple Acquisition Methods, the user can easily switch between the available methods any time the devices are *Idle*. To view the list of available methods, on the top toolbar select *Edit* > *Acquisition Method* to open the *Instrument Method List Editor*.

File	Edit	View	Tools	Help			
	Find S	Spectru	m				
	Span						
	Measurement Standards						
	Product Configuration						
	Acqui	isition N	/lethod				

This will open a separate window titled *Instrument Method List Editor*.

🔁 Instrument Method List Editor	_			
C:\MAX Data\Acquisition\Instrument Methods				
🕂 🖍 🗅 🗱 🚡	\$			
Method	Instrun	nent		
Default Method	MAX-IR			
Example - Combustion	MAX-IR			
Example - Sample Gas Analysis	MAX-IR			
MAX-IR	MAX-IR			
	Select	Close		

The column on the left lists the name of each available method, and the column on the right lists the Product Configuration that each method is linked to.

Select the method to be run by clicking on its name in the list. The selected method will be highlighted in blue. Click the Select button to open the highlighted method.

The Acquisition Method can also be viewed and selected from Detailed View. On the top toolbar, click *View* > *Detailed View*.



# MAX Acquisition 4.0 - MAX-IR File Edit View Tools Help Monitor View Detailed View Diagnostic View Data Filters Show Run Description... Show Spectrum File Details... Show Data Table... Show Error Logging...

In the Runtime UI panel on the top left of the screen, the active Acquisition Method is listed above the Play Button (For Example: "MAX-iR").



Click the Select button to open the Instrument Method List Editor.

🔁 Instrument Method List Editor	_		×
C:\MAX Data\Acquisition\Instrum			
🕂 🖍 🖻 💥 🚹			礅
Method	Instrun	nent	
Default Method	MAX-IR		
Example - Combustion	MAX-IR		
Example - Sample Gas Analysis	MAX-IR		
MAX-IR	MAX-IR		
	Select	Clo	ose

Select the appropriate method from the list as needed.



The following sections explain the additional features of MAX Acquisition that support operation of the instrument and data analysis.

#### View Data Table

On the top toolbar, click *View > Show Data Table...* to open the data table for an active run.



All raw concentration results for the reported-on gases are tabulated here. The table will update each time a new spectrum is acquired. Each spectrum is tabulated with its time stamp and file name.

Spectrum	Date-Time	Acetaldehyde ppm	Acetylene [19 ppm	Acrolein [191 ppm	Ammonia [19 ppm	Carbon Dioxi %	Carbon Mono ppm	Hydrogen Ch ppm	Methane [19 ppm	Methanol [ ppm
ample Measurement_0000062.LAB	6/23/2021 4:24:14 PM	-0.143	0.620	-0.157	-0.117	8.249	0.437	-0.142	0.059	-0.057
ample Measurement_0000063.LAB	6/23/2021 4:24:46 PM	0.274	0.062	-0.270	-0.155	8.533	0.165	0.001	0.122	-0.214
ample Measurement_0000064.LAB	6/23/2021 4:25:18 PM	-0.130	-0.054	0.251	-0.029	8.247	0.102	-0.057	0.144	-0.149
ample Measurement_0000065.LAB	6/23/2021 4:25:50 PM	-0.118	0.037	-0.065	0.057	8.261	0.144	0.067	0.076	-0.122
ample Measurement_0000066.LAB	6/23/2021 4:26:21 PM	-0.132	-0.093	-0.210	-0.203	8.232	0.007	-0.026	0.208	-0.169
	<									

If the "Track Active Spectrum" box is checked at the bottom of the window, the selected spectrum (highlighted in blue) will automatically advance the user to the next data point in the table each time a new one is acquired. Unchecking this box will allow the user to toggle through any item listed item in the table without being automatically advanced to the most recently collected data point.

If acquisition is paused, the gas list in *Detailed View* will reflect the results from scan that is selected from the data table.

#### Find Spectrum and View Spectrum File Details

The list of all acquired spectrum in the active data set can be accessed by clicking Edit > Find Spectrum... A separate window will open titled "Find Spectrum." The file name and time stamp of each spectrum in the data set are listed here.

of Spectra	a: 15			
Validated	Spectrum	Comments	Time/Date	
	Nitrogen Background_0000012.LAB		15:56:21 06/23/2021	
	Nitrogen Background_0000013.LAB		15:56:53 06/23/2021	
	Nitrogen Background_0000014.LAB		15:57:25 06/23/2021	
	Nitrogen Background_0000015.LAB		15:57:57 06/23/2021	
	Nitrogen Background_0000016.LAB		15:57:57 06/23/2021	
	Sample Measurement_0000016.LAB		15:58:28 06/23/2021	
	Sample Measurement_0000018.LAB		15:59:00 06/23/2021	
	Sample Measurement_0000019.LAB		15:59:32 06/23/2021	
	Sample Measurement_0000020.LAB		16:00:04 06/23/2021	
	Sample Measurement_0000021.LAB		16:00:35 06/23/2021	
	Sample Measurement_0000022.LAB		16:01:07 06/23/2021	
	Sample Measurement_0000023.LAB		16:01:39 06/23/2021	7

A spectrum can be searched by file prefix or number using the search dialog box on the top right of the window. A count of the total number of spectra in the data set is tabulated above the list.

To view the spectrum file details, select the desired scan (it will be highlighted in blue) and click the Details... button on the bottom right of the window. This will open the raw spectrum and all values associated with the spectral file, including resolution, apodization, and laser frequency.



Click close to return to the Find Spectrum window.

Alternatively, the spectrum file details can be opened by clicking View > Show Spectrum File Details... This will display the details of the scan that the hashed green trace is on in the concentration plot.

#### Spanning Data

The software provides users the option to span concentration results of individual gases. Typically, a gas would be spanned based on a direct reading from a certified standard, which is common for certain compliance testing applications.

Gas Id	Span Multiplier	Span Offset	Set Using Spectrum	Reading Was	Actual Was
Acetaldehyde [191C] [75-07-(	1.00000	0.00000		0.00000	0.00000
Acetylene [191C] [74-86-2]	1.00000	0.00000		0.00000	0.00000
Acrolein [191C] [107-02-8]	1.00000	0.00000		0.00000	0.00000
Ammonia [191C] [7664-41-7]	1.00000	0.00000		0.00000	0.00000
Butane [191C] [106-97-8]	1.00000	0.00000		0.00000	0.00000
Carbon Dioxide [191C] [124-3	1.00000	0.00000		0.00000	0.00000
Carbon Monoxide [0-4000 pr	1.00000	0.00000		0.00000	0.00000
Carbon Monoxide [0.1-10%]	1.00000	0.00000		0.00000	0.00000
Ethane [191C] [74-84-0]	1.00000	0.00000		0.00000	0.00000
Ethylene [191C] [74-85-1]	1.00000	0.00000		0.00000	0.00000
Formaldehyde [191C] [50-00-	1.00000	0.00000		0.00000	0.00000
Hydrogen Chloride [191C] [76	1.00000	0.00000		0.00000	0.00000
Methane [191C] [74-82-8]	1.00000	0.00000		0.00000	0.00000
Methanol [191C] [67-56-1]	1.00000	0.00000		0.00000	0.00000
Nitric Oxide [191C] [10102-4:	1.00000	0.00000		0.00000	0.00000
Nitrogen Dioxide [0-400 ppm	1.00000	0.00000		0.00000	0.00000
Acetaldehyde [191C] [75-07-0	] ———				
Reading: Offset:		Multiplier:	Actual:		
( 0.00000 + 0.0000	) X (	1.00000	= 0.00000	ppm	

To apply a span to a gas, on the top toolbar click Edit > Span... to open the Edit Span Data window.

