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Operating Instructions
Raman RunTime v6.6

Endress+Hauser
People for Process Automation

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1 About this document

1.1 Document function

This manual provides details on configuring and using Raman RunTime for process applications, but it is not intended to replace Raman Rxn system analyzer installation and training from Endress+Hauser representatives.

This Raman RunTime software manual is approved for use with the following analyzer configurations:

- Raman Rxn2 and Raman Rxn4 single-channel and four-channel embedded analyzers with 532, 785, or 1000 nm.
- Raman Rxn2 Starter single-channel and four-channel embedded analyzers with 785 nm.
- Raman Rxn2 Hybrid and Raman Rxn4 Hybrid embedded analyzers with 785 nm.
- RamanRxn2 and RamanRxn4 non-embedded analyzers with 785 nm.
- RamanRxn2 and RamanRxn4 non-embedded analyzers with 1000 nm.
- Raman Rxn5 embedded analyzer with 532nm.

CAUTION

▶ The performance of procedures, the use of controls, or the adjusting of the analyzer other than as specified in the manual may result in hazardous radiation exposure.

1.2 Safety symbols

Warnings

Structure of Information	Meaning
WARNING **Causes (/consequences)** Consequences of noncompliance (if applicable) ▸ Corrective action	This symbol alerts you to a dangerous situation. Failure to avoid the dangerous situation can result in a fatal or severe injury.
CAUTION **Causes (/consequences)** Consequences of noncompliance (if applicable) ▸ Corrective action	This symbol alerts you to a dangerous situation. Failure to avoid this situation can result in minor or more serious injuries.
NOTICE **Cause/situation** Consequences of noncompliance (if applicable) ▸ Action/note	This symbol alerts you to situations which may result in damage to property.

Symbols on the device

Symbol	Description
	The Laser Radiation symbol is used to alert the user to the danger of exposure to hazardous visible laser radiation when using the Raman Rxn system.
	The High Voltage symbol alerts people to the presence of electric potential large enough to cause injury or damage. In certain industries, high voltage refers to voltage above a certain threshold. Equipment and conductors that carry high voltage warrant special safety requirements and procedures.

Symbol	Description
	The WEEE symbol indicates that the product should not be discarded as unsorted waste but must be sent to separate collection facilities for recovery and recycling.
CE	The CE Marking indicates conformity with health, safety, and environmental protection standards for products sold within the European economic area (EEA).

1.3 List of abbreviations

Term	Description
ALT	Alternate
BIS	Bureau of industry and security
Btu	British thermal unit
°C	Celsius
CRS	Calibration reference standard
CSM	Calibration switching module
DCS	Distributed control system
EEA	European economic area
°F	Fahrenheit
FC	Fiber channel
GPa	Gigapascals
GPA	Gas processors association
HCA	Raman calibration accessory
HV	Heating value
INTLK	Interlock
IP	Internet protocol
IPA	Isopropyl alcohol
ISO	International organization for standardization
kJ	Kilojoule
kPa	Kilopascal
LAN	Local area network
LED	Light emitting diode
LNG	Liquefied natural gas
LOD	Limit of detection
NAT	Network address translation
nm	Nanometer
OPC	Open platform communications
PDF	Portable document format
psi	Pounds per square inch
psia	Pounds per square inch absolute
RTU	Remote terminal unit
SOP	Standard operating procedure

Term	Description
SPC	Spectrum file format
TCP	Transmission control protocol
TLS	Transport layer security
UA	Unified architecture
UDP	User datagram protocol
USB	Universal serial bus

1.4 Documentation

All documentation is available:

- On the media device supplied (not included in the delivery for all device versions)
- On the Endress+Hauser mobile app: www.endress.com/supporting-tools
- In the Downloads area of the Endress+Hauser website: www.endress.com/downloads

This document is an integral part of the document package, which includes:

Part Number	Document Type	Description
4005856	Raman RunTime Automation OPC v6.6	Current list and history of OPC Tags for Raman RunTime.
4005855	Raman RunTime Automation Modbus v6.6	Current Modbus Map for Raman RunTime.
4005857	HTTPS Automation Interface v6.6	Details on using HTTPS protocol to transfer supported file types to Raman RunTime.

1.5 Registered trademarks

Modbus®
Registered trademark of SCHNEIDER AUTOMATION, INC.

SIMCA®
Registered trademark of Sartorius Stedim Biotech.

GRAMS IQ™
Registered trademark of Thermo Fisher Scientific.

PEAXACT
Trademark of S-Pact

Aspen Unscrambler™
Registered trademark of AspenTech

Solo/PLS_Toolbox
Trademark of Eigenvector research, Inc.

2 Safety

2.1 Product safety

CAUTION

Laser Safety Notice. Endress+Hauser Raman analyzers utilize laser sources as an excitation source.

- When using the Raman RunTime near an operating instrument, follow all safety requirements outlined in the operating and safety documents of the analyzer and Raman probe(s) being used.

2.2 IT safety

IT security measures, which provide additional protection for the device and associated data transfer, must be implemented by the operators themselves in line with their security standards.

2.2.1 Device-specific IT security

In addition to creating users for password protection of system functionality, Raman RunTime's security features protect against your Raman Rxn system unauthorized usage with the following features:

- Customized embedded system presents a non-standard attack surface.
- For-purpose operational profile eliminates unauthorized user behaviors.
- Network accessibility limited to analyzer core services.
- Only authenticated updates digitally signed by Endress+Hauser can be applied.
- No capability for running non-Endress+Hauser software.
- Unauthorized system modifications are automatically purged upon reboot.

2.2.2 Remote access from web browser

Raman RunTime can be accessed using a desktop web browser from a remote workstation that meets the following requirements.

Client system requirements

- Google Chrome or Microsoft Edge (for remote access)

There are two ways to access the Raman RunTime user interface remotely:

- **Standard.** Navigate to *http://<IPaddress>:3593* or *http://<hostname>:3593*.
- **Secure.** Navigate to *https://<hostname>:3594*. The client must be able to resolve the analyzer hostname for secure connections. Refer to *Network configuration* →🗎 for a list of ports that need to be open on the network for secure remote access.

The IP Address and hostname of the analyzer can be viewed and configured under **Options > System > Network**.

When Security within Raman RunTime is enabled, attempts to access Standard remote access are redirected to the Secure remote access URL.

Refer to *Certificates* → 🗎 for instructions on avoiding privacy warnings by configuring trust on client workstations.

2.2.3 Security settings

Security can be enabled to block non-authorized users from performing Raman RunTime functions. By default, security is set to **OFF**. When security is **ON**, access to restricted functionality requires the name and password of an authorized user.

User accounts with different access levels can be added to Raman RunTime. When the security feature within Raman RunTime is enabled, the system automatically locks itself after 10 minutes of inactivity.

To turn security settings on

1. Navigate to **Options > System > Security**.
2. Toggle Security to **On**.

A notice appears that states that a system administrator password must be set.

3. Click **OK** and enter a password for the system administrator. Verify the password in the second password step.

   Record the system administrator password. It is required to turn security on and off, and to create new users.

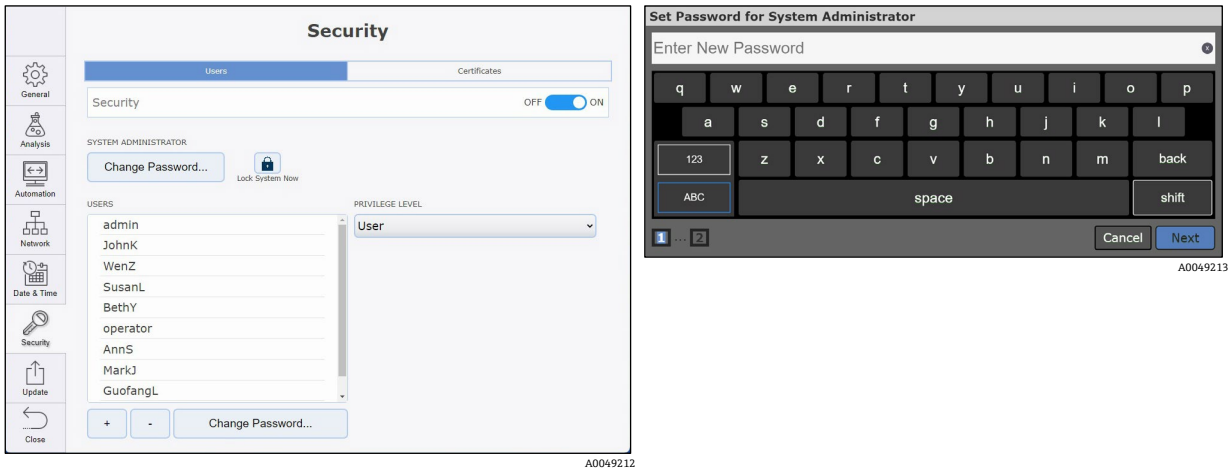


Figure 1. Setting up security

When the Administrator password is verified, the system security turns on. Refer to *User interface* → 🗎 for a description of the Raman RunTime dashboard.

To lock the system after enabling security

1. Click **Lock System Now**.
2. Click **OK** on the confirmation messages.

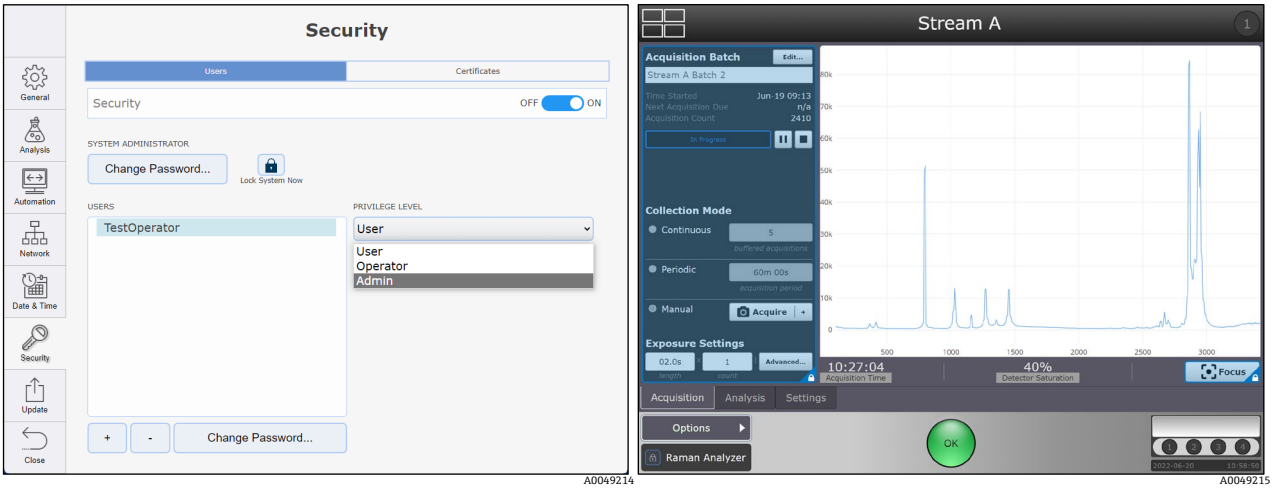


Figure 2. Security settings, adding users, and restricted access

On the Raman RunTime dashboard, a **Blue** lock appears over the following restricted features:

- Pausing or stopping a batch
- Acquisition settings
- Model selection
- Stream settings
- Focus
- System options
- Exporting a new diagnostics report
- Internal and probe calibration

The system can also be locked by clicking **Lock** in the lower left corner of the dashboard, next to the Raman Analyzer name.

2.2.4 Certificates

Raman RunTime delivers certificate management for secure remote access with a self-signed root CA certificate for encrypting HTTPS communication. IT services can deploy trusted root CA certificates to managed workstations, making trust automatic and invisible to end users, without per-workstation effort.

Each analyzer can be configured to use either Raman RunTime's default root certificate or a custom root certificate. The default root certificate is available on all analyzers running Raman RunTime v6.5 or newer, and custom root certificates can be copied from one analyzer to another. For ease of management, it is recommended that all analyzers accessed from the same client workstations use the same root certificate.

Default and custom root certificates can be managed on the Certificates tab of the Security screen in Settings. To grant trust on a workstation to the Raman analyzer, first save the root certificate to a file, then add the analyzer's root CA certificate to the Trusted Root Certification Authorities store on the workstation, as below.

To save the root certificate

1. From the workstation, navigate to *https://<hostname>:3594* in a qualifying web browser. This connects you to the Raman analyzer.

   If trust has not been configured, web browsers present a privacy warning. This warning is expected in a secure network environment.

2. Bypass the warning to access the analyzer by selecting **Advanced** and clicking **Proceed to <hostname>**.

   The remote access dashboard displays.

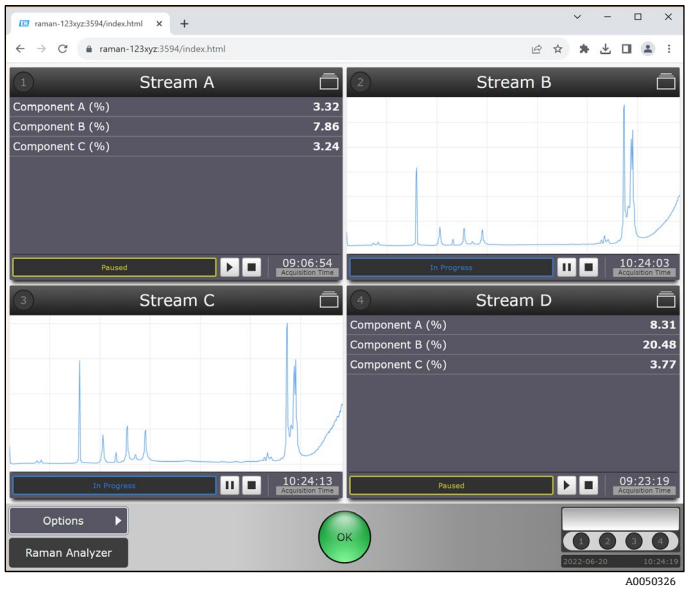


Figure 3. Remote access dashboard

3. Click **Options**, then **Settings**.
4. On the **Settings** screen, select the **Security** tab, then the **Certificates** tab.

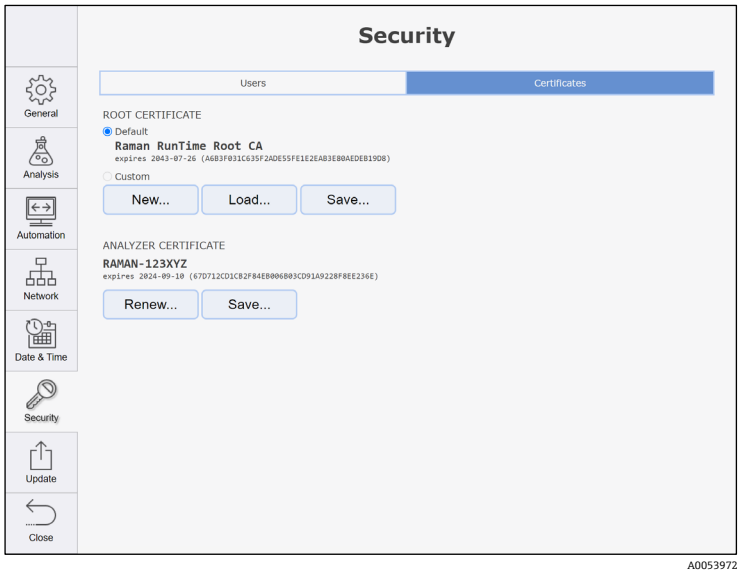


Figure 4. Root certificate options

5. **Save** the root CA certificate to a file. The "Save" button in the root certificate section of the settings screen saves the active root CA certificate to a locally attached flash drive. You can also download the certificate to a remotely connected client.

To add the analyzer root CA certificate to the workstation Trusted Root Certification Authorities store

1. Double-click the exported certificate file.
2. In the Certificate **General** tab, click **Install Certificate**.
3. In the Certificate Import Wizard, select **Current User**, then **Next:**
   a. Select the Place all certificates in the following store then click Browse.
   b. Select Trusted Root Certification Authorities.
   c. Click **Next**, and then **Finish**.
4. In the security warning dialog box, the Analyzer's hostname displays. Click **Yes** to install the certificate.

Granting trust to the analyzer's certificate is now complete. Upon restarting the compatible web browser and navigating to *https://<hostname>:3594*, the certificate shows as installed and trusted.