The user has the option of applying a multiplier or offset to the raw concentration reading of each gas. Select the gas for spanning by selecting it form the list (it will be highlighted in blue).

To span a gas based on the average response of a direct reading, the concentration value must be inputted into the dialog box below "Actual." Click the "Set Span" button, and the appropriate multiplier will be applied to span the "Reading" to the "Actual" value.

The table will list the span multipliers and span offsets applied to each component. It will also detail the spectrum used to span the gas along with both the raw and spanned results.

Click "Clear Span" to remove any span multipliers or offsets from the selected gas.

Click Close to return to the original view.



If an error occurs while MAX Acquisition is open, it will be listed in the Error Log.

On the top toolbar, click *View > Show Error Logging...* to open the Error Logging Window.

🕑 Error Lo	ogging Window	_	0	: כ
Filter:	Warn ~			
Туре	Time/Date	Description	_	
Error	12:05:35 10/31/2022	MAX FTIR: Failed to open spectrometer 'MAC_00_02_2C_08_11_01'		
Error	12:07:41 10/31/2022	Counter(2) - MAX FTIR: Failed to open spectrometer 'MAC_00_02_2C_08_11_01'		
Error	12:09:46 10/31/2022	Counter(2) - MAX FTIR: Failed to open spectrometer 'MAC_00_02_2C_08_11_01'		
Error	12:11:51 10/31/2022	Counter(2) - MAX FTIR: Failed to open spectrometer 'MAC_00_02_2C_08_11_01'		
Copy to	Clipboard	Clear		Close

Any potential errors that impact instrument communications or performance will be listed in this window. In the example above, the computer could not connect to the spectrometer.

The information listed in this window can be filtered by error severity using the dropdown menu on the top left. The options are *Trace, Debug, Info, Warn, Error, and Fatal.* 

😔 Error L	ogg	ing Wind	dow	- 0	×
Filter:	Tra	ce ~			
Туре		Irace	Date	Description	
Info	12	Debug	/31/2022	RetryCommand failed on: OpenBoard	^
Debug	12	Info	/31/2022	MAX FTIR: MAX-IR SDK Version: 2.63	
Info	12	Warn	/31/2022	RetryCommand failed on: OpenBoard	
Error	12	Error	/31/2022	Counter(2) - MAX FTIR: Failed to open spectrometer 'MAC_00_02_2C_08_11_01'	
Debug	12	Fatal	/31/2022	MAX FTIR: MAX-IR SDK Version: 2.63	
					$\sim$
Copy to	Clip	oboard	)	Clear	;

For more information on error descriptions and troubleshooting, please refer to Chapter 10 (10 Troubleshooting).

## NOTICE

For troubleshooting assistance, please contact Technical Support at 1-800-532-4752. Select "option 2" for Unity Lab Services technical support. For instrument type, select "option 6" for Molecular, Vibrational Spectroscopy Based Spectrometers.

## Archiving Data

The Archive tool in MAX-Acquisition is necessary for periodically saving backups of your acquisition method(s), quant method(s), Product Configuration, gas references, and measurement standards. In the event of a computer crash or unintentional changes to the data acquisition method, archives can be used to restore previous versions. Archived methods can also be crucial for receiving fast support, since they allow replication the customer's system so method edits can be made efficiently while minimizing interruptions to data collection.

Please follow the steps outlined below to archive your data:

- 1. Stop or pause data collection.
- 2. At the top toolbar, select Tools, Archive Data...



3. A separate window will pop up titled "Archive Save Options"



- 4. Select Browse... and navigate to the desired save directory.
  - Windows File Explorer will open in a separate window.
  - The default save location for archived files is C:\MAX Data\Output\Archives.
  - Enter the desired file name for the saved archive (ex: Combustion Test #1 2022-10-31).
- 5. Select Save to return to the archive window.
- 6. Check the boxes so that they match the image below. These options are sufficient for routine backup of methods.



😌 Archive	e Save Options	_		×				
Archive:	Combustion Test #1 202	2-10-31.zip	Bro	owse				
Save								
🖌 🗹 Data :	set							
🖌 Quan	✓ Quant Method							
Meas	✓ Measurement Standards							
✓ Reference	ence Profiles							
🖌 Acqui	sition Method							
🗸 Produ	✓ Product Configuration (includes all methods)							
Error	Logs							
	-							
		Or	0	col				
		UN	J Can	icei j				

- For certain support concerns, Error logs may also be required.
- $\circ$  Specific archive options may be provided by the Technical Support team for certain support requests.
- 7. Select OK to save the archive.
- 8. Another Windows File Explorer window will open to the save location of the archive.
   o Every archive is saved as a compressed folder (.zip).
- 9. Select Close and return to the Acquisition window.
- 10. Press Play to resume data collection once the archive backup is complete.

# 6 MAX-iR Diagnostics

This chapter explains how to perform routine MAX-iR diagnostic checks to ensure instrument calibration. The user must understand the basic software tools to navigate the software and run the diagnostics, so please review this information in Chapter 5 MAX-Acquisition Software Overview and Features before starting this section.

## NOTICE

If the MAX-iR is used for compliance testing, instrument diagnostics must be checked once per day prior to any sample data acquisition. See Chapter 8 Recommended Operating Procedures for the recommended diagnostics testing frequency.

### Diagnostic View

MAX-Acquisition must be *Idle* to open *Diagnostic View*, so click Stop to end a current run if needed. On the top toolbar click *View* > *Diagnostic View*. All diagnostic tests are performed in this viewing mode.

There are two important diagnostic panels that demonstrate instrument performance: the *Water Band* tab and the *Signal to Noise Ratio (SNR)* tab. The water band tab allows the user to confirm that the system resolution and the calculated IR frequencies are correct. If either measurement are outside their performance metrics, the user is encouraged to pause data collection until both are within their metrics. The SNR tab allows the user to confirm that the instrument will have the required signal-to-noise to perform the required measurements and that the detector response is linear.



#### TABLE 13. DIAGNOSTIC TEST DESCRIPTIONS

Test	Purpose	Sample Inlet Gas
Water Band	Allows the user to check the instrument resolution and set the laser frequency (these tests are critically important for good data quality).	Ambient air or process gas
SNR	Displays the Single Beam spectrum and tabulates the SNR in different spectral regions. Also calculates the detector linearity.	Nitrogen

The Stability tab is utilized to determine the instruments sensitivity to temperature changes and is not required for normal instrument operational diagnostics checking.

## Verify Instrument Settings

## NOTICE

As soon as Diagnostic View is opened, verify that the gas cell temperature setpoint is correct. It should be set to the same temperature as the sample data collection. Specifically, the temperature setpoint should be the same as the selected Acquisition Method.

If the gas cell temperature setpoint is correct, no action is required.

If the gas cell is set to the wrong temperature, the reading in the Runtime UI will be highlighted in red. To verify or modify the temperature setpoint, click the *Settings...* button.



A window titled *Instrument Settings* will open:

😌 Instrument Se	ettings			-		×
Resolution:	1 ° cm <sup>-1</sup>	Time per Spectrum:	60.000 Sec			
Average # Scans:	10 ~	Lower Range:	500 cm <sup>-1</sup>			
AutoRef:	4 X ~	Upper Range:	6000 cm <sup>-1</sup>			
Apodization:	Cosine ~					
Averaging:	Adjust CenterBurst 🛛 👻					
Sweep Direction:	Both ~					
Fractional Aligned	n Centerburst					
Cell Temp:	35.0 °C					
Wait for minim	al cell temperature to be reached bef	ore starting				
Minimal:	180 °C					
				ancel	O	

Modify the gas cell temperature setpoint if needed. **Do not change any other instrument settings**. The settings in the image above (aside from Cell Temp) are the default settings required to run the diagnostics and should not be changed. If these settings are changed, the diagnostic results will be incorrect and invalid.

If the Cell Temp setpoint was modified, click OK to apply the changes and close the window. If no change was made, click Cancel to close the window.

**Optional:** If you do not wish to save the spectra collected during the diagnostics, in the Runtime UI check the box to *Pause Spectrum Collection*.

# Summary of Performance Specifications

The table below outlines the specifications criteria for each diagnostic check. The following sections detail how to check these diagnostics in the software.

Diagnostic Check	Specification
Signal Intensity (Intensity units)	> 0.04 (MAX-iR, DTGS)
	> 2.00 (MAX-iR, StarBoost)
Detector Linearity (% of Max Signal)	< 0.1%
Track Peak At	3133.068 cm <sup>-1</sup>
Peak Location	3133.068 ± 0.02 cm <sup>-1</sup>
FWHM	1.04 ± 0.04 cm <sup>-1</sup>
Computed Laser Frequency	Original Laser Frequency ± 0.08 cm <sup>-1</sup>

TABLE 14. DIAGNOSTIC PARAMETER SPECIFICATION SUMMARY

## Water Band Test

- 1. Select the Water Band tab.
  - Set Track Peak At to 3133.068 cm<sup>-1</sup>
- 1. Click Play  $(\bigcirc)$  to begin the test and collect diagnostics spectra.
- 2. Sample ambient air or process gas for few seconds to introduce ambient-level moisture into the gas cell.
  - The zero filled sample spectrum (blue line) should be between ~0.1 and 0.4 abs.



#### 3. Check the Peak Location.

 If the water Peak Location is not 3133.068 ± 0.02 cm<sup>-1</sup>, click Set Frequency. This will change the laser frequency so that the water line is properly centered at 3133.068 cm<sup>-1</sup>.

#### 4. Check the Resolution.

Observe the FWHM. It should be 1.04 ± 0.04 cm<sup>-1</sup>. There is no adjustment to optical alignment that will correct the resolution. If it is outside this range, check to see that the resolution is set to 1cm<sup>-1</sup> and the apodization is set to cosine. If it remains outside this range, contact Technical Support (see Contact Information and Technical Support).

#### 5. Check the Laser Frequency.

Confirm that the Computed Laser Freq. value and the Original Laser Freq. value are within ± 0.08 cm<sup>-1</sup> of each other. Monitor the Computed Laser Freq. for 5-10 more scans. If the Computed Laser Freq. drifts more than ± 0.08 cm<sup>-1</sup> from the Original Laser Freq., click Set



*Frequency* again. The water peak location and the laser frequency values are linked and both will change when the *Set Frequency* button is pressed.

- Monitor the Peak Location, FWHM and Computed Laser Freq. for 5-10 more scans to verify the instrument continues to meet the specifications without drifting.
- 7. Press Stop ( $\bigcirc$ ) to end the run.

## NOTICE

Take a screenshot of the Water Band Test results for recordkeeping and as mandatory documentation for applications such as compliance testing.

#### **SNR** Test

- 1. Select the SNR tab.
- 2. Click Play to begin the test and collect diagnostics spectra.
- 3. Flow 2-5 LPM nitrogen directly into the Sample Inlet.

#### 4. Check Signal Intensity

- Record the *Max Height* of the *SBeam* spectrum (shown below) and confirm it is within the specification for the detector configuration. The *Max Height* is the highest signal in the Single Beam Spectrum.
  - The *Height %* is the current signal height with reference to when the tool was started.
  - The *Height* is the current height of the maximum signal.



#### 5. Check Detector Linearity

- Record the Linearity of the single beam spectrum (shown above) and confirm that is < 0.1%. 0 Linearity is the % of signal observed beyond the detector cutoff.
- 6. Stop the flow of nitrogen to the gas cell.
- 7. Press Stop  $(\bigcirc)$  to end the run.

## NOTICE

If the instrument fails any diagnostic criteria or the laser frequency drifts more than 1.0 cm<sup>-1</sup>, please contact Technical Support (see Contact Information and Technical Support).

- 8. Return to Default View to Begin Data Acquisition
  - o If the Signal Intensity, Detector Linearity, FWHM (Resolution), and Laser Frequency are all within their respective specifications, press the Back button in the top right corner of the panel to return to the default view.

The instrument is now ready to collect sample data. If the laser frequency was set to a new laser frequency, a new background spectrum will be required.

# 7 Data Acquisition and Reporting

This chapter describes the basic steps necessary to acquire data in the MAX-Acquisition software.

#### Data Storage

All spectra data are stored indefinitely on the control PC.

- 1. Chose a location for Data Storage
  - Above the Runtime UI, press the *Save To...* button to open the *Save Folder Location* window.
  - The default directory for saving dataset folders is C:\MAX Data\Samples.
  - To choose a different directory for saving data, click *Browse…* and select the desired file path.

😔 Save Folder Location	1			_		l	×
Dataset folders will be	Dataset folders will be saved to this directory.						
C:\MAX Data\Samples					E	Brows	se
Automatically Seq	uence Folder Names						
Project Name:	Project						
Naming Pattern:	Project+Year-Mon\Day\#Seq ~						
Example:	Project 2022-08\18\#2						
					_	_	
Reset			C	Ж		Cano	el

## NOTICE

Spectral data should be saved to the local C:\drive and not sent directly to a network. This ensures data collection is not interrupted by any network communication issues. Data should always be backed up to a secondary location by the end user.