3 Product description

Endress+Hauser's Raman RunTime embedded software is the control platform for the Endress+Hauser suite of Raman Rxn analyzers. Raman RunTime software is intended for easy integration with standard multivariate analysis and automation platforms to enable a real-time, *in situ* process monitoring and control solution. Raman RunTime presents an OPC and Modbus interface, which provides clients with analyzer data as well as analyzer control functions.

3.1 Raman analyzers

⚠ CAUTION

▶ When the Raman Rxn analyzer's main power switch and laser key are turned **ON**, probes should be shuttered or covered. Laser safety must always be considered.

Raman Rxn2 and Raman Rxn4 embedded analyzers

Raman RunTime software is embedded into the following analyzer configurations:

- Raman Rxn2 and Raman Rxn4 configured as a single- or four-channel embedded analyzer (532 nm, 785 nm, or 1000 nm wavelength laser)
- Raman Rxn2 single-channel, embedded analyzer starter configuration (785 nm only)
- Raman Rxn2 or Raman Rxn4 hybrid analyzer configuration (785 nm only)

Raman Rxn5 embedded analyzer

Raman RunTime software is fully embedded into the Raman Rxn5 analyzer (532 nm).

Raman Rxn non-embedded analyzers

Raman Rxn non-embedded analyzer configurations that support Raman RunTime software are outlined in the table below. New configurations are only available with Raman RunTime version 6.1+, while older models are compatible with earlier software versions.

Raman RunTime software can be used for those customers wishing to continue using older versions of their existing Raman Rxn analyzers, including the RamanRxn2 and RamanRxn4 non-embedded four-channel analyzers configured with either 785 nm or 1000 nm. The 1000 nm non-embedded configuration has a single-channel option, but the 785 nm does not.

Use with non-embedded analyzers can be accomplished by running Raman RunTime as the control platform via an optional external controller, which can be the original HMI or the current HMI. Both external controllers are functionally equivalent. The current shipping HMI is referred to as either the current HMI or HMI2 in Endress+Hauser documentation which is what is described hereafter.

	Base Unit		Channels		Controller		Version Compatibility		
Analyzer	**Rxn2**	**Rxn4**	**Four**	**Single**	**Embedded**	**HMI**	**Embedded**	**Original HMI**	**Current HMI**
Rxn 532	●	●	●	●	●	●	6.2+	6.2+	6.2+
Rxn Enclosure 532	—	●	●	●	●	●	6.2+	6.2+	6.2+
Rxn 785	●	●	●	●	●	●	6.0+	5.1+	6.2+
Rxn Enclosure 785	—	●	●	●	●	●	6.0+	5.1+	6.2+
Rxn Hybrid 785	●	●	—	—	●	—	6.2+	—	—
Rxn Hybrid Enclosure 785	—	●	—	—	●	—	6.2+	—	—
Rxn Hybrid Transmission 785	●	●	—	—	●	—	6.2+	—	—
Rxn Hybrid Transmission Enclosure 785	—	●	—	—	●	—	6.2+	—	—
Rxn Starter 785	●	—	●	●	●	—	6.2+	—	—
Rxn 1000	●	●	●	●	●	●	6.0+	5.1+	6.2+
Rxn Enclosure 1000	—	●	●	●	●	●	6.0+	5.1+	6.2+

	Base Unit		Channels		Controller		Version Compatibility		
Raman Rxn 1000	●	●	—	●	—	●	n/a	5.1+	6.2+
Raman Rxn Enclosure 1000	—	●	—	●	—	●	n/a	5.1+	6.2+

3.2 User roles, access permissions, and password management

To add a new user

1. From the Raman RunTime dashboard, click **Options**, then click **System**.
2. Select the **Security** tab.
   To add a new user, security must be enabled.
3. Turn on the **Security** toggle, then click **OK** in the **Enable Security** dialog box.
4. Click **+** to add a new user.
5. In the **Add User** prompts, enter the following information:
   - Enter a username. Click **Next**.
   - Create and verify the new user's password. Click **Finish**.
6. Specify the **Privilege Level** for the user. See below for privilege level definitions.
   The user's privilege level is applied.

3.2.1 User privilege levels

There are three user privilege levels: user, operator, and administrator. The user level is the most basic, followed by operator with more privileges. The administrator can perform all actions. User privileges are detailed below:

User Level	Action
User	▪ Change channel display name ▪ View summary and detail of active batch acquisitions ▪ View calibration information ▪ View diagnostics ▪ Perform exports including basic, diagnostic, and full
Operator	User level actions plus: ▪ View active batch acquisitions ▪ Perform calibration and view calibration information ▪ Perform verification and view verification results ▪ Start/stop batch acquisitions ▪ Focus ▪ Snapshot ▪ Ad hoc analysis ▪ Select from pre-loaded models and enable/disable prediction on specific channels ▪ Restart
Admin	No Restrictions. Operator level restrictions plus: ▪ Add/remove models ▪ Configure models including changing the display name, enabling or disabling components, and setting properties ▪ Configure network ▪ Change system display name ▪ Configure date and time ▪ Configure Open platform communications (OPC) ▪ Change security settings and manage users ▪ Apply embedded software updates

3.2.2 Password management and issues

Users can change their own password. To do so, click **Change Password** in the bottom left corner of the login keyboard screen. Raman RunTime system administrators can also change their passwords in the same way.

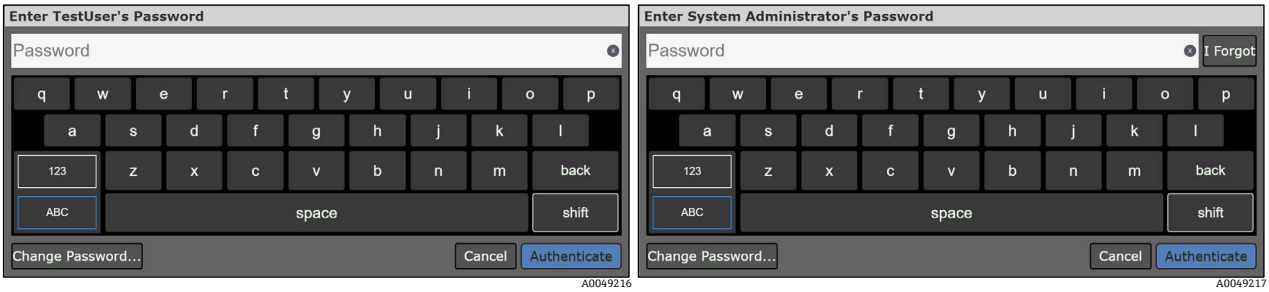


Figure 5. Enter user password dialog box (left) and enter system administrator password dialog box (right)

To recover a lost or forgotten password

To recover a lost or forgotten password for an assigned user, the user must contact their Raman RunTime system administrator to help reset their password. The system administrator can reset at password by following the procedure below.

1. From the Raman RunTime dashboard, navigate to **Options > System > Security.**
2. Log into the system administrator account on this screen.
3. Select the user requesting a password reset.
4. Select **Change Password** at the bottom of the screen.

Furthermore, if the Raman RunTime system administrator forgets their own password, they can select the **I Forgot** icon in the top right corner of their system administrator password entry screen.

After doing so, they are provided with a code and are instructed to contact Endress+Hauser Support and share this code. In response, they receive a reset code to enter at their prompted screen. They can then select **Authenticate** and proceed to set their new password on the screen that follows:

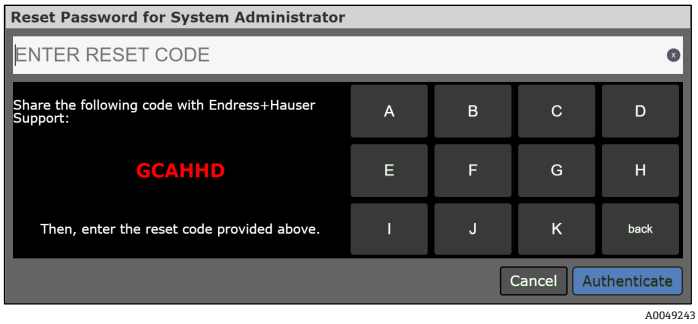


Figure 6. Password recovery screen for a Raman RunTime system administrator

4 Software operation

All Endress+Hauser Raman analyzers use Raman RunTime. Available functions within Raman RunTime may vary between products. These differences are indicated in the relevant sections of this manual.

4.1 User interface

The Raman RunTime dashboard displays four quadrants for four-channel analyzers. Each quadrant displays a probe or stream and a **Status** bar for a quick view of warnings and acquisition status. Single-channel analyzers display only 1 main channel or probe window, while analyzers with hybrid configurations display 2 channel or probe windows: 1 for the Rxn-20 probe channel, and the other for the non-Rxn-20 Alternate (ALT) probe.

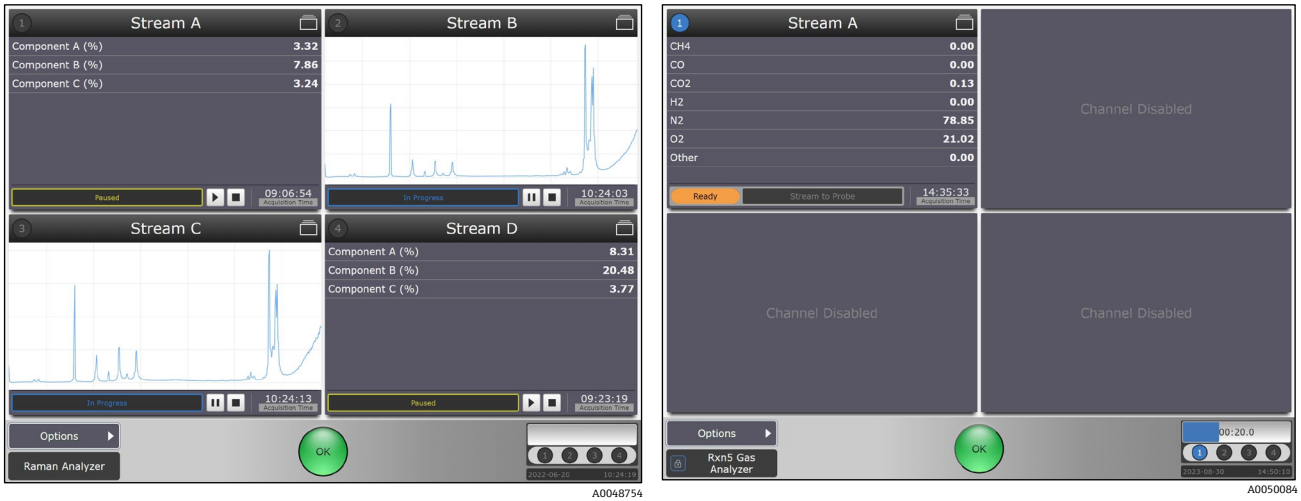


Figure 7. Raman RunTime dashboard in a Raman Rxn2 or Raman Rxn4 four-channel analyzer (left) and Raman Rxn5 analyzer (right)

Analysis details are accessed from each probe or stream window. To switch back and forth between the dashboard and batch detail views, click the **Title Bar** for each stream or probe. Views of current spectrum vs. process values (model results) can also be swapped by clicking on the **Stream** window display. System settings, calibration, and diagnostics are found on the **Options** menu.

Analyzer status indicators

The circular **Status** button located at the bottom center of the main screen has three modes: **Green**, **Yellow**, and **Red**. When the **Status** indicator is **Green** with an **OK** in the center, there are no detectable problems.

Figure 8. Green OK status indicator

When the **Status** indicator turns **Yellow** with a flashing **Warning** in the center, the analyzer is in caution status. Click the yellow **Warning** indicator for a description of the status.

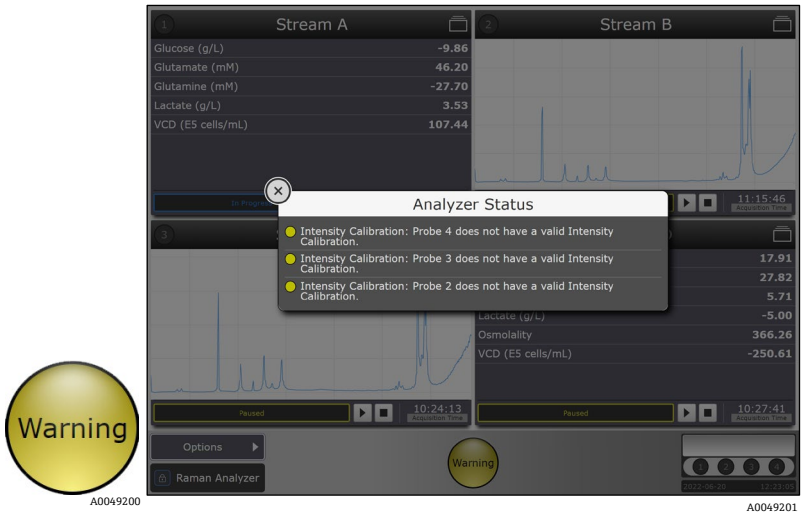


Figure 9. Explanation for yellow warning

For analyzers with unused channels/probes, the warning indicator turns **Yellow**. This indicates there are uncalibrated channels. To resolve this erroneous warning, unused channels can be disabled. To disable a channel or probe, see *Unused channels and probes* → 🗎.

When the **Status** indicator turns **Red** with an Error in the center, it signifies a more serious problem that needs immediate attention. Click the **Red** status indicator for an explanation of the error. The error message disappears automatically once the problem is resolved.

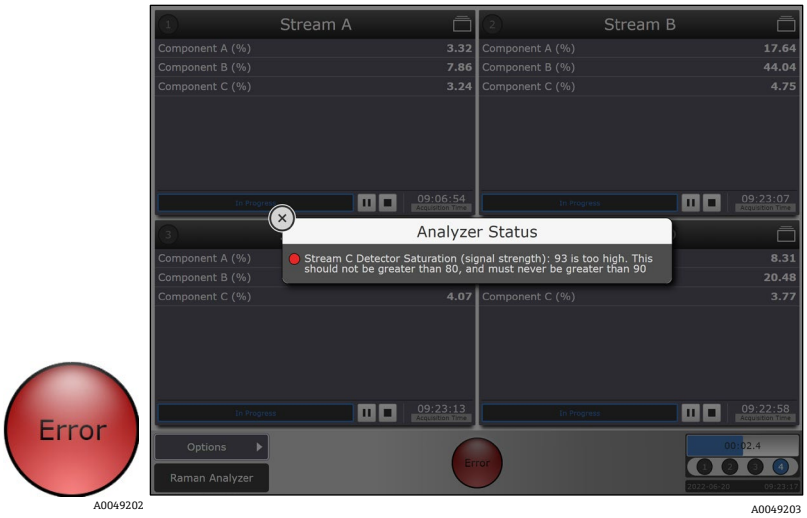


Figure 10. Explanation for red error

Raman analyzer progress bar

The Raman analyzer progress bar is shown in the lower right corner of both the main screen and the detail view. The status bar continually updates to display the time remaining in the current acquisition. The lower portion of the progress bar shows the current system date and time.

Figure 11. Progress bar

4.2 How to start

For first-time set up of RunTime, follow these steps:

1. Connect power, Ethernet, and probes
2. Calibrate the touch screen
3. Set the time and date
4. Customize network settings
5. Customize analyzer and probe names

For instructions relating to power and Ethernet cables, refer to the appropriate Raman analyzer manual. Refer to probe documentation for probe connections.

After performing initial setup of the analyzer, let the system stabilize for at least two hours before proceeding to calibration.

4.2.1 Calibrate the touch screen

To calibrate the touch screen

1. From the dashboard, click **Options** then select **System**.
2. On the **General** tab, click **Calibrate Touch Screen**.
3. Follow the on-screen prompts.

   To achieve better calibration, use the edge of your fingernail when following on screen prompts and touching the requested touch points.