- 2. Setup Automatic Data Naming Structure (Optional)
  - Check the box next to "Automatically Sequence Folder Names" in the popup panel above.
    - This allows the spectral data files to automatically be saved into a new folder daily.
  - Type a *Project Name* into the text box replacing "Project".
    - In the example to the right, it was "Scrubber Emissions"
  - Select a Naming Pattern from the drop-down menu.
    - The recommended naming pattern is "Project+Year-Mon\Day\#Seq".
    - This organizes daily dataset folders into monthly directories, shown in the example to the right.
- Scrubber Emissions 2019-11
   19
   20
   21
   22
   23
   24
   27
   28
   24
   29
   30
   30
   31
- Click OK to return to the main MAX Acquisition interface panel.

## Data Acquisition

This section describes how to manually acquire sample data in Detailed View.

## NOTICE

If you were provided an automated Acquisition Method with Workflow, check the worksteps programmed in the Method before acquiring data. Some steps described need not be performed manually.

- 1. Begin data collection in Detailed View
  - In the Runtime UI, click Play ( $\triangleright$ ). The status indicator should say Acquiring ( $\bigcirc$ ).
- 2. Collect a background spectrum.
  - $\circ$  Flow 2-5 LPM of UHP (N3.0) N<sub>2</sub> to the gas cell.
  - In MAX-iR tab, click the "Take Background" button. The button will turn blue while the background spectrum is being acquired, and the next acquired spectrum will be used as a background to Zero the subsequent data.

## NOTICE

A new background is needed whenever a new laser frequency is set.

Monitor the sample spectrum for any absorbances from contamination (water, CO<sub>2</sub>, etc.) in the gas cell. If sharp peaks are observed in the H<sub>2</sub>O or CO<sub>2</sub> regions that are near > 0.1 abs in intensity, continue to purge the gas cell with UHP (N3.0) N<sub>2</sub> until the absorbances stabilize. Take a new Background. Monitor the next 5-10 scans to ensure there is no longer contamination in the gas cell. Representative background spectra of nitrogen gas are shown in the figure below providing a guide as to appropriate signal levels. Repeat these steps as needed.



DTGS Nitrogen background at 1 cm-1 resolution



MCT Nitrogen background using 2 x 8 cm-1 (AutoRef) - note the fine features due to ppm level water and optical filter



InAs Nitrogen background using 2 x 8 cm-1 (AutoRef) - note the fine features due to ppm water and optical filter

- *3.* Begin sampling the gases of interest.
  - Flow 2-10L of sample to the gas cell.
- 4. Monitor the Work Steps in the Workflow (Optional)
  - If you are using an Acquisition Method with Workflow, advance through the steps by using the left and right arrow buttons.
  - To view the next or previous work step hover the cursor over the left and right arrow buttons.

#### 5. Stopping data collection

• Use the Pause button (<sup>(III)</sup>) if you wish to suspend data collection while waiting to collect further data within the current folder.



- To manually stop acquisition, click the Stop () button. If the acquisition is stopped and the data are being sequenced to the next data folder, the current folder will be closed and the next one generated.
- If you are using an Acquisition Method with Workflow, data acquisition may either stop automatically or restart the workflow in a new data set once complete. Refer to your worksteps.
- Each time data acquisition is stopped, a Summary Results file (.QTA) file will be saved to the folder containing spectral files. If the *Data Recorder* is included in your *Product Configuration*, a database entry will also be published when acquisition is stopped.

## Excel Reporting in MAX-Acquisition

QTA files can be exported to Microsoft Excel. Optionally, the Acquisition Method can be configured to automatically generate an Excel report at the conclusion of the *Workflow* data collection or when the data collection is manually terminated. This section describes how to export results to Excel and how to set up automated Excel reporting in MAX-Acquisition.

## NOTICE

*The Reporting templates are stored in C:\MAX Data\data\Reports* 

## NOTICE

A license for Microsoft Excel is not included with purchase. The software allows exporting the QTA summary results to Excel format, but unless you purchase a license for Microsoft Excel, they cannot be opened on the control PC.

#### Manually Export Results to Excel in MAX-Acquisition

Results can be exported to Excel at any point during a run, if acquisition is paused (<sup>10</sup>), and/or at the conclusion of the run, when data acquisition is stopped (<sup>10</sup>).

## NOTICE

Data acquisition must be stopped or paused before proceeding further.

- 1. In Detailed View, just above the Gas List section, click the Excel (I) button to setup the summary results to export to an Excel reporting template.
- 2. Click the Save As button in the popup window (see figure to the right).
  - Choose a file name and location for the exported Excel spreadsheet.
  - Click *Save* to return to the Excel Export Options popup.
- 3. From the Excel Template drop down menu, select the appropriate reporting template.

Excel Export Option	ons		0	^
Quant Results 2022-11-14.xlsx Save As				As
Excel Template:	Detail			~
Open after export	t			
?	Ok		Can	cel

- 4. Check the box next to Open after export to automatically view the report after saving (provided you have a license for Excel resident on the PC).
  - Click *Help* (?) in the popup window to see a list of the variables that are exported to Excel.
- 6. Save and Return to Detailed View.
  - Click OK to save (Cancel to reset) the file
  - If Excel is installed, it will open for viewing the report in Excel format.

~

## NOTICE

Data acquisition must be stopped before proceeding further.

#### 1. Open the Acquisition Method Editor

- In the main Max Acquisition software top toolbar, click *Edit* > *Acquisition Method* to open the Acquisition Method List Editor.
- From the Method List Editor, select the Acquisition Method for the application then click Edit (
  ).

## 

💽 🖉 🖂 👻 🔍 💭 😥 🕫 🗼 🔩 🖓 Sam

#### 2. Setup Data Acquisition Storage Information

- In the Acquisition Method Editor, click on the Info tab (see figure below) to display current reporting information.
- Choose the location where the report(s) will be saved:
  - The default location is the *Spectrum Data Folder*, the folder containing the FTIR spectra.
  - To save reports to an alternative directory, click Select to browse for the desired directory. In the example below the folder "C\MAX Data\Daily Reports" was created and selected.

💽 Instrument Method Editor - MAX-IAQ	-		×
Info         Quant Method         Workflow         Image: Constraint of the second se			
Instrument Method Name: MAX-iAQ			
r Reporting Save Reports to Folder: Ru	n Reports		
Spectrum Data Folder     MAX-iAQ Daily     Other Folder     Select	Report		1 ^
			v
On Error: Retry Indefinitely *			
Description:			
Reset Check Back	ОК	Car	cel

#### 3. Setup Reports for Each Dataset Collected

- Under *Run Reports*, double click the top slot and select which *Report Type* you want to run.
  - Detail or Summary are two default reports provided.
  - The reports can be user modified in Excel and saved under another name in File Explorer.
- $\circ$   $\quad$  Double click on the next open slot to add another Report.
- Choose up to four reporting templates.



• Once the reports and storage location have been configured (see figure below), click *OK* to save the selections or *Cancel* to clear them, and then return back to the main MAX Acquisition panel.

## NOTICE

Note that these reporting settings will now be applied to all subsequent datasets collected with the Acquisition Method.

# 8 Recommended Operating Procedures

There are no scheduled parts maintenance for the MAX-iR. Routine calibration checks and instrument diagnostics should be used to identify any issues requiring maintenance or repair. These routine assessments are required to maintain optimal instrument performance and should only be performed by trained and experienced personnel. General specifications are provided below, however these may change depending upon the application.

Daily Checks	Description	Purpose	Specification
Zero Background	Direct measurement of UHP (N3.0) №2. Repeat daily or whenever new laser frequency is set.	Collect background. For StarBoost configurations, collect filter interference spectrum.	Check that the sample spectrum has no negative absorbances to ensure no contamination.
Alarm Status	Monitor the status of all alarms daily.	Demonstrates the Hardware is working properly.	All alarms green

TABLE 15. DAILY MAX-IR PERFORMANCE CHECKS

#### TABLE 16. PERIODIC MAX-IR DIAGNOSTIC CHECKS\*\*\*

FTIR Checks	Description	Purpose	Specification
Peak Signal Intensity	QUARTERLY: Measurement of peak intensity of single beam spectrum	Demonstrates FTIR has enough signal strength to achieve the required MDLs	See SNR Test
Detector Linearity	QUARTERLY: Measurement of average detector signal in specified spectral region.	Demonstrates the detector response is linear with respect to changing energy intensity required for constant calibration	See SNR Test
Resolution	QUARTERLY: Measurement of the FWHM of a specific Water Band.	Demonstrate that the FTIR peak resolution is still within specifications.	See Water Band Test
Laser Frequency	QUARTERLY: Verify that the laser frequency is still within the permitted values.	This allows for good spectral matching.	See Water Band Test
Clean Gas Cell	YEARLY: If Peak Signal Intensity is low then clean gas cell and mirrors.	Removes any film or debris from the mirror and window surfaces which impacts the amount of light allowed to get to the detector.	See MAX-iR Gas Cell Maintenance Procedures

\*\*\* Diagnostic checks must be done daily if using the MAX-iR for compliance testing.

## **Calibration Checks**

After initial installation, the performance of the MAX-iR should be assessed using a certified gas cylinder as a calibration transfer standard (CTS). The CTS is analyzed to verify the MAX-iR response.

The measured value, an average of 10 independent scans, should be within ±5% of the certified cylinder value. No span value should ever be applied to the CTS calibration. A method can be configured to alarm if the measurement of the calibration cylinder is outside of this specification when running a CTS.

For calibration gas and CTS gas component recommendations, please contact Technical Support (see Contact Information and Technical Support for details).

# 9 MAX-iR Preventive Maintenance

This chapter provides a guide to the hardware preventative maintenance procedures for the MAX-iR FTIR Gas Analyzer. Preventative maintenance is required to maintain optimal instrument performance, and these procedures should only be performed by trained and experienced personnel. While many of these items can be completed by the user, it is recommended the user take advantage of the MAX-Advantage support program.

#### Preventative Maintenance Schedule

Schedule	Procedure	Specification
Quarterly	Check MAX-iR Peak Signal Intensity	See SNR Test
	Check MAX-iR Detector Linearity	See SNR Test
	Check MAX-iR Resolution	See Water Band Test
	Check MAX-iR Laser Frequency	See Water Band Test
Annually	Clean MAX-iR Gas Cell Mirrors and Replace O-rings	See
		MAX-iR Gas Cell Maintenance Procedures

 TABLE 17. PREVENTIVE MAINTENANCE SCHEDULE

## Spare Parts and Consumables

The following serviceable items are consumables and are not covered under warranty. The user should maintain an on-site inventory of consumables, as shown in the table below.

TABLE 18. MAX-IR CONSUMABLES

Description	Yearly Qty	Replacement Interval
Kit, MAX-iR Gas Cell o-Rings	1	Replace when cleaning gas cell mirrors.
MAX-iR Gas Cell Windows*	2	
$\circ$ KBr Gas Cell Window, MgF <sub>2</sub> Coated		Remove and replace when cleaning gas cell mirrors.
• CaF <sub>2</sub> Gas Cell Window		Do not remove when cleaning. Replace if damaged.
<ul> <li>ZnSe Gas Cell Window, AR Coated</li> </ul>		Do not remove when cleaning. Replace if damaged.
<ul> <li>ZnSe Gas Cell Window</li> </ul>		Do not remove when cleaning. Replace if damaged.
• BaF <sub>2</sub> Gas Cell Window		Do not remove when cleaning. Replace if damaged.
MAX-iR Gas Cell Window o-Ring	2	Replace with gas cell window.
MAX-iR Gas Cell Window PTFE Washer	2	Replace if original is lost or damaged.

\*Application dependent. Refer to MAX-iR Part Numbers and Configurations for details.

Thermo Fisher Scientific maintains a spare parts depot in East Windsor, CT. For critical spare parts with extended delivery times (denoted below), the user should consider maintaining spare parts on-site to minimize downtime.

 TABLE 19. MAX-IR CRITICAL SPARE PARTS

Description	Yearly Qty	Replacement Interval
Pressure Transducer*	1	Critical spare. Only replace if needed.
<ul> <li>Kit, 1atm Pressure Transducer</li> </ul>		
<ul> <li>Kit, 5atm Pressure Transducer</li> </ul>		
Kit, Gas Cell Mirror, Objective	1	Critical spare. Only replace if needed.
Kit, Gas Cell Mirror, Field 1		Critical spare. Only replace if needed.

\*Application dependent. Refer to MAX-iR Part Numbers and Configurations for details.

## MAX-iR Gas Cell Maintenance Procedures

#### Required Tools

In general, the mirror and windows do not need to be cleaned or replaced unless there are issues with signal intensity that cannot be attributed to any other component.

Parts / Tool	Description
Screwdriver	Philips head
Allen Wrenches	2.5mm, 3mm, 4mm
Long Shaft Allen Wrench	5mm
Lens paper	Lint free lens paper or lens cloth – do not use Kleenex or paper towels
Water & Soap	Warm Tap Water & Dawn Dish Soap
Small flashlight	Used to inspect the gas cell windows
Gas Cell Mirror o-Ring Kit	MAX-iR Gas Cell O-ring – Qty 1

## 

Take care when working with the gas cell and the sample line as they may still be hot. Allow at least 4 hours for cooling before handling the gas cell or sample lines.

#### Removing the MAX-iR Gas Cell

Using the Phillips head screwdriver remove the 6 outer screws of the MAX-iR top cover – two on each side and two on the top back flap of the cover.

• Using the 3mm Allen wrench loosen (do not remove) the two screws holding the gas cell cover on and pull the cover up and off the gas cell.



- Facing the back of the MAX-iR, note the orientation of the bulkhead shields. Use the 2.5mm
   Allen wrench to remove two lower screws as well as the two upper screws holding the bulkhead shield in place. Remove the shields and set them aside.
- Using a Phillips head screwdriver, remove the 4 screws holding the Sample In/Sample Out access panel in place. Remove the access panel and set it aside.