4.2.2 Customize network settings

To customize the identity for communication protocols and network settings

1. From the dashboard, click **Options** then select **System**.
2. Click **Network**.

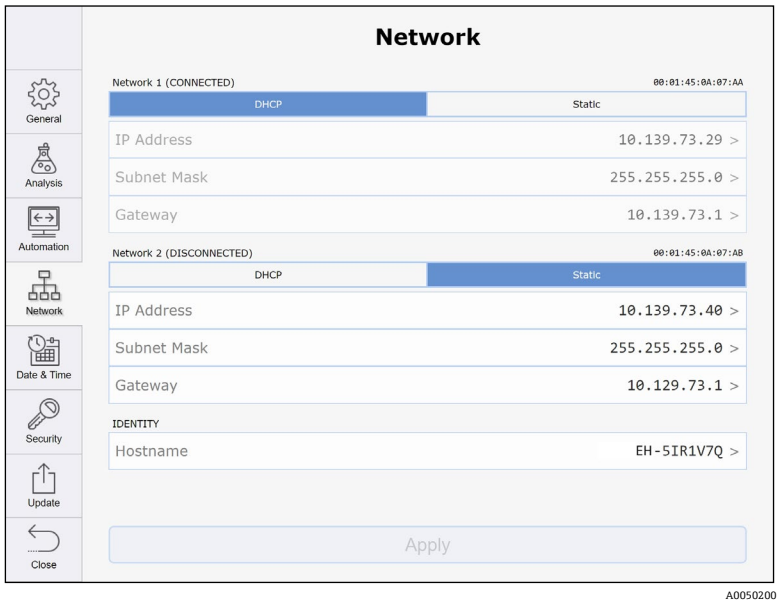


Figure 12. System settings – network tab

3. Click the **Hostname** field.
4. Enter a custom name and click **Apply**. The hostname is how the Raman Rxn system is identified through communication protocols.
5. (Optional) Enter the static IP information, as applicable, then click **Apply**. If using DHCP, the IP address is obtained automatically.

4.2.3 Set the date and time

Setting the analyzer date and time is critical step. Spectral acquisition, spectral files, and communication protocols are managed by the analyzer's date and time.

To set the date and time:

1. From the dashboard, click **Options** then select **System**.
2. Click **Date & Time**.

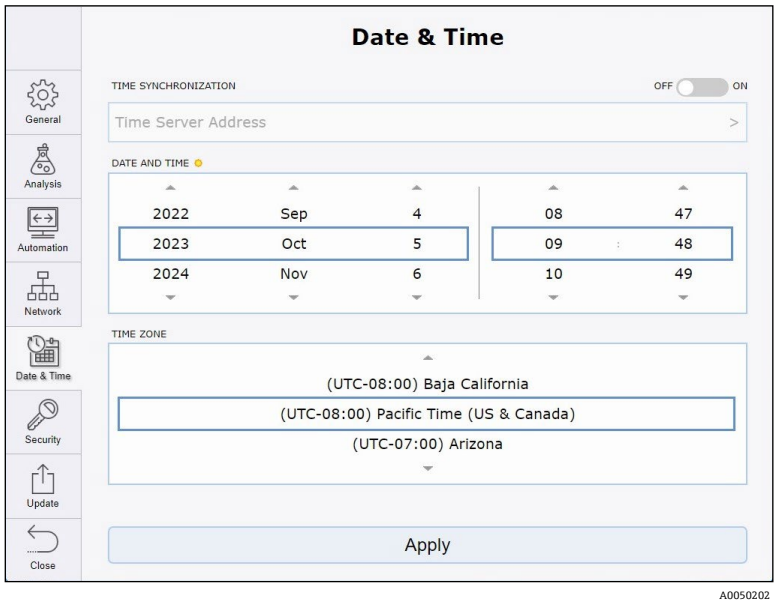


Figure 13. System settings – date & time tab

3. Choose one of the following:
   - Specify the time, date, and time zone. If setting the date and time manually, ensure the time zone is set up correctly before proceeding to other adjustments.
   - Enable **Time Synchronization**. Provide a time server address on the local network.
4. Click **Apply**.

4.2.4 Customize the analyzer name

To customize analyzer and probe names

1. From the dashboard, click **Options** then select **System**.
2. Click **General**.
3. Select the **Instrument Name** field. The default name is "Raman Analyzer".
4. Enter a custom name, for example, Raman Rxn2-785 SBAAAF12000, then click **Apply**.

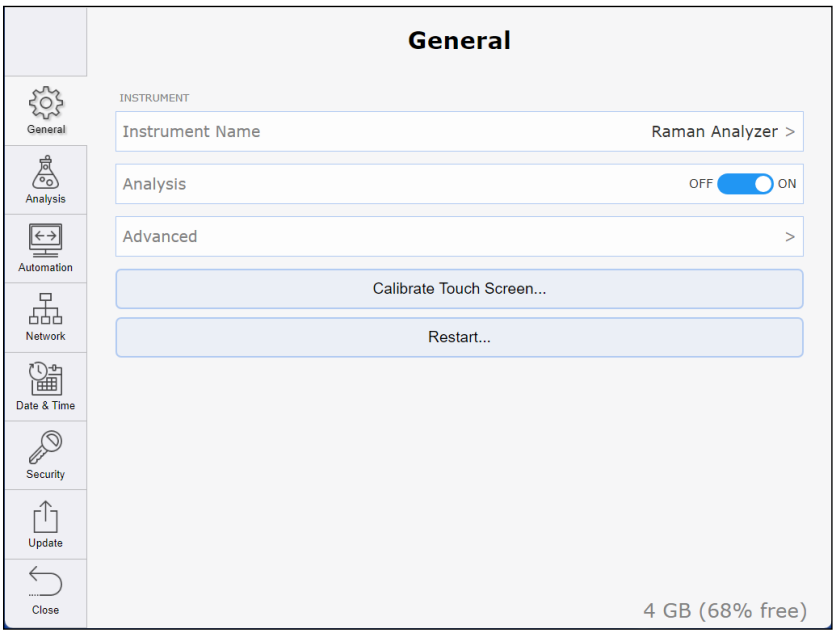


Figure 14. System settings – general page

The analyzer name is how the system is identified in diagnostic exports and within calibration reports.

4.2.5 Customize probe or stream names

To specify names for each probe or stream on the dashboard

1. From the dashboard, click the title bar of the probe you wish to name.
   The stream or probe detail view displays.

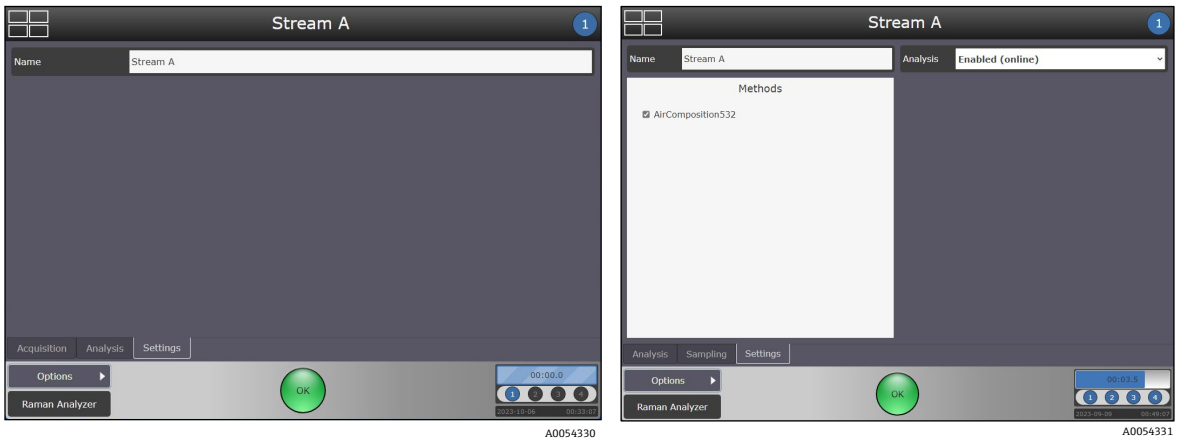


Figure 15. Stream details – settings tab (Raman Rxn2 and Raman Rxn4, left) (Raman Rxn5, right)

2. Select the **Settings Tab** and click **Name**.
3. Enter the name of the probe and click **Apply**.

After performing initial setup of the analyzer, let the system stabilize for at least two hours before proceeding to calibration.

4.2.6 Customize the X-axis (legacy spectroscopy models only)

Raman RunTime features an advanced configuration option for customizing the x-axis range and spacing of spectral data. The x-axis scaling feature accommodates customers who utilize legacy models built from spectral data acquired in HoloGRAMS version 4.2.0.12 and HoloPro version 3.3.0.14, which may be incompatible with the standard range and spacing on the X-axis of spectra in Raman RunTime.

X-axis customization applies only to the spectral data used for real-time analysis. Spectral data accumulated on the system and retrieved after collection, through using either the batch export feature or by reading batch .spc files from a network file share, always shows the standard range and spacing. New model development should always be based on standard range and spacing.

X-axis standard spacing of 1.0 cm^{-1} should not be modified unless necessary to enable execution of legacy models with strict x-axis requirements.

To customize the x-axis

1. From the dashboard, click **Options** then select **System**.
2. Click **General**, then click **Advanced**.
3. Click **X Axis**.

   The X Axis screen displays.

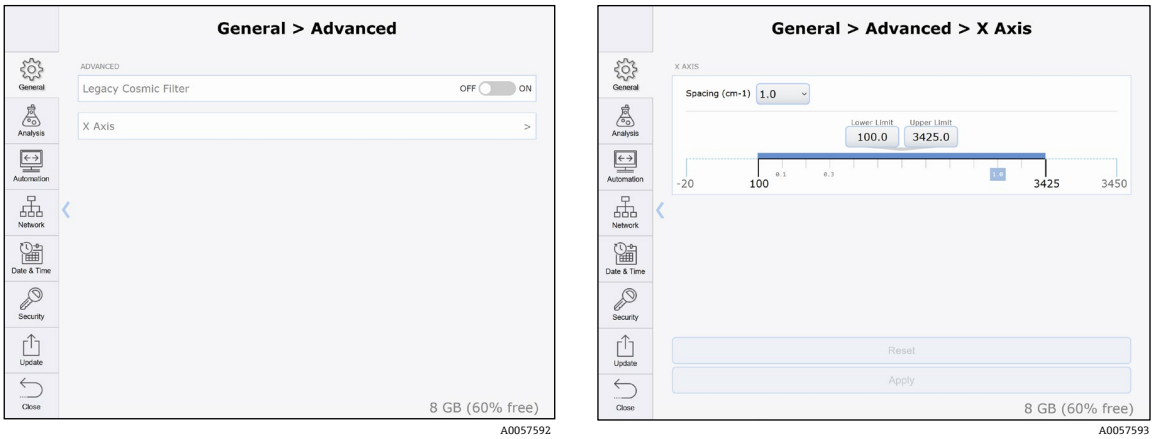


Figure 16. Advanced settings screen (left) and X Axis screen (right)

4. Click the **Spacing** list and select one of the following:
   - 0.3 cm^{-1}
   - 0.1 cm^{-1}
5. (Optional) Adjust the x-axis range by setting the lower and upper limits. These values represent Raman Shift values of the first and last points in the spectrum.
6. Click **Apply**.

X-axis settings are applied when executing any model or collecting a sample spectrum on any channel of the analyzer. The customized x-axis is also reflected in real-time spectral data published via OPC. However, the customized x-axis is not reflected in spectral data displayed in on-screen plots or accumulated on the system for later retrieval.

4.3 Calibration and verification for Raman Rxn2, Raman Rxn4, and hybrid configurations

Raman RunTime does not allow spectra to be collected without passing internal and probe calibrations. All calibrations are required before spectral acquisition. Passing the verification step is not required but is highly recommended.

Follow these instructions to perform internal calibration on your Raman Rxn2 or Raman Rxn4 analyzer for the first time. For analyzer and probe setup before calibration, refer to the manuals for your analyzer and probe(s). For probe calibration and verification, refer to the calibration kit instructions related to your kit.

Viewing the calibration and verification screen

Navigate to **Options > Calibration**. Calibration windows for the different Raman Rxn2, Raman Rxn4, and hybrid analyzer configurations are shown in Figures 17, 18, and 19. The Calibration screen displays the most recent verification.

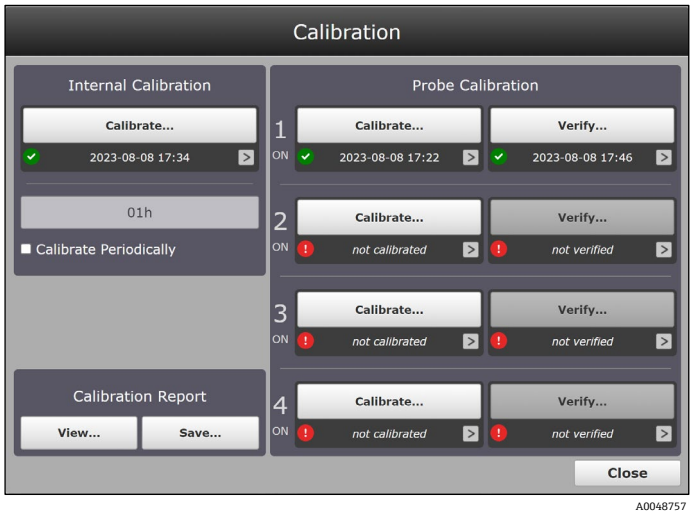


Figure 17. Calibration window for a Raman Rxn four-channel analyzer

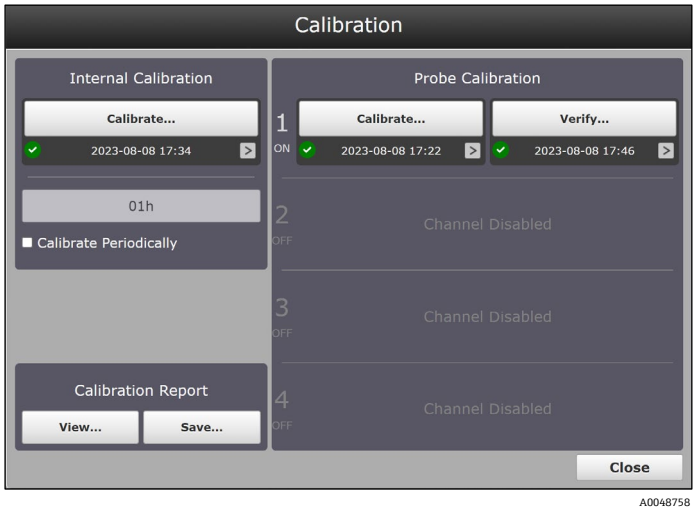


Figure 18. Calibration window for a Raman Rxn single-channel analyzer

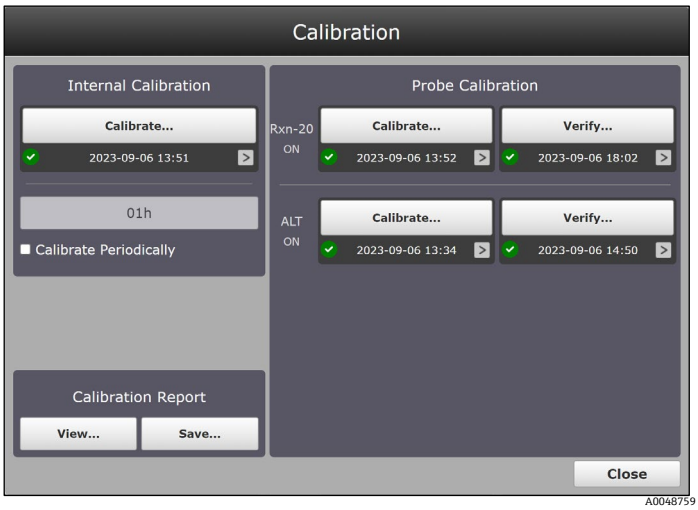


Figure 19. Calibration window for a Raman Rxn analyzer with hybrid configuration

Because not all probes use the Raman Calibration Accessory (HCA) for calibration, the Intensity Calibration window looks different for other calibration devices. Refer to the applicable probe, optic, or calibration device manual for additional information.

4.3.1 Performing Raman Rxn2 and Raman Rxn4 internal calibration

Raman Rxn2 and Raman Rxn4 analyzers have internal calibration standards for spectrograph and laser wavelength. The internal calibration options are:

- **Automatic.** If the instrument is already calibrated, this setting compares the current analyzer response to calibration specifications and applies an algorithmic correction if it is minorly out of specification. This setting also recalibrates if the spectrograph wavelength, laser wavelength, or both are out of specification. If the analyzer is uncalibrated, this performs an alignment calibration, followed by a full wavelength calibration and full laser wavelength calibration.
- **Recalibrate X Axis.** Forces full wavelength and laser calibrations without first checking whether the analyzer is within spec.
- **Recalibrate All.** This setting causes the alignment calibration to be repeated before performing full spectrograph wavelength and laser wavelength calibrations. Note that when **Recalibrate All** completes, the intensity calibrations and verifications of all probes are invalidated.

Performing internal calibration at least once per day (1d 00h) is recommended.

To perform internal calibration

1. Ensure all probes are capped.
2. Click **Calibrate** under Internal Calibration.

   The Calibrate Instrument dialog appears.

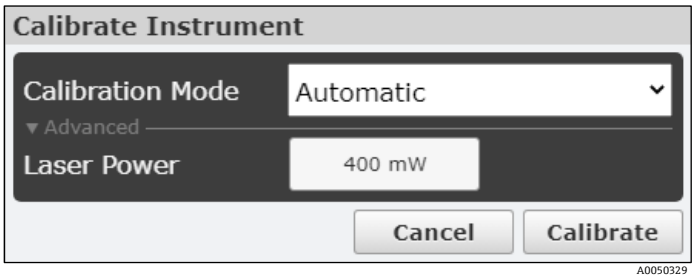


Figure 20. Internal calibration standards for spectrograph and wavelength

3. Do one of the following:
   - For initial startup, click the **Calibration Mode** list and select **Recalibrate All**. Click **Calibrate**.
     The **Recalibrate All** option is only required at initial start-up or when the analyzer is moved or serviced.
   - For subsequent calibrations, click the **Calibration Mode** list and select **Automatic**. Click **Calibrate**.
4. (Optional) Select the **Advanced** drop-down list to change the laser power setpoint. Input the desired setpoint for Laser Power and click **Calibrate**.

To set automatic daily or periodic internal calibrations

1. Ensure all probes are capped.
2. Click **Calibrate** under Internal Calibration.
3. On the Calibration screen, select **Calibrate Periodically**.
4. Click the time button above the periodic calibration setting to set the frequency. Periodic calibration is configurable in one-hour increments.

4.3.2 Probe calibration for single-channel, four-channel, and hybrid configurations

Probe calibrations for Raman Rxn2 and Raman Rxn4 analyzers can be performed using two different calibration devices:

- The Raman calibration accessory (HCA)
- A probe-specific calibration and verification kit that utilizes a Calibration Reference Standard (CRS)

Refer to the specific probe and applicable supplementary optics manual to determine the appropriate calibration device. Refer to the appropriate calibration device manual for details on how to calibrate the specific analyzer and probe combination.

When performing a probe calibration for a specific channel, the other active channels should be paused to eliminate the risk of ambient light or white light entering the probe under calibration and affecting the analysis of those channels.

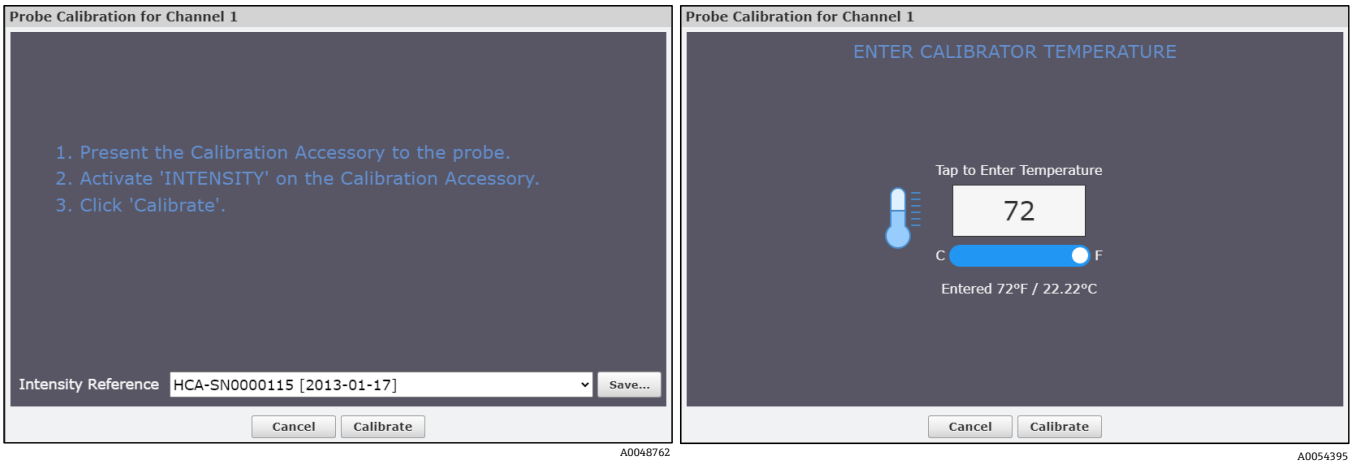


Figure 21. Probe calibration, HCA standard (left) and probe calibrator temperature (right)

4.3.3 Probe verification

For the Raman Rxn2 and Raman Rxn4 analyzers, a probe verification establishes calibration results using a standard reference sample, such as 70 % isopropanol (IPA), cyclohexane, or acetone (LNG only). This step is not required to collect a Raman spectrum, but it is highly recommended.

NOTICE

- The use of certain standard reference samples can permanently damage some Endress+Hauser Raman probes. Consult the documentation for your specific probe(s). These instructions detail the recommended standard reference materials and verification steps for that probe.

Refer to the operating instructions that come with your probe and optic devices, as well as and the instructions provided with the calibration or verification kit.

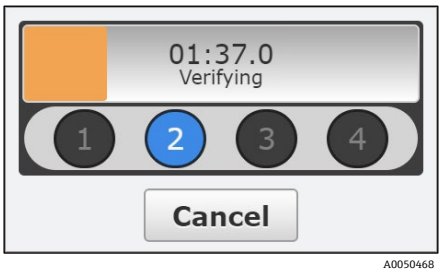
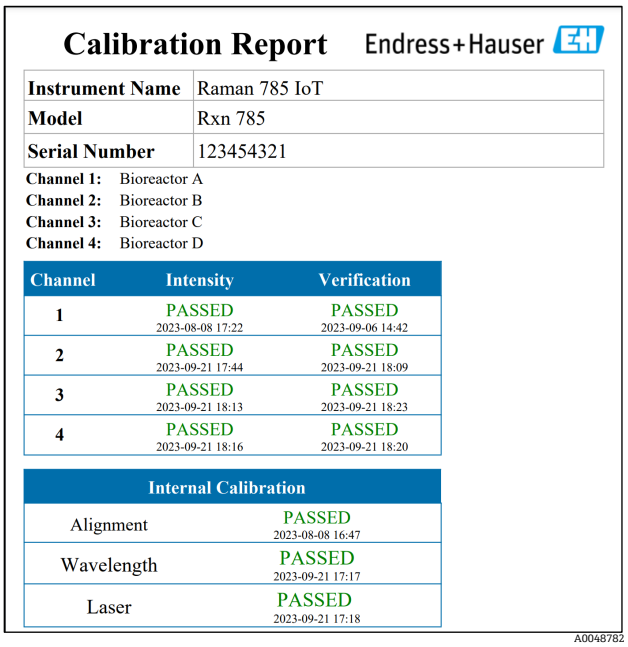


Figure 22. Verification timer

4.3.4 Calibration and verification reports

To view calibration and verification reports

1. On the lower left of the screen under **Calibration Report**, click **View** to see the calibration and verification report. A summary of the internal calibration report appears at the top of the screen.



Calibration Report Endress+Hauser

Instrument Name	Raman 785 IoT
Model	Rxn 785
Serial Number	123454321

Channel 1: Bioreactor A
Channel 2: Bioreactor B
Channel 3: Bioreactor C
Channel 4: Bioreactor D

Channel	Intensity	Verification
1	PASSED 2023-08-08 17:22	PASSED 2023-09-06 14:42
2	PASSED 2023-09-21 17:44	PASSED 2023-09-21 18:09
3	PASSED 2023-09-21 18:13	PASSED 2023-09-21 18:23
4	PASSED 2023-09-21 18:16	PASSED 2023-09-21 18:20

Internal Calibration	
Alignment	PASSED 2023-08-08 16:47
Wavelength	PASSED 2023-09-21 17:17
Laser	PASSED 2023-09-21 17:18

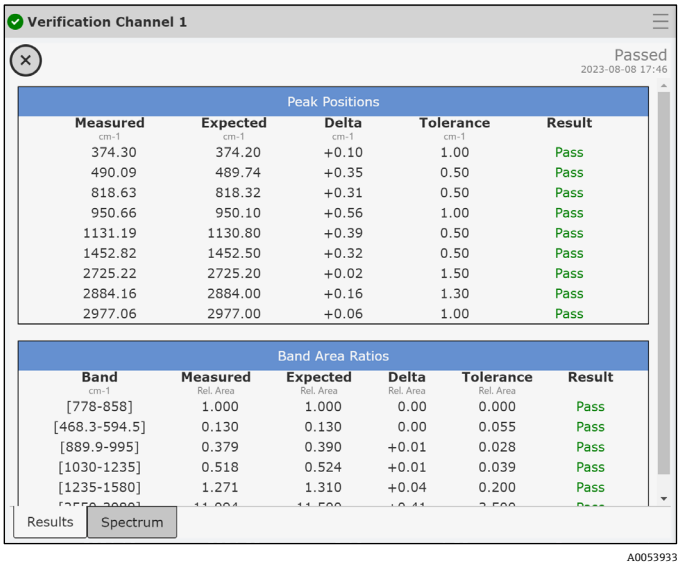
A0048782

Figure 23. Calibration and verification report

2. Scroll through the full calibration and verification report.
3. Click **Close** at the bottom of the report window to exit.
4. On the Calibration screen, click **Save** to save the full calibration and verification report as a .pdf file to a USB memory stick. The calibration report can also be accessed remotely via network Raman RunTime connection or via OPC.

To view probe verification results

1. From the Raman RunTime dashboard, select **Options**, then **Calibration**.
2. Click in the status area under the **Verify** button to display the verification report.



Verification Channel 1

Passed
2023-08-08 17:46

Peak Positions

Measured cm-1	Expected cm-1	Delta cm-1	Tolerance cm-1	Result
374.30	374.20	+0.10	1.00	Pass
490.09	489.74	+0.35	0.50	Pass
818.63	818.32	+0.31	0.50	Pass
950.66	950.10	+0.56	1.00	Pass
1131.19	1130.80	+0.39	0.50	Pass
1452.82	1452.50	+0.32	0.50	Pass
2725.22	2725.20	+0.02	1.50	Pass
2884.16	2884.00	+0.16	1.30	Pass
2977.06	2977.00	+0.06	1.00	Pass

Band Area Ratios

Band cm-1	Measured Rel. Area	Expected Rel. Area	Delta Rel. Area	Tolerance Rel. Area	Result
[778-858]	1.000	1.000	0.00	0.000	Pass
[468.3-594.5]	0.130	0.130	0.00	0.055	Pass
[889.9-995]	0.379	0.390	+0.01	0.028	Pass
[1030-1235]	0.518	0.524	+0.01	0.039	Pass
[1235-1580]	1.271	1.310	+0.04	0.200	Pass

Results Spectrum

A0053933

Figure 24. Probe verification report

3. Click the **Spectrum** tab to view the verification spectrum.

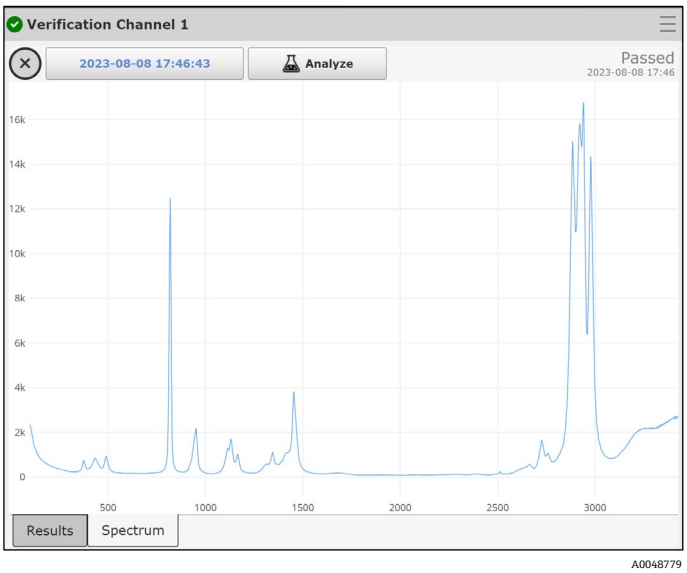


Figure 25. Probe verification spectrum viewer

4. Select the following:
   - Click the **date/timestamp** button in the upper left of the screen to add a spectrum or to export this verification spectrum. Adding a spectrum allows you to overlay, visualize, and analyze spectral changes between a few different spectra.

     The **Export** button saves the verification spectrum to an external USB memory stick that can be inserted in auxiliary USB ports on the front and rear of the device. A network connected drive can also be used for *.spc file export.
   - Click **Analyze** to view or apply a new model.

4.4 Channel verification and calibration for Raman Rxn5

The Raman Rxn5 gas analyzer automatically performs internal calibrations with each analysis without user intervention or configuration. As such, the Calibration screen only displays probe calibration functions.

The Calibration screen shows each channel with the date of the most recent calibration and verification. On this screen you can access channel calibration or verification, including the date and time of calibrations and verifications, pass or fail results, and details of each calibration.

Calibrate and Verify buttons at the top of each channel are used to run a new verification or calibration. Running a new calibration is typically recommended only when a verification fails.

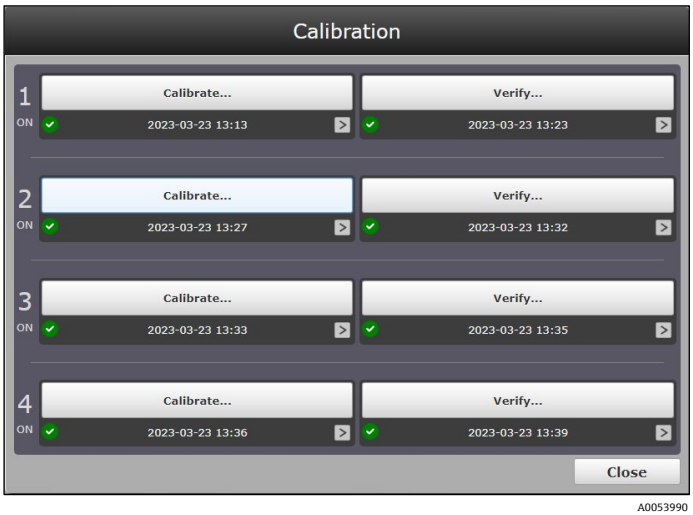


Figure 26. Calibration window for a Raman Rxn5 analyzer

Prior to verifying any channel, the analysis for all channels on the system must be disabled, as described in *Data collection for the Rxn5* → 🗎.

To perform a new calibration or verify the existing calibration for a channel, from the dashboard **select Options > Calibration**.

To view the details of a calibration or verification

1. Click the date below **Calibrate** or **Verify** to select the details you wish to view.

   The calibrations screen displays the most recent calibrations or verifications displays for each method.

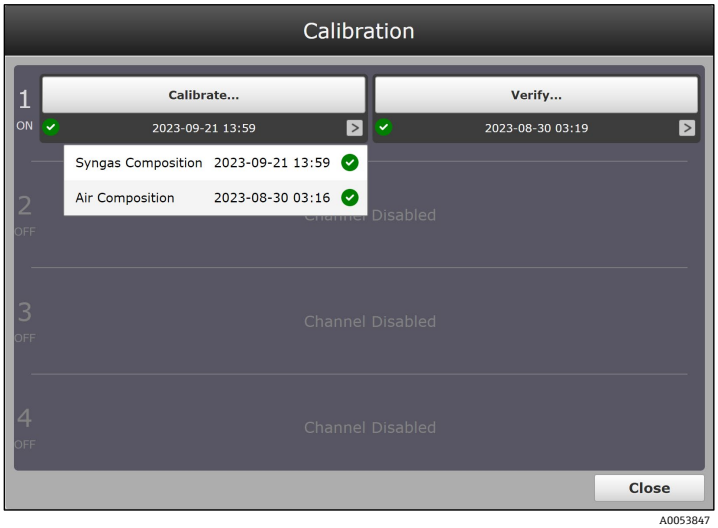


Figure 27. Calibration reports for multiple methods on a Raman Rxn5 analyzer

2. Select the desired calibration or verification.

   A detailed view of the calibration or verification spectrum displays.