- Disconnect the electrical connections going to the gas cell. There are two yellow thermocouple connections and two white Molex power connections that are adjacent to the pressure transducer that need to be removed.
- The yellow connections are removed by squeezing the sides and gently pulling them out.
- The white connectors are removed by pushing down on the top clip and gently pulling them out.
- Using the long-handled 5mm Allen wrench, loosen the 4 capture screws two on each side of the gas cell base - that are holding the gas cell in place. Pull the gas cell up – note you may



have to use a flat head screwdriver in the specified notches to gently pry the base up to loosen it.



• Carefully remove the gas cell from the MAX-iR by pulling the left side (with the window retainers) towards the outside first, so the window retainers come out first.

#### Replacing the MAX-iR Gas Cell Windows

- 1. Inspect the Windows for fogging
  - Without removing the windows, use the flashlight and shine it on the gas cell windows to see if there is any fogging.
  - If the windows are clean, proceed to next section to replace or clean the MAX-iR gas cell.

#### 2. Replace the Windows and Window O-rings

- Use the figure below for reference. For ease of window replacement, it is recommended that the field mirror (mirror with windows) be removed before replacement of the windows. Refer to the next section for the proper procedure to remove the mirror.
- Gently remove the grey insulation from the window retainers, pulling the top above the top window retainer. Be careful not to tear the insulation.
- Remove and set aside the two outer O-rings on the outside of the two window retainers (A).
- Using the 3mm Allen wrench remove each of the three window retainer screws and remove the retainers (B).
- Remove the white PTFE gasket (this will be reused so do not throw it away).
- Remove the window and the bottom O-ring out of the gas cell cavities (C, D). The windows
  may be stuck and require some force to remove. Put the mirror face down on a flat surface
  with a cloth and gently push the windows out using a Q-tip from the other side. It may require
  pressure around the corners of the window for it to be removed. (Damage to the window is
  common when removing them, only remove them if necessary or if they are being replaced).



- Make sure the O-ring groove is clean and dry (a Q-tip) is ideal for cleaning, drying or removing debris
- o Insert a new O-ring (D) and new window (C) into the gas cell cavity (red arrow).
- Only 5 mm thick by 25 mm to 25.2 mm diameter round windows can be utilized by MAX-iR.
- The best procedure to insert a new window is to hold it above the opening and then drop it onto the O-ring. Trying to place the window in the opening may cause it to cock and this can crack the window. If the window goes in at an angle do not try to push into place (this will cause damage to the window). Gently flip the mirror over and catch the window with a gloved hand or onto a soft cloth on a flat surface.
- Reinsert the PTFE gasket on top of the window.
  - Note: The white PTFE gasket located between the retainer (B) and window (C) should only be replaced if it is damaged (see below).



- Replace the retainer (B) and then gently tighten down the retainer with the three screws in a circular pattern until all three screws are completely tight. repeat for the other window.
- Replace the outer sealing O-rings (A).
- Confirm that the insulation is on the window retainers and the inlet / outlet plumbing on the rear of the gas cell before attempting to reinstall the gas cell. Be gentle it can tear easily.



#### 3. Replace the Gas Cell back into the MAX-iR

- To replace the gas cell into the MAX-iR, follow the reverse instructions as shown in the section above Removing the MAX-iR Gas Cell.
- The gas cell is positioned properly if it is firm in place and does not rock side to side. Gently tighten the four captive baseplate screws until completely tight to the baseplate.
- Confirm that the remaining insulation is in place. Especially the two pieces located underneath the mirrors on both ends.
- $\circ$   $\;$  Replace the insulating cover making sure the foam does not tear or fold over.
- Tighten 3 mm screws to hold the cover in place
- Make sure the cover slips all the way down against the optics box cover and that it is not standing off of the back plate (should be a ¼ inch below the vertical back plate).
- Reconnect the 4 electrical connections, starting with the two white Molex connections and then the two yellow thermocouple connections.
- Replace the back plate of the MAX-iR that includes the plumbing bulkhead shields.

## 

Before reinstalling the gas cell, verify that all 12 heater plate screws on the top and bottom are tight. Failure to do so may result in poor heating and / or damage to the heaters.

#### Replacing or Cleaning MAX-iR Gas Cell Mirrors

## NOTICE

In most cases, cleaning the Objective Mirror (F) should be sufficient. Only clean the Field Mirror (C) if necessary.

- 1. Remove the Gas Cell from the MAX-iR
  - Follow the same instructions as shown in the section above Removing the MAX-iR Gas Cell.
- 2. Remove the Gas Cell Mirrors
  - Use the figure below for guidance.
  - Remove and set aside the two outer O-rings on the outside of the two window retainers (A).
  - Using the 2.5mm Allen screwdriver, loosen the six screws holding each of the heater plates to the gas cell (green circles). Do not remove.
  - Using the 4mm Allen screwdriver, remove the three screws (B) holding the Field Mirror (if needed) (C) and Objective Mirror (F) to the gas cell body.
  - Pull both mirrors off the gas cell body and remove the two O-rings (D, E).

## NOTICE

Take care that you put the correct O-rings back on the gas cell as they are different sizes. D is the Field Mirror O-ring while E is the Objective Mirror O-ring.


### 

In the next step below you must use lint free lens paper or lens cloth – do not use Kleenex or paper towels or you will permanently scratch the surface of the mirrors.

- 3. Clean the mirror surface
  - Inspect the mirror surfaces for contamination.
  - Wearing Latex lab gloves to hold the sides of the mirror, use warm tap water (distilled will not work well) to gently rinse the surface of the objective mirror over a sink or appropriate waste disposal area.
  - If a residue remains on the objective mirror surface, Dawn Dish Soap can be utilized to clean the mirror surface.
    - Apply a small drop of Dawn dish soap to the mirror surface. Very gently, a gloved finger can be used to spread the soap across the mirror surface, until the soap suds fully
    - Use warm tap water to thoroughly rinse the mirror surface and remove all soap.
  - Rinse mirror with distilled water (if available).
  - $\circ$  Dry the mirror with high pressure N<sub>2</sub> or clean dry air (CDA), to remove all visible traces of water. Then inspect again for any contamination. Clean again if needed; if residue still remains, use a lint free lens paper or cloth (diagrammed

Make sure the entire mirror is completely dry prior to returning it to the gas cell.



#### 4. Reassemble the gas cell

- Replace both the Objective and Filed mirror O-rings with new ones.
- Use the figure and instructions above in Step #2 of Replacing or Cleaning MAX-iR Gas Cell Mirrors and reverse the order to reassemble the mirrors onto the gas cell.
- The mirrors should be tightened until the screws stop turning. If the screw has a gummy feeling while tightening, it is possible the O-ring is trapped outside its intended groove. If this happens it is recommended to replace the trapped O-ring with yet another new O-ring for proper sealing.
- 5. Replace the Gas Cell back into the MAX-iR
  - To replace the gas cell into the MAX-iR follow the reverse instructions as shown in the section above **Removing the MAX-iR Gas Cell**.

### 

Before reinstalling the gas cell, verify that all 12 heater plate screws on the top and bottom are tight. Failure to do so may result in poor heating and / or damage to the heaters

#### **Replacing Fuses**

The power inlet module has two fuses to protect against overcurrent or short circuit. If necessary, be sure to replace with fuses of the same rating, as indicated on the system label.

- 1. Shut off the power to the MAX-iR
  - $\circ$   $\;$  Switch the Power switch on the back of the unit to OFF.
  - $\circ$   $\;$  Disconnect the system power cord from the back of the unit.
- 2. *Remove the fuse block from the power inlet module* 
  - Use a flat head screwdriver to pull the block out.



**3.** Replace both fuses and insert the power inlet module back into the unit. Plug in the cord, switch on the power switch to turn the power back on to the unit.

## 10 Troubleshooting

This chapter provides guidelines to frequently asked questions relative to troubleshooting the MAX-iR and associated software.

Issue	Solution		
No communication with Temperature or Pressure sensor after software installation	Disconnect USB from computer or MAX-iR and reinstall software.		
The computer went to sleep which disrupted data collection and caused a connectivity issue	1.	Install the updated software version (if applicable)	
	2.	Go to Start > Settings > Power & Sleep.	
	3.	For both sleep options, please select "Never".	
	4.	Power off the MAX-iR.	
	5.	Go to Start > Power > Restart.	
	6.	Once the computer has restarted, power on the MAX-iR.	
Software not acquiring temperature and/or pressure	1.	Verify that the serial USB connection cable is connected between the MAX-iR and the computer.	
	2.	In the MAX-Acquisition Software, go to Edit > Product Configuration. Select the current Product Configuration so it is highlighted in blue, then select the pencil icon to edit it.	
	3.	Once the editing window opens, select the MAX-iR Temperature and Pressure Sensor module. Next to COM Port, click <b>Search</b> to allow the software to automatically identify the appropriate COM port.	
	4.	If the software identifies a COM port, select OK then Save the changes to the Product Configuration before resuming data collection.	
	5.	If a COM port is not identified, unplug the ethernet cable as well as the serial USB connection from the PC. Re-connect the ethernet and serial cables.	
	6.	Retry the search. Once identified, select OK then Save the changes to the Product Configuration before resuming data collection.	

Software not connecting to spectrometer	<ol> <li>Verify that the ethernet cable is connected between the MAX-iR and the computer.</li> </ol>		
	<ol> <li>In the MAX-Acquisition Software, go to Edit &gt; Product Configuration. Select the current Product Configuration so it is highlighted in blue, then select the pencil icon to edit it.</li> </ol>		
	<ol> <li>Once the editing window opens, select the MAX-iR Spectrometer monospectrometer Instance, click <i>Search</i> to allow the softwar automatically identify the appropriate spectrometer.</li> </ol>		
	4. If the software identifies a spectrometer, it may give a message indicating that the laser frequency may need to be set. Typically, this occurs when it is the first time that the computer is connected to the hardware.		
	<ol> <li>Select OK then Save the changes to the Product Configuration before resuming data collection.</li> </ol>		
	6. If a spectrometer is not identified, unplug the ethernet cable from both the MAX-iR and PC. Re-connect the ethernet cable to both the MAX-iR and computer. Retry the search. Once identified, select OK then Save the changes to the Product Configuration before resuming data collection.		
Gas cell not heating	Check the power connections and the thermocouple connections under the top cover (next to the pressure transducer)		
No Water Band during Diagnostics	Add ambient air to the gas cell. This should contain enough water to allow for proper calculation of the laser frequency and water band frequency.		
Poor laser frequency calculation	Confirm that the water peak is between ~0.1 to 0.4 abs for best calculation of water and laser frequencies. If the water absorbance is too low, add ambient air to the gas cell. If the water absorbance is too high, turn on N <sub>2</sub> briefly to the gas cell and then stop the flow, so that the moisture is between the recommended absorbances.		
Calculated laser frequency outside of standard range	Laser frequency is more than $\pm 2$ cm <sup>-1</sup> from 15799 cm <sup>-1</sup> . Confirm that the water peak is between ~0.1 and 0.4 abs.		
	If still outside of range, please contact Technical Support for instructions or how reset to proper laser frequency (see Contact Information and Technica Support).		
FWHM of Water Band	If FWHM is outside recommended guidance, confirm that the water band is between ~0.1 and 0.4 absorbance and measure again.		
	If the FWHM is significantly higher than 1.04 cm <sup>-1</sup> , check resolution setting of instrument. Then check the gas cell windows for fogging.		
	If the gas cell was recently removed, confirm gas cell is properly seated.		
Gas Cell Temperature Incorrect in Diagnostics	The gas cell temperature is set in the Acquisition Method. It is recommended that diagnostics are run at the same temperature that data will be collected Select the Acquisition Method that corresponds with the data collection prio to running diagnostics. This will ensure the diagnostics are run at the correc temperature.		

CTS Failed	1. Verify that the gas cylinder is properly connected and that there are no leaks.		
	<ol> <li>Confirm that the ethylene calibration in the Quant Method matches the temperature, pressure, and resolution settings in the Acquisition Method.</li> </ol>		
	3. Check MAX-iR Diagnostics (see Water Band Test and SNR Test).		
	4. Repeat CTS measurement.		
Quant is 'NaN'	Confirm the quantification region is in a region of the spectrum that there i signal present, and that the absorbance spectrum is being calculated for tha region. If not, the quantification region must be moved to a valid region.		
Algebraic values not displayed	If the algebraic is a batch average over a particular <i>Workstep</i> , the value will not publish until that workstep is complete.		
Low Signal Strength	If the MAX-iR is used to analyze process or environmental samples, the gas cell may be contaminated. Consider cleaning the Objective mirror and/or replacing the windows if they are damaged. See MAX-iR Gas Cell Maintenance Procedures.		
Signal Strength Alarm	If the signal is below 10, consider increasing the gain. If the signal is above 90, it is important the gain setting be reduced to prevent over-range of the digitizer. This will produce poor data quality like wavy baselines and single beam spectra.		
Desired Acquisition Method does not appear in list	Verify that the correct Product Configuration is selected.		
Error Message: Setting Resolution: 1	The resolution did not set properly. Close MAX-Acquisition then re-open it.		
Error Message: X Hours Since Last Neon Calibration	Contact Technical Support (see Contact Information and Technical Support).		
Pressure Transducer does not agree with calibrated Baratron measurement	The pressure transducer in the MAX-iR comes calibrated and should not require any adjustments. If it is suspected that the pressure transducer is not measuring correctly, please contact Technical Support (see Contact Information and Technical Support).		