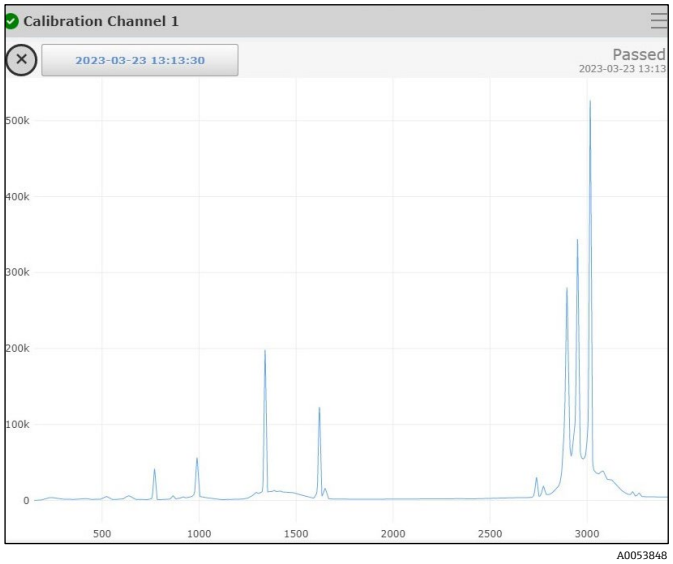


Figure 28. Calibration spectrum details

3. On the calibration or verification details screen, you can do one of the following:
   - Click the **date** button in the top left corner to export or add spectra.
   - Click the ☰ menu in the top right corner to view calibration or verification details, including method and reference.
4. Click outside of the window to return to the Calibration screen.

4.4.1 Raman Rxn5 channel verification

From the Calibration screen, you can view a channel's verification scores, verification spectrum, or associated calibration spectrum. Click **>** to view these verification details. Click outside of the window to return to the Calibration screen.

To verify a channel

1. Click **Verify** for the desired channel on the Calibration screen.

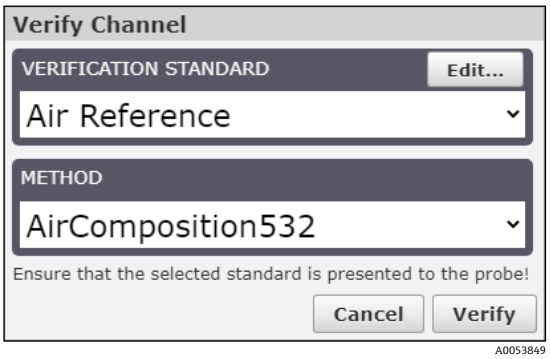


Figure 29. Verify channel selections

2. Select:
   - **Verification standard.** The verification standard is similar to a calibration reference. Verification consists of scoring the method's performance against the known composition of the reference gas.
   - **Method.** When the selected reference is a gas, a corresponding analytical method must also be specified.
3. Click **Verify**.

   The Verifying progress displays.

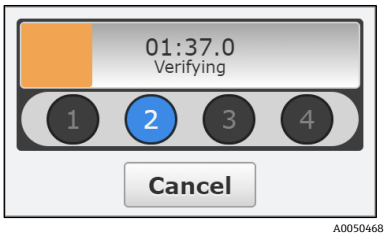


Figure 30. Verification progress

   When the verification is complete, the Calibration screen shows the results of the verification.
4. From the Calibration screen, click **Close** to return to the dashboard.

The validation is now complete, and the system returns to sampling.

4.4.2 Raman Rxn5 channel calibration

Before verifying a channel, the analysis for all channels on the system must be disabled, as described in *Data collection for the Rxn5* → 🗎.

To calibrate a channel

Before the initial calibration of a channel, a method and appropriate reference gas must be selected for that channel.

1. Click **Calibrate** for the desired channel on the Calibration screen.

   The Calibration dialog appears.

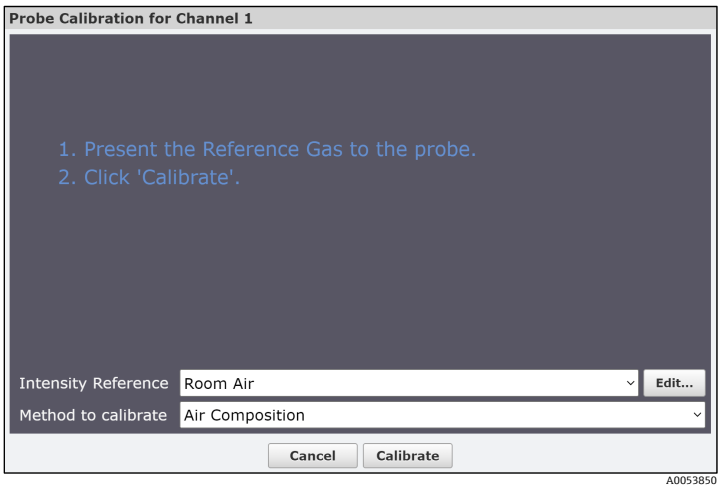


Figure 31. Calibration dialog

2. Select:
   - **Intensity reference.** For gas-phase applications, the Intensity Reference is the calibration gas for the associated method.
   - **Method to calibrate.** When a gas is selected as the intensity reference, then the secondary choice of "Method to Calibrate" specifies which analytical method the calibration applies to. When the Intensity Reference selection is instead a broadband calibrator such as the Raman calibration accessory (HCA), then there is no secondary choice of method to calibrate.

   For gas-phase analyses, if the reference gas composition does not contain the correct components for the Method, an error message occurs. Select the correct reference to remove the error message.
3. Click **Calibrate**.

   The Calibration progress displays.

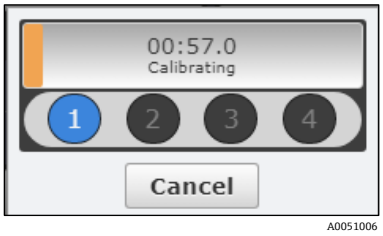


Figure 32. Calibration progress

When the calibration is complete, the Calibration screen displays the results of the calibration. The Result state of a newly calibrated channel is 'Unverified'. The new calibration needs to be verified to complete the process. Follow the steps outlined in *To verify a channel* → 🗎 to verify the channel.

4. (Optional) Click **>** on a channel to view its calibration scores, verification spectrum, or calibration spectrum. Click outside of the window to return to the Calibration screen.
5. From the Calibration screen, click the **Close** button to return to the dashboard. The calibration is now complete. The system must be re-enabled to return to its normal sampling cycle, as described in *Restarting the system* → 🗎.

4.5 Adding and replacing calibration gas

To add a new calibration gas

When a new method is added to a channel, a compatible reference gas must be created for that method.

1. Select the channel this reference gas applies to and click **Calibrate...**.
1. Click the **Intensity Reference** list and select **New Reference Gas...**.

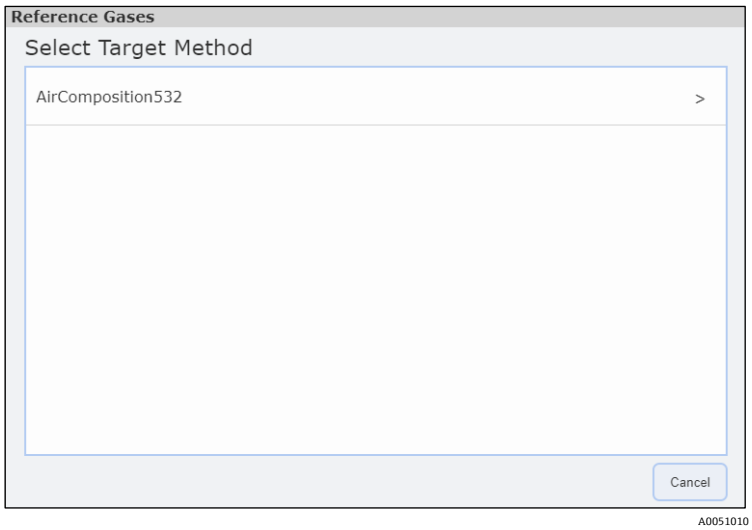


Figure 33. Select target method

2. Select the target method from the list in the Select Target Method dialog.

   This opens the Set Composition dialog and creates a component list from all the components in the selected method. By default, all composition values are 0.000 mol %.
3. Enter the following:
   - **Name** for the reference gas
   - **% Composition** for each gas in the list. Enter the composition values from the new calibration gas cylinder.

   When this process is completed, ensure the Total value at the bottom of the dialog is 100.
4. Click **Save** to update this Reference gas.

The new method appears in the Gas References dialog and in the pull-down menu for Reference in the Calibration Parameters dialog.

To replace a calibration bottle

Use the Calibration screen to update the reference or calibration gas when an existing calibration gas bottle is being replaced.

5. On the Calibration screen, click **Calibrate** on the channel for which the calibration gas bottle is being replaced.

   The probe calibration screen displays.
6. Click the **Intensity Reference** list and select the reference gas to be replaced.
7. Click **Edit**.

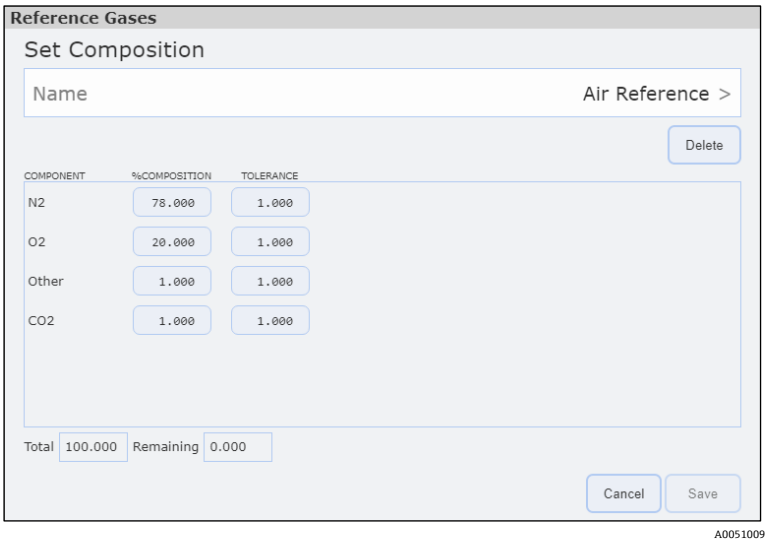


Figure 34. Set reference gas composition

8. In the Set Composition window, click the **% Composition** box for each gas in the list and enter the composition values from the new calibration gas cylinder.

   When this process is completed, ensure the Total value at the bottom of the dialog is 100.
9. Click **Save** to update this Reference gas.

5 Data collection

This chapter discusses methods for collecting and viewing data through Raman RunTime. It is divided into two sections:

- Data collection for Raman Rxn2, Raman Rxn4, and hybrid configurations
- Stream details for the Raman Rxn5

5.1 Data collection for Raman Rxn2, Raman Rxn4, and hybrid configurations

In Raman Rxn analysis, batches are collections of data over discrete periods of time with defined beginnings and ends. Batches are particularly useful in applications such as reaction monitoring. Collection modes such as continuous data, focus, snapshot, and manual are not considered part of a batch.

Active batches can be paused or stopped at any time using the corresponding buttons. When collection is paused or stopped, Raman RunTime automatically proceeds to the next probe in sequence or waits until the next periodic acquisition for another probe.

Pausing a batch can be used to not disturb the sample/spectrum while interrupting the experiment, such as exposing a reactor to room light or extracting a sample. It is recommended to pause at the start of a new sample because the current spectrum/sample terminates.

Stopping acquisition of a Raman RunTime batch means the same experiment cannot be restarted — new spectra needs to be stored under a new “batch” name and collection of spectra. If there is a chance the user might need to return to the experiment, be sure to pause rather than stop the acquisition process.

Batch names can be up to 60 characters maximum.

5.1.1 Collection modes

The collection modes available in Raman RunTime include continuous, periodic, manual, focus, and snapshot. Batch settings for collection mode and exposure settings are saved. This makes it easy to start a new batch that is like the previous one.

It is not necessary to use the same collection mode for each probe. Collection mode differences and how they affect sampling sequence are described in the following sections.

Exposure length and counts (number of co-added exposures, also referred to as accumulations) need to be specified for every collection mode except focus. Focus may be used to determine exposure length.

- **Exposure Length.** How long the laser is exposed to the sample for collection of a single spectrum.
- **Count.** The number of times the exposure repeats for a single spectrum.

The goal of determining the appropriate exposure length is to avoid overexposing the detector. Increasing the count improves the signal-to-noise ratio, but each added count doubles the total collection time. Determining the optimum number of counts is a balance between data quality and the desired total acquisition time per analysis.

- Ideal detector saturation is between 40 % and 70 %.
- Avoid detector saturation below 10 % and above 80 %.

Exposure settings can also be changed during an active experiment. It is not necessary to pause to change exposure settings. New settings take effect on the next sample acquisition.

5.1.2 Dark exposures

Dark exposures are utilized to remove non-sample data from the measurement. 532 nm and 785 nm detectors naturally have stable dark levels, so dark exposure requirements for these systems are minimal and mostly automatic. However, 1000 nm detectors have intrinsically less stable dark levels and require extra dark exposure modification.

It is best to collect a dark exposure after the system has stabilized for about 2 hours after start-up. If the analyzer has been relocated, it should stabilize for at least one day with the laser on before collecting a new dark exposure. Note that this is not applicable to moving short distances on a Raman Rxn2 cart.

To collect a dark exposure for storing and repeated use, such as for routine exposure settings, allow the analyzer and laser to remain on for 2 hours before dark exposure collection if the laser has been turned off.

Dark exposure for Raman Rxn2 532 nm and 785 nm analyzers

There is only one user initiated dark exposure setting for 532 nm and 785 nm systems, located on the Advanced button under Exposure Settings. The Status indicator specifies when a dark exposure is active and how long is remaining.

- Leave the Force New Dark check box deselected. This is the default setting for 532 nm and 785 nm systems.
- Force New Dark collects and applies a new dark every time a spectrum is collected. This is not recommended for most applications because it doubles the collection time.

Dark exposures are automatically collected at the beginning of acquisition whenever an exposure or count setting has been changed.

- If a dark exposure has already been collected and stored for the same Length and Count setting, e.g. for another probe or during a previous experiment, then the system uses the stored dark exposure.
- To expire an old dark exposure and force a new one at any length and count interval, select the Force New Dark check box for at least one interval, then turn it off.

If a dark exposure is needed when acquiring in continuous or periodic mode, one is collected at the start of the first acquisition and used for all subsequent spectra. This causes the first spectral collection interval to take double the time of subsequent intervals.

Dark handling for Raman Rxn-1000 nm single-channel and four-channel analyzers

On 1000 nm systems, dark exposures are collected automatically at the end of every acquisition. The number of dark exposures collected at the end of each acquisition is determined by the Dark Exposures setting under the Advanced button.

Dark subtraction mitigates non-sample contributions in the measurement due to “dark current”, when the Dark Exposures setting is approximately one half of the count setting.

- In processing the final spectrum, the trailing dark exposures taken after the sample is measured are combined with leading dark exposures taken before the sample is measured.
- Trailing dark exposures from one acquisition are used as the leading dark exposures for the next acquisition. This reduces the time needed to collect the requisite number of dark exposures for a given acquisition.

New leading dark exposures are collected at the beginning of every acquisition when any of the following conditions are met:

- The length setting has changed since the most recent dark collection.
- The most recent dark collection completed more than 10 minutes prior.
- The Force New Dark option is selected under the Advanced button.

Due to the conditional nature of leading dark collection, there is the potential for inconsistent acquisition times, especially on the first acquisition after starting a new experiment or rebooting the instrument, or when using periodic or manual collection. Selecting Force New Dark can be used to achieve consistent acquisition times, when doing so is more beneficial than minimizing acquisition time.

5.1.3 Focus mode

Focus mode is used to position non-contact optical probes or determine appropriate collection settings for a given sample or process. No spectra are saved from Focus mode. Focus spectra are for visual evaluation only. Please consult the manual for the probe being used to determine how to configure it before using focus mode.

During focus mode, the spectrum and current signal value are constantly updated on the screen. The update frequency is determined by the position of the blue Detail slider. This allows for dynamic feedback of signal level during the alignment process.

To use focus mode

1. Position probe to sample and click **Focus** under the probe details view.

   A suggested exposure displays. The example below shows 1.7s to 3.0s for a sample of 70 % IPA.

Figure 35. Focus mode example

#	Description
1	Current signal
2	Detail slider
3	Maximum signal
4	Suggested exposure display

2. Move the blue Detail slider to decrease or increase the focus time (as needed). Samples yielding weak signals may provide more information with slower focus settings.
3. Using feedback from the signal and max values, reposition the sample or probe to achieve the maximum signal level.
   - Signal and max values provide a comparison of the current signal level and the largest signal that has been measured during the focus process for the current probe/sample position. The current signal changes with repositioning of the probe/sample. Each time the signal exceeds the maximum value, number reflecting max value is updated.
   - When current is equal to or very close to the max value, this is the best focus of the system and the highest signal-to-noise.
4. Click **Reset** to reset the max signal.
5. Click **Stop** to exit focus mode.

5.1.4 Snapshot mode

Snapshot mode is similar to Focus in that no spectra are saved. Snapshot is intended for quick, single acquisitions to measure laser power, try out different length and count settings for a sample, or more commonly to quickly assess spectral quality either visually or by applying a model.

It is recommended to use Snapshot mode for *in situ* verification of starting materials, especially for long experiments like bioprocesses. Using this method, verification spectra can be collected quickly without needing to adjust batch exposure settings.

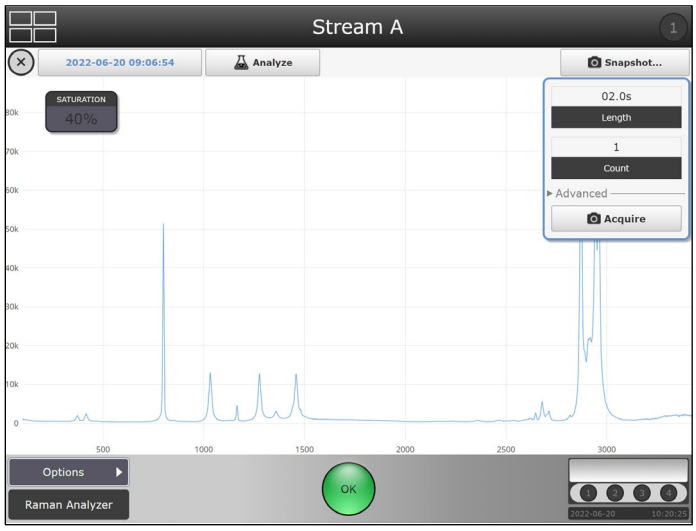
To access Snapshot mode

1. From the dashboard, click a probe title bar to select the probe detail view.

   The probe detail view with spectral plot displays.

2. Click within the spectral plot.

   The spectra overlay plot appears.



A0048788

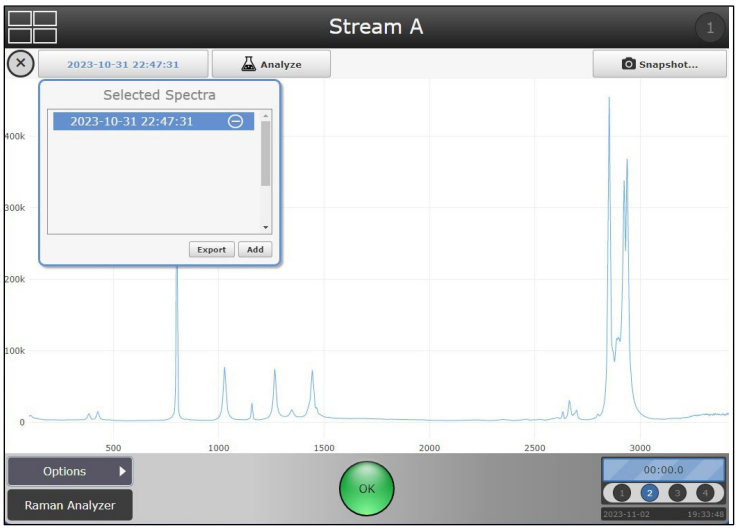
Figure 36. Snapshot mode options

3. Click **Snapshot**.
4. Select an exposure length and count, then click **Acquire**:
   - The snapshot spectrum overlays the most recent spectrum if an experiment is already in progress, such as shown below.
   - The snapshot spectrum is not stored with the current batch data; it is for on-screen tests only.

To overlay the snapshot spectrum over spectra from previous batches or experiments

1. In Snapshot mode, click the spectrum name displayed as a **Blue** date and time in the top right header.

   Clicking the spectrum name located to the left of Analyze button displays a selected spectra drop-down list.



A0054346

Figure 37. Select spectra in snapshot mode

2. Click **Add** and browse to select the reference spectra.

   The select batch dialog displays.
3. Select the batch you wish to overlay.

   The select spectrum dialog displays.

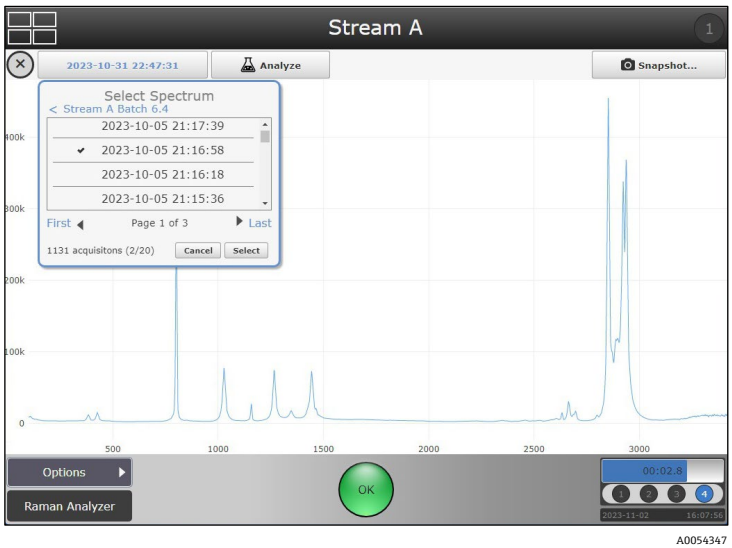


Figure 38. Select spectrum in snapshot mode

4. Select the spectrum you wish to compare. Click **Select**.

   When a new snapshot is collected, it automatically becomes active and is displayed in blue. The spectrum is principal and can be changed by selecting/highlighting it in the spectrum list.

Multiple spectra can be added to the overlay, but only a single spectrum is distinguished as the active spectrum. The active spectrum is always blue and listed by name in the header.

To apply a model in Snapshot mode

Applying a model in snapshot mode is ad hoc analysis. During ad hoc analysis, only the principal spectrum will be processed by the selected model.

1. In Snapshot mode, click **Analyze.**

   Available models are listed in a models dialog.

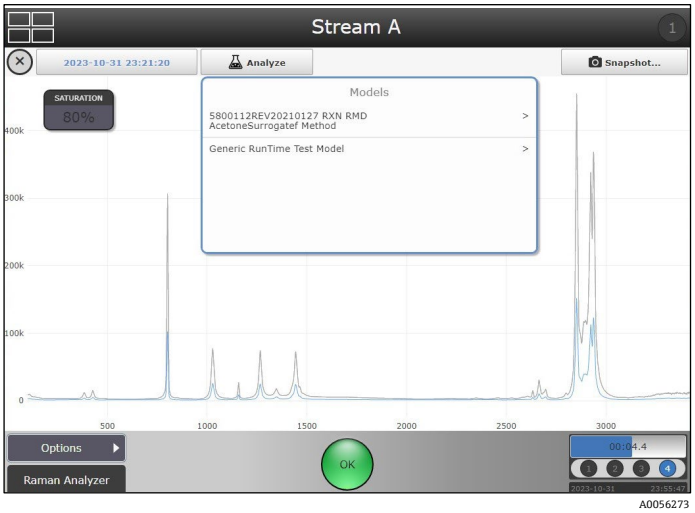


Figure 39. Analyze function in snapshot mode

2. Select a model.

   The model components are listed in the model dialog.

3. Select expand or collapse to view specific component attributes.

   To exit the spectra overlay view, click anywhere on the quadrant name or click **Exit** ⊗.

5.1.5 Manual mode

Use the Manual collection mode to acquire spectra that are triggered manually with the Acquire button. A batch/experiment name can be specified to group manual samples together for spectra storage and sample names can be specified for each spectrum.

To acquire spectra manually

1. Navigate to the probe details screen.
2. Create a new acquisition batch:
   a. Click **Edit**.
      The batch management window appears.
   b. Click **New.**
      The enter batch name dialog appears.
   c. Enter a unique batch name and click **Apply**.

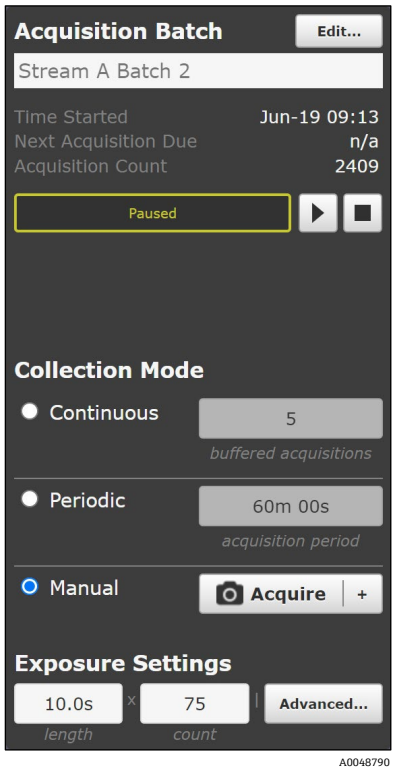


Figure 40. Manual collect mode options

3. Enter the manual collection mode settings:
   a. Under Collection mode, select **Manual**.
   b. Click **Play** A0054341 .
      The Acquisition Batch shows “In Progress” but no spectra is collected until triggered (by clicking **Acquire** in a later step below).
   c. Use the **Up** or **Down** arrows to adjust the length and count values in Exposure Settings.

Figure 41. Exposure settings as described with length (left) and count (right)

d. (Optional) If a custom sample name is desired, click **+** next to **Acquire** to enter a sample name.

Figure 42. Keyboard that pops up to rename the sample

e. Click **Acquire** to collect a spectrum.

4. Click **Stop** A0054048 to end the sequence of manual samples stored together.

To collect another spectrum, specify a new sample name (if desired), change Exposure Settings as needed, then click **Acquire** again.

5.1.6 Continuous mode

Continuous collection mode cycles through each active probe as quickly as possible. It is recommended for method development when collecting frequent reference samples, and for monitoring and control when models are active.

To set up a continuous collection

1. Create a batch under **Edit > New** and specify a new batch name.
2. Set the collection mode to **Continuous**.
3. Enter the exposure and buffer settings. For information on buffered acquisitions, see *buffered acquisition* → 🗎, below.

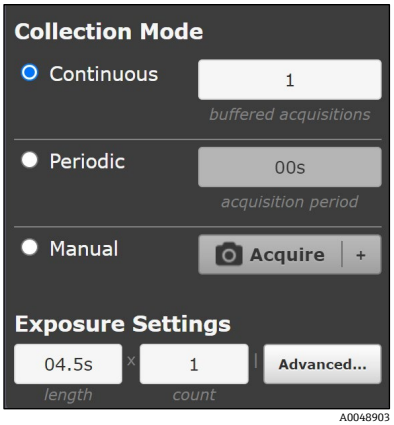


Figure 43. Collection mode details for continuous mode

4. Repeat for all active probes and click **Play** in the desired probe sequence.

Pausing, stopping, adding new batches, and rebooting could affect the probe sampling sequence in continuous mode. If cycle order matters, periodic mode is recommended.

Buffered acquisition

Buffered acquisition provides a way to receive updated spectra and model values more frequently, without sacrificing accuracy or repeatability. The buffered acquisitions setting specifies the number of consecutive acquisition cycles to combine in each reported spectrum by adding together the individual acquisition spectra. During buffered acquisition, the spectrum and model values are updated at the end of each acquisition cycle.

When buffered acquisition is selected, only the combined spectrum is reported. Individual acquisition spectra are not reported. As a result, active models operate on the combined spectrum, not on the individual acquisitions. For

applications requiring long collection intervals, buffered acquisition is not recommended when more than one probe is active.

As collection alternates among multiple probes, combining consecutive acquisitions on a given probe runs the risk of including outdated process spectra if other active probes have long intervals.

To configure buffered acquisition that achieves the same total target collection time as non-buffered acquisition, reduce the count setting and increase the buffered acquisitions setting, keeping their product the same. For example:

- If exposure settings of 10s x 60 with 1 buffered acquisition are used, spectra and process values update only at the end of the full spectrum collection cycle, approximately every 10 minutes.
- If settings of 10s x 6 with 10 buffered acquisitions are used, then spectra and process values update approximately every 1 minute.
- Each reported spectrum includes 10 minutes of total acquisition time, because each update adds together the ten most recent acquisitions of 10s x 6.

Setting buffered acquisitions to the default value of 1 disables the feature, resulting in conventional acquisition in which each spectrum is independent of previous spectra.

5.1.7 Periodic mode

Periodic collection mode acquires spectra at specified intervals and is typically used during method development to allow spectra to sync with samples being drawn from reactors or other timed process events. Buffered acquisitions are not an option in periodic mode.

To set up a periodic batch

1. Create a batch under **Edit > New** and specify a new name.
2. Set the collection mode to **Periodic**.

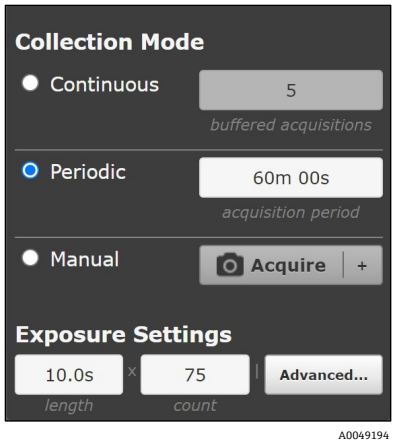


Figure 44. Periodic mode batch details

- In the example shown here, periodic acquisition is scheduled for 60 min.
- The batch details show when the next acquisition is due and how many counts of spectra have been collected for the current batch.
- If spectral acquisition is active in periodic mode, the Next Acquisition Due reads “now.”

3. Set the exposure settings and acquisition period.
4. Repeat for all active probes and click **Play** in the desired probe cycle order, for example, 1, 2, 3, 4 or 1, 3, 2, 4.

5.2 Stream details for the Raman Rxn5

The RunTime dashboard for Rxn5 displays the most recent results for each of the four streams. Each stream's data is displayed in a separate quadrant.

The quadrant display for a given stream shows the percent of each component in that stream as determined from the last analysis of that stream, as well as optional derived values such as Gross Heating Value and Wobbe Index. The time stamp of the last sample is also displayed. The Options menu provides access to system settings, diagnostics, and calibration.

Finally, a large indicator in the lower left corner of each quadrant displays the current sampling status of that stream. The indicator displays Ready with an orange background when a stream is ready to collect data, Disabled when a stream has been disabled, and Prepare when the Raman Rxn5 analyzer is preparing a sample for acquisition.

Figure 45. Raman Rxn5 dashboard

#	Description
1	Details icon
2	Sampling status indicator
3	Status button
4	Progress bar

5.2.1 Data collection

For the Raman Rxn5, global data collection settings are found on the system settings screen. Detailed settings can also be set based on the channel.

The Analysis setting allows an advanced user to enable or disable analysis for all channels of the instrument.