Poor Spectral Residuals or quantitative results	1. Confirm the laser frequency is correct.		
	2. Confirm the resolution is correct for the method being used.		
	3. Confirm that all gases present in the sample are in the method.		
	4. Confirm that water and carbon dioxide are listed as interferences.		
	5. Confirm the quant region is within the spectral range of the system.		
	<ol> <li>Confirm that multiple regions are not being utilized by reviewing the location of the residual.</li> </ol>		
	7. Confirm the calibration and sample gas are at the same temperature.		
	8. If all settings are correct, try utilizing the fencing algorithm within the calibration editor to reduce the residuals.		
	<ol> <li>Additionally try using "Forward" only in the MAX-iR settings instead of "Both"</li> </ol>		
MAX Software needs to be installed	Whenever the MAX Software package needs to be installed, the license key needs to be active on the associated computer and all MAX software programs must be closed. If updating the software, do NOT uninstall the previous software version or it will result in permanent loss of data, calibrations, methods, etc.		
Quant Method was modified	If the Quant Method is modified, the updates can be saved by selecting File > Save Quant Method As		
Instrument Method is in Read Only	To modify the Instrument Method, data collection must be stopped. If data collection is active or paused, the software will display the Instrument Method editor in Read Only view to prevent modifications.		
	editor in Read Only view to prevent modifications.		
۹ Bad Scan occurred	editor in Read Only view to prevent modifications. If the MAX-iR experiences any sudden contact, such as getting bumped into, hit, etc. a bad scan may occur. It is best practice to set up all sample lines prior to data collection and to take care to avoid harsh contact with the MAX-iR.		
A Bad Scan occurred .ow Signal Alarm	editor in Read Only view to prevent modifications. If the MAX-iR experiences any sudden contact, such as getting bumped into, hit, etc. a bad scan may occur. It is best practice to set up all sample lines prior to data collection and to take care to avoid harsh contact with the MAX-iR. Forward/backward sweep – need additional info		
A Bad Scan occurred Low Signal Alarm Computer crashed and software is not working	<ul> <li>editor in Read Only view to prevent modifications.</li> <li>If the MAX-iR experiences any sudden contact, such as getting bumped into, hit, etc. a bad scan may occur. It is best practice to set up all sample lines prior to data collection and to take care to avoid harsh contact with the MAX-iR.</li> <li>Forward/backward sweep – need additional info</li> <li>It is recommended that data, Instrument Methods, and Quant Methods are backed up in case of a computer crash. If the computer crashes and the MAX Software package is not responding, update and restart the computer. If the issue persists, re-install the MAX Software package.</li> </ul>		
A Bad Scan occurred Low Signal Alarm Computer crashed and software is not working While the MAX-iR was open, the Watlow was manually adjusted	<ul> <li>editor in Read Only view to prevent modifications.</li> <li>If the MAX-iR experiences any sudden contact, such as getting bumped into, hit, etc. a bad scan may occur. It is best practice to set up all sample lines prior to data collection and to take care to avoid harsh contact with the MAX-iR.</li> <li>Forward/backward sweep – need additional info</li> <li>It is recommended that data, Instrument Methods, and Quant Methods are backed up in case of a computer crash. If the computer crashes and the MAX Software package is not responding, update and restart the computer. If the issue persists, re-install the MAX Software package.</li> <li>All the Watlow settings in the MAX-iR are preconfigured so that the MAX Software package controls all temperature settings in the MAX-iR. Therefore, it is recommended that the Watlow is never modified or adjusted manually. If the Watlow settings are modified or adjusted, they will need to be reset back to factory settings. If this occurs, please contact Technical Support (see Contact Information and Technical Support).</li> </ul>		

	If KBr with MgF2 windows are in use, the windows may become fogged or even dissolve in the presence of liquid moisture. This will likely result in loss of signal that cannot be attributed to another factor.	
Liquid moisture may have gotten into the gas cell	If any of the alternative windows are used, the gas cell will likely need to be heated to 191C and purged with N2 to remove the moisture. Alternatively, the gas cell can be cleaned as well.	
	If you are unsure of the type of windows that you have in your MAX-iR, please contact Technical Support (see <b>Contact Information and Technical Support</b> ).	
Gas cell window will not remove from the mirror	It is important to note that the gas cell windows can easily get damaged or broken when removed. As a result, it is recommended that spare windows are kept on hand. Windows are easier to remove when they are warm, but the gas cell should never be hot during maintenance, or it could result in injury.	
	A trick that can be utilized to help remove the window is to use a clean, dry q tip to gently push along the outer edge of the window to help push the window out. Do NOT touch anywhere near the center of the window or it could result in damage to the window.	
When replacing the gas cell window, the window keeps going in place crooked	It is important to ensure that the window o-ring is replaced when the window is replaced. The washer should only be replaced if it is damaged or deformed.	
	When replacing the gas cell window, it is important to keep the window level over the hole in the mirror with the mirror laying flat. The best means of setting the window into place is by "dropping" it.	
Gas cell mirror was cleaned, but there is still residue on the mirror	Always follow the steps outlined in Replacing or Cleaning MAX-iR Gas Cell Mirrors. If the gas cell mirror still has a residue after , contact Technical Support (see Contact Information and Technical Support).	
Retainer plates around the Sample In and Sample Out were removed	There are 2 metal retainer plates that are located around the Sample In po as well as 2 that are located around the Sample Out port. For MAX-i maintenance, they may need to be removed. When putting them back int place, they should be installed so that there is not a gap between the re insulation ring and the retainer plates. Take care not to damage the re insulation ring during this process to avoid creating a cold spot.	
The foam insulation was damaged during MAX-iR maintenance	The insulation material is brittle and can easily be damaged or broken. It is important to take special care of it while working on the MAX-iR. If the insulation material becomes damaged at any time, please contact your sales representative to order a replacement.	
Error Message States "No connection could be made because the target machine	If this error message appears when connecting to the spectrometer, it typically indicates a part of the MAX Software package was not installed properly or has been deleted. Close all MAX Software programs and re-install	
actively refused it. 127.0.0.1:5002"	the MAX Software. If this becomes a recurring issue, contact Technical Support (see Contact Information and Technical Support).	

# Appendix: O-ring Chemical Compatibility

Gas (as bulk)	Viton	FFKM (Kalrez)	PTFE (Teflon)
Ammonia	U	S	S
Hydrogen Chloride	S	S	S
Hydrogen Bromide	S	S	S
Hydrogen Fluoride	S	S-	S
Phosphine	N/A	S	S
Diborane	N/A	S	S
Arsine	S	S	S
Silane	S	S	S
Trichlorosilane	N/A	S	S
Boron Trifluoride	N/A	S	S
Nitrogen Trifluoride	N/A	S	S
Carbon Tetrafluoride	S	S	S
Sulfur Hexafluoride	S	S	S
Phosgene	N/A	S	S
Hydrogen Cyanide	S	S	S
Carbonyl Fluoride	N/A	S	S
Fluorine	S-	S-	U
Bromine	S	S	S
Hydrogen	S	S	S
Argon	S	S	S
Oxygen	U	S	S
Nitrogen	S	S	S
Carbon Dioxide	S	S	S
Carbon Monoxide	S	S	S
Methane	S-	S	S
Ethane	S	S	S
Ethylene	S	S	S
Propylene	S	S	S
Propane	S	S	S
Ethylene Oxide	U	S	S
Ozone	S	S	S
S (satisfactory)			
S- (slightly satisfactory)			
U (unsatisfactory)			
N/A (no available data)			