To turn analysis on or off

1. From the dashboard, click **Options** then click **System** to view the System Settings screen.

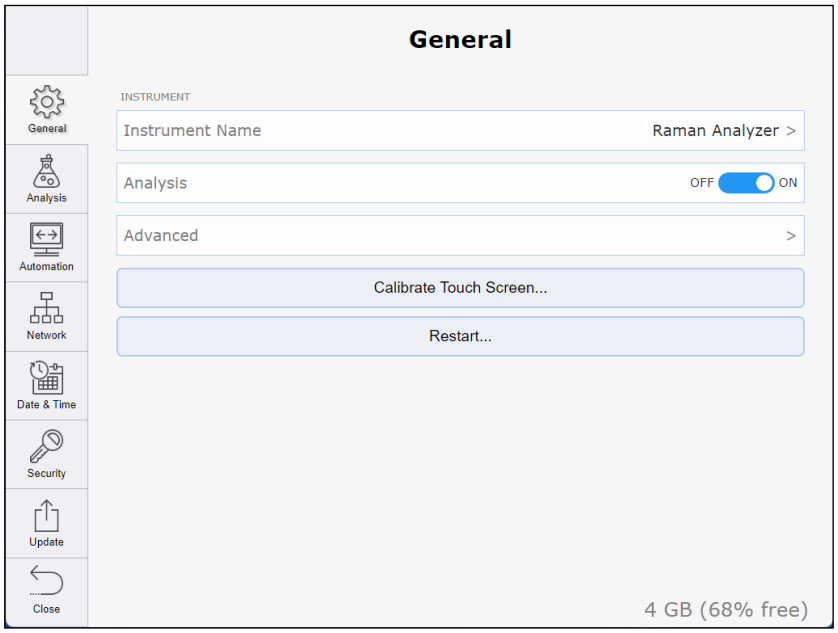


Figure 46. System settings – general page

2. Click the **Off — On** toggle to enable or disable analysis for all channels of the instrument.

5.2.2 Stream detail view

The Stream detail view displays additional information for a particular stream. Each section of the stream detail view is discussed below. The stream detail view has three tabs: Analysis, Sampling, and Settings, which are described in the following sections.

To access the stream detail view, click the **Details** icon from the dashboard. To return to the dashboard, click the **Quadrants** icon in the upper left corner of the Stream Detail View.

5.2.3 Analysis tab

The Analysis tab shows the analysis from the last acquisition and the spectrum from that acquisition. Average temperature and pressure from the most recent acquisition are displayed and update along at the end of the acquisition cycle, with the other data. Detector saturation is also shown. Detector saturation increases as sample pressure increases in gas phase. Detector saturation is used to optimize the performance of the analyzer.

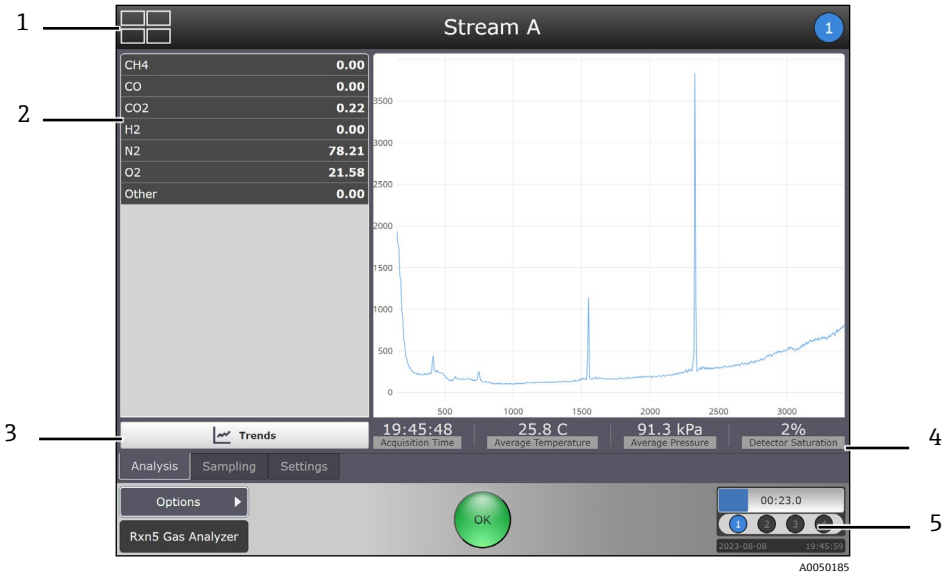


Figure 47. Stream detail – analysis tab

#	Description
1	Quadrants icon
2	Components measurement
3	Trends
4	Average probe temperature, pressure, and detector saturation
5	Progress bar

5.2.4 Trends

The Trends window displays a trend chart of the stream components for a selected time period.

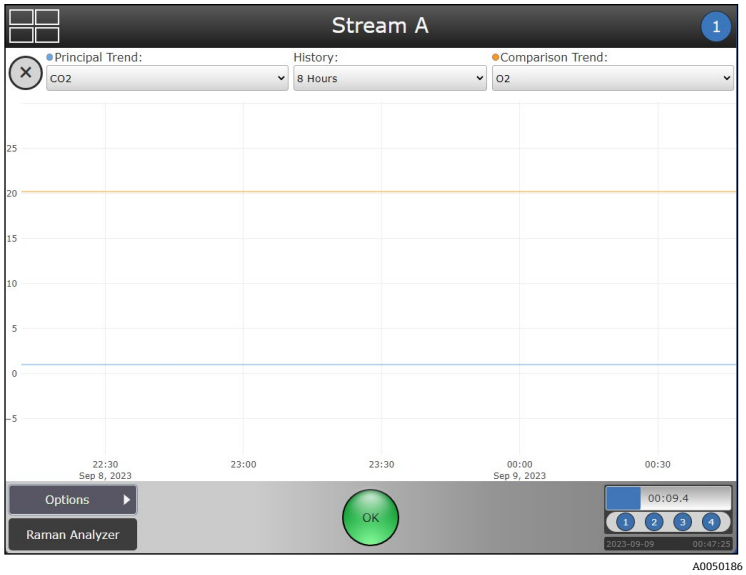


Figure 48. Stream detail – trends tab

Select a principal trend, a time frame, and a comparison trend on this screen:

- **Principal trend.** Select the component you want to view as a principal measurement trend.
- **History.** Select the time period to display on the graph, from 8 hours up to 10 days.
- **(Optional) Comparison trend.** Select the comparison trend you want to view. This option can only be selected if a Principal trend has been selected.

5.2.5 Sampling tab

The sampling tab enables operators to coordinate the Raman Rxn5 analyzer with the sampling system. You can define individual sampling states and set up analysis sampling sequences using those states. Each stream is configured independently.

Creating sampling states

Users with operator permissions can create, modify, and delete Sampling States as well as Sampling Output signals within the states. Sampling States are mutually exclusive. The Sampling States sub-tab is shown below.

Each Sampling State consists of one or more Sampling Output signals. Each Sampling Output signal consists of a Signal to Send, which is True or False, and the Time to Wait, which is the pause in seconds or minutes before sending the next signal, for up to four digital outputs.

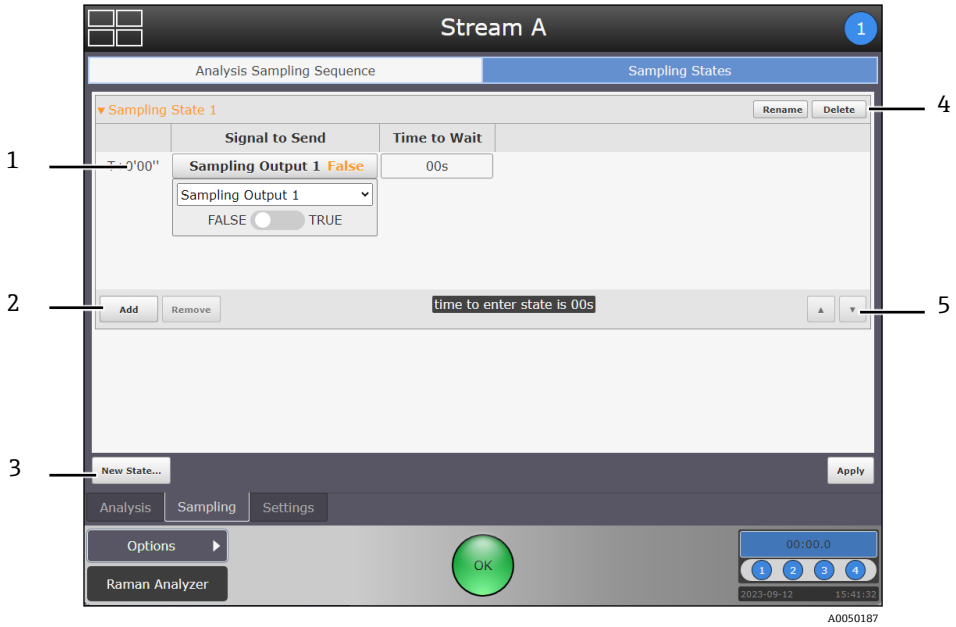


Figure 49. Sampling states tab showing states sub-tab

#	Description
1	Sampling outputs
2	Add or remove sampling output
3	New state button
4	Rename or delete sampling state
5	Arrows to move sampling outputs up or down

To create a new sampling state

1. Navigate to the **Sampling States** tab from the **Stream Details** screen.
2. Click the **New State** button.
3. Using the on-screen keyboard, enter a meaningful name for the new state, for example, “Stream to Bypass”.
4. Click **Apply**.

To rename or delete a state, select it by tapping its row and then clicking the **Rename** button or the **Delete** button.

To create a new sampling output signal for a particular state

1. On the Sampling States screen, select the sampling state you want to modify.
2. Click **Add**.
3. Select the following for each sampling output signal:

- Select either **True** or **False**.
- Select a **Time to Wait**.

4. Click **Apply**.

To remove a sampling output signal

1. Select the signal you want to remove.
2. Click the **Remove** button.

   A confirmation dialog appears.
3. Click **OK**.

5.2.6 Managing sampling sequences

The Analysis Sampling Sequence tab enables operators to configure the sampling sequences, including determining the order of the sampling states and the amount of time for the sampling system to remain in a given state.

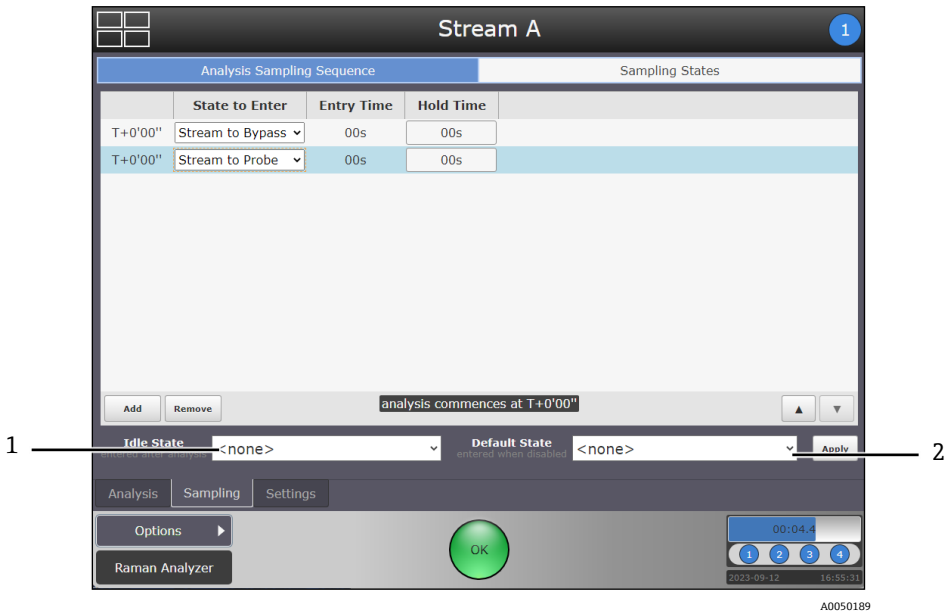


Figure 50. Analysis sampling sequence tab

#	Name	Description
1	Idle state	The state between one cycle and the next during live analysis. For the Rxn5 analyzer analysis is continuous, and you do not need to change the Idle State setting from its default state of <none>. If you do need to set the Idle State, click the drop-down list to select the desired state. States are created on the Sampling States tab.
2	Default state	The state a stream goes into when it is disabled. Click the drop-down list to select the Default State. Consult best practice guidelines to select the Default State, for example, to best conserve the product when the stream is disabled.

5.2.7 Settings

The Settings Tab is shows settings for analysis states and parameters for a stream.

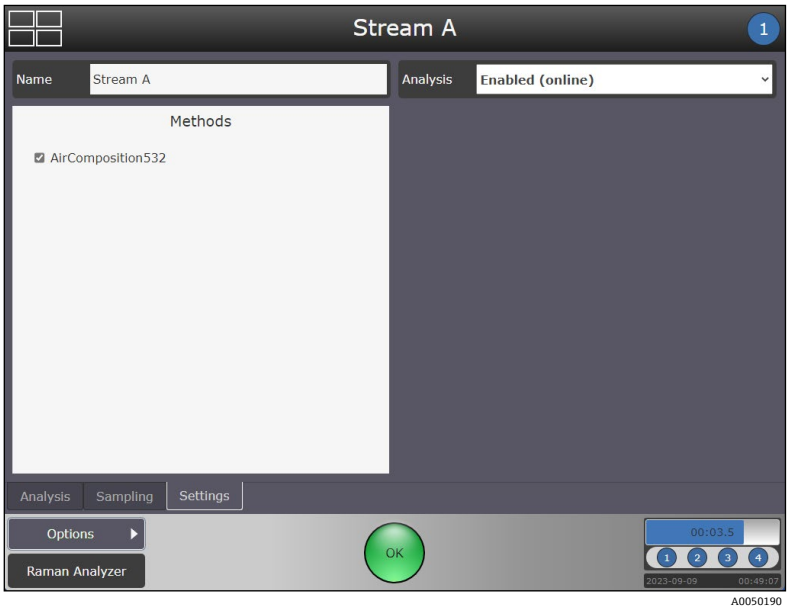


Figure 51. Stream detail settings tab

Methods

All methods available for this stream are displayed on the left half of the Stream Detail screen. Selecting the check box next to a method enables that method to process collected data and present results.

Analysis

The Analysis list allows the advanced user to set the analysis state of each stream. Options include:

- **Disabled**. Stops analysis from occurring for that stream.
- **Enabled (online)**. Starts analysis for the stream. The enabled option means results are available to an external DCS if it has been configured.
- **Enabled (offline)**. Starts analysis for the stream. Enabled offline does not send results to an external DCS. The enabled offline feature is used while servicing an instrument.

6 Models and Methods

This chapter provides instructions on loading and managing analytical models and methods in Raman RunTime. Raman Rxn2, Raman Rxn4, and hybrid configuration systems enable the use of models outlined in the section below. Raman Rxn5 analyzers use methods created in the Endress+Hauser Raman Method Designer (RMD).

6.1 Model and process value names

Model titles and y-variable names, called process values in Raman RunTime, should be changed in the final models to reflect the desired display names and OPC tags. For OPC communication, it is important use a consistent naming scheme because each time a model title or assay name is changed, the OPC tags change accordingly (and need to be reconfigured for OPC communication).

Use the following recommendations for process values:

- Include units, for example g/L or mM. Model outputs within Raman RunTime do not automatically display units.
- Avoid using periods and commas in model titles and assay names.
- Special characters such as “&” and “%” work with some OPC configurations but should always be tested and removed from model or process value names as needed.
- There can be multiple models for each process value type. This allows for easy prediction comparisons during model development/validation phases, and the use of multiple process value models per batch, for example Gluc M1, Gluc M2 or VCD Day 1-6, VCD Day 7-14.

Raman data library can be used to ensure consistent process value naming. For more information, refer to *Data Fields* in *Raman data library User Operating Instructions* (BA02367C).

6.2 Models for Raman Rxn2, Raman Rxn4, and hybrid configurations

Raman RunTime supports executing models generated in Raman data library, SIMCA® (Sartorius), GRAMS IQ™ (Thermo Fisher Scientific), PEAXACT (S-Pact), Aspen Unscrambler™ (AspenTech), and Solo/PLS_Toolbox (Eigenvector). These multivariate models are typically based on in-line Raman spectra correlated to off-line analytical measurements and can be used to turn raw spectra into meaningful process values in real time. Model results can be viewed on-screen as well as communicated via OPC and Modbus.

Raman RunTime supports the following model file versions:

- Raman data library 2.0
- SIMCA® versions 13 through 18
- GRAMS IQ™ versions 9.3 and previous
- PEAXACT version 4, 5, 5.4, 5.6, 5.7, and 5.9
- Aspen Unscrambler™ version 11
- Solo/PLS_Toolbox version 8.9, 9.0, and 9.3

6.2.1 Loading models into Raman RunTime

To load and select a new analysis model

1. Save the desired project files from the modeling package to a USB memory stick and connect it to the USB port on the front of the Raman analyzer. Alternatively, models can be loaded from a network connected folder.
2. From the dashboard, select **Options > System > Analysis > Add Model** and browse to the appropriate model file. Repeat for additional files.

   The file names appear in the Analysis window.

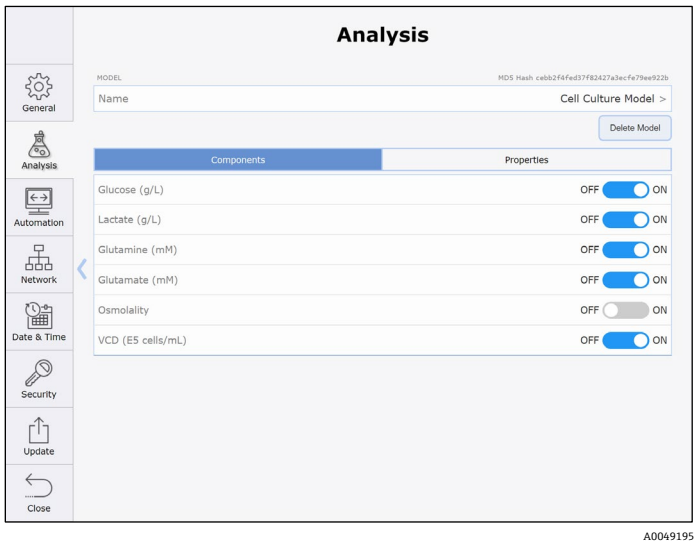


Figure 52. Analysis screen to select model(s)

3. Select a file name to turn model components and properties on/off. Repeat for additional files.
4. Return to the dashboard and navigate to the Details screen for one probe.
5. Select the **Analysis** tab and enable the model files on or off. Repeat for additional probes.

6.3 Defining parameters

When the model or method utilized in Raman RunTime has support for parameters, they can be managed and defined in the **Parameters** tab on the **Analysis** screen. Available parameters are specific to each model or method and are determined by the model or method developer.

Many parameters have default values. For parameters without default values, a valid value should be entered. Parameters without default values can be identified by the presence of a **Trash** icon next to them.

For example, the sample temperature is normally provided using an external temperature sensor and is stored with the acquisition. If no value is provided for the Manual Sample Temperature parameter, the system uses the temperature stored with the acquisition to produce temperature-corrected results. When a valid value is entered into the Manual Sample Temperature parameter, it overrides the value stored with the acquisition. To return to using external sample temperature, delete the Manual Sample Temperature parameter.

When a value has been entered into any parameter that has no default value, the value can be changed but it cannot be cleared. To revert to the system setting, the defined parameter must be deleted by clicking the **Trash** icon for this parameter.

6.3.1 Default parameters

Parameters shown with a default value cannot be deleted. Default Raman RunTime parameters are set at the factory and can be changed as needed. The **Reset** icon to the right of the field restores the default value. If these parameters are not changed from their defaults, the method works but the results may not be as intended.

RunTime can be configured to ignore any value by using the Parameters list under Analysis settings.

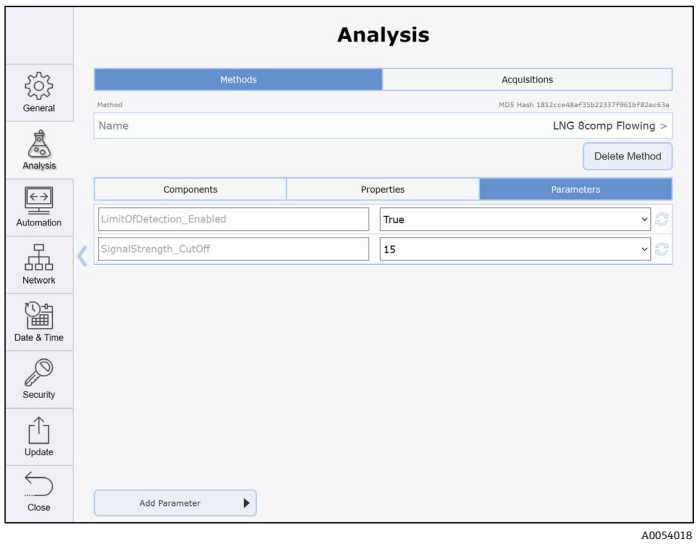


Figure 53. Default parameters

Limited parameters

A drop-down list of the possible values is displayed when the parameter has a fixed number of valid entries.

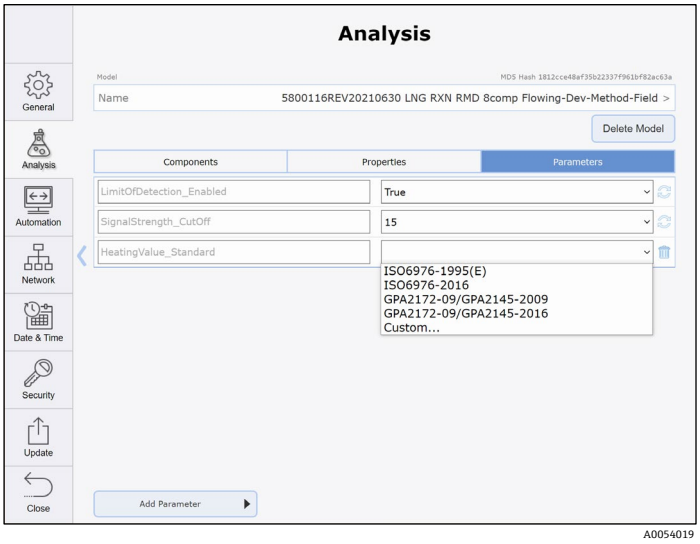


Figure 54. Limited parameters

Default parameters for LNG applications (Raman Rxn4 analyzer)

The following parameters are applicable to Raman Rxn4-based LNG applications only. For a list of parameters that apply to your application, review the parameters listed in your method or model.

Limit of Detection (LOD) enable

Key Name LimitOfDetection_Enabled

Description Set this value to True to force the reported component values to report as zero when a component is below its detection limit.

Possible Values
- True
- False

Default True

Recommended True

Signal strength cutoff

Key Name SignalStrength_Cutoff

Description Signal strength is just a scaled sum of Raman peak areas. It is meant to distinguish between a full pipe and an empty pipe. Therefore, the signal strength cutoff must be set between full and empty pipe. If signal strength drops below the cutoff, all outputs are reported as zero. Note that signal strength is not a measure of instrument performance. The signal strength of a full pipe varies by installation and sample composition. An empty pipe typically has a signal strength of 0-3 and full pipe has a signal strength that is variable, with typical values ranging from 30 to 150.

Possible Values Numeric, typically in the range of 5-25

Default 15

Recommended About 2/3 between empty and full pipe

Other concentration

Key Name OtherConcentration

Description Mass balance by normalization is a standard part of the quantitative method. Using mass balance forces the sum of the concentrations of all measured components to add to 100 percent, with the assumption that there are no unmeasured components. Invisible components represent atoms or molecules which do not generate a Raman signal or cannot be measured under the analysis conditions. If the concentration of these 'invisible' components is known, the sum of their concentrations can be input as the 'Other' concentration. The mass balance step is then calculated based on the value of 100 minus the other concentration and can result is an improvement in the accuracy of the method results. This feature is rarely used for LNG measurements.

Default None, interpreted as zero

Manual sample temperature

Key Name TemperatureCompensation_SampleTemperatureC

Description During normal operation, the sample temperature (for temperature compensation) is read from the acquisition data. The temperature value from the acquisition can come from MODBUS, OPC, or a direct sensor reading. However, if a manual sample temperature is provided, it overrides the sample temperature provided from the acquisition. Deleting the manual temperature by using the Trash icon next to the key value reverts to using the temperature in the acquisition data.

Default None (this allows key deletion). Values entered should be in units of ˚C

Recommended -20 ˚C to +50 ˚C

Heating value standard

Key Name HeatingValue_Standard

Description The heating value standard is a published document containing both data and instructions for how to calculate various heating values and related quantities. Calculations are based on the composition and base temperature. Some quantities also require metering temperature and pressure. Each standard expects specific values for the temperatures and pressures caution should be used when selecting the desired standard. See instructions for those particular parameters.

Possible Values
- GPA2172-09/GPA2145-2009
- GPA2172-09/GPA2145-2016
- ISO6976-1995E
- ISO6976-2016

Default None

Recommended ISO6976-2016

Heating value units

Key Name HeatingValue_Units

Description Heating value units vary according to standard, but translation abilities are provided by the predictor. However, it is important to note that the different standards produce slightly different results so a translation from the native units of one standard to the native units of another standard may not exactly agree with using the standard directly. The numerator and denominator are examined independently to determine if translation should occur.

Allowed Values
- MJ/cubic meter
- kJ/cubic meter
- Btu/cubic foot

Default None

Heating value base temperature

Key Name HeatingValue_BaseTemperature

Description Each standard has several tables of combustion data which were collected using different base temperatures for the calorimeter. Choosing the base temperature determines which table of data is used. The ISO standard uses several base temperatures, while GPA standard uses only one.

Allowed Values

GPA
- 60 °F

ISO
- 0 °C
- 15 °C
- 20 °C
- 25 °C
- 288.15 K (same as 15 °C)
- 15.55 °C

Default None

Heating value metering temperature

Key Name HeatingValue_MeteringTemperature

Description This parameter is used to calculate compressibility, which is used to convert from ideal gas law conditions to real, or extended, gas law conditions. Only certain values are allowed for each standard.

Allowed Values

GPA
- 60 °F

ISO
- 0 °C
- 15 °C
- 20 °C
- 25 °C

Default None

Heating value metering pressure

Key Name HeatingValue_MeteringPressure

Description This parameter is used in a similar fashion to the metering temperature. It is used to convert from ideal to real heating value. Only certain values are allowed for each standard.

Allowed Values

GPA
- 14.65 psi
- 14.696 psi
- 14.73 psi

ISO
- 101.325 kPa

Default None

Heating value output values

Key Name HeatingValue_OutputValues

Description The heating value output values are a list of calculated values made available to RunTime by the method developer. For LNG the complete list is available, but for surrogates only the Wobbe Index is made visible because the others are not needed. Not all of the exposed values need to be used or displayed.

Allowed Values Ideal Wobbe Index, unless utilized for LNG

6.3.2 Adding parameters

To add a new parameter to the list of default parameters

1. Click **Add Parameter**.
   The parameter name is case sensitive.

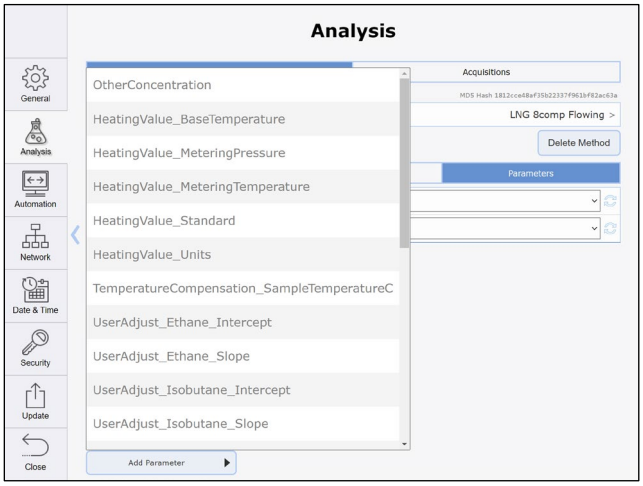


Figure 55. Adding a parameter

2. Choose a valid parameter from the list.

When the parameter is not needed, it should be deleted using the **Trash** icon.

6.3.3 Modifying parameter outputs

Use the **Components** tab on the **Analysis** screen to enable or disable parameter outputs. This function allows you to select which outputs you want to see.

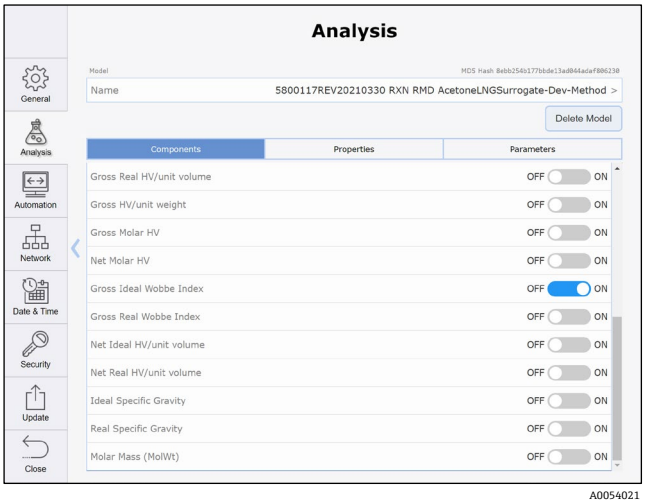


Figure 56. Enabling and disabling a parameter

6.4 Methods and acquisition for Raman Rxn5

The Methods tab on the System Settings Analysis screen enables the user to manage the methods installed on the analyzer and adjust acquisition parameters. The Acquisitions tab on the System Settings Analysis screen allows you to adjust the time to sample, calibrate, and verify a sample stream.

6.4.1 Loading and selecting methods

Under the Methods tab, selecting one of the listed methods displays the method components. On this page, the method name can be changed, the method can be deleted from the system, and reporting of individual components can be turned off.

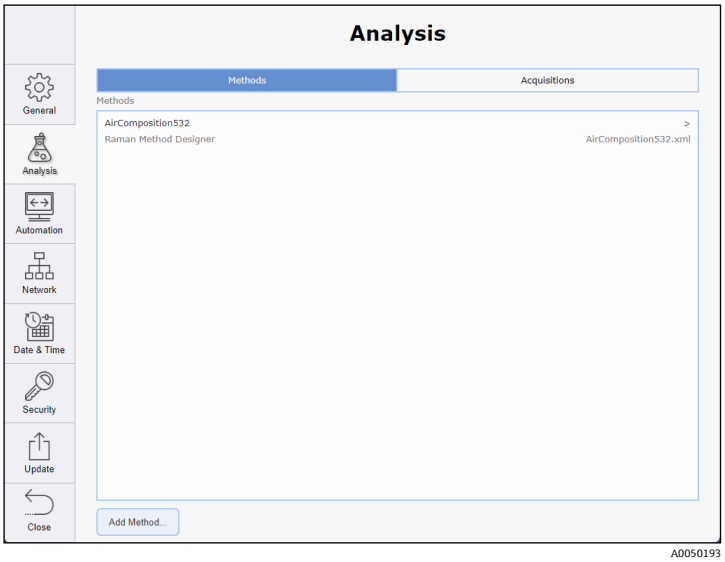


Figure 57. System analysis – method page

To load and select a new analysis method

1. Save the desired project files from the method package to a USB memory stick and connect it to the USB port on the front of the Raman analyzer. Methods can also be loaded through remote access from a network connected folder. See *Remote access* → 📖.

2. Select **Options > System > Analysis > Add Method** and browse to the appropriate method file. Repeat for additional files.

   The file names display in the Analysis window.

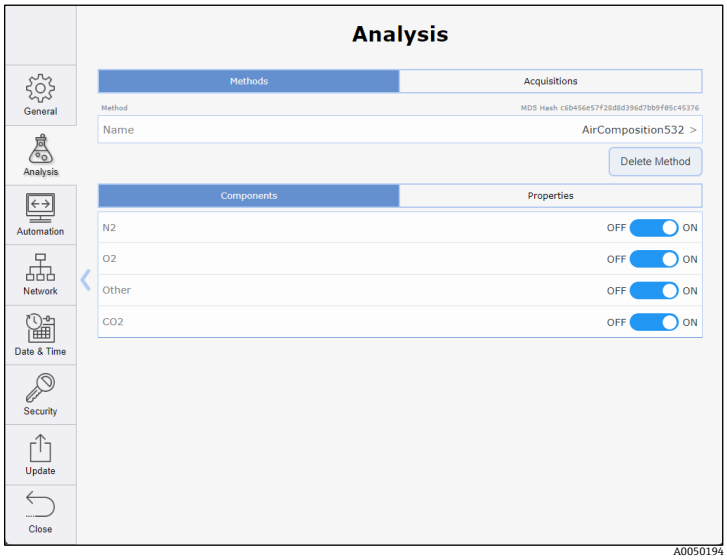


Figure 58. Analysis screen to select methods

3. Select a file name to turn method components and properties on/off. Repeat for additional files.
4. Clock **Close** to return to the dashboard. Select the Details for one stream.
5. Click **Settings** and enable the method files on or off. Repeat for additional streams.

6.4.2 Managing acquisition time

Under the Acquisitions tab, the total acquisition time for sampling, calibration, and verification can be adjusted. Automated exposure control in the system software ensures that the hardware settings are adjusted as necessary.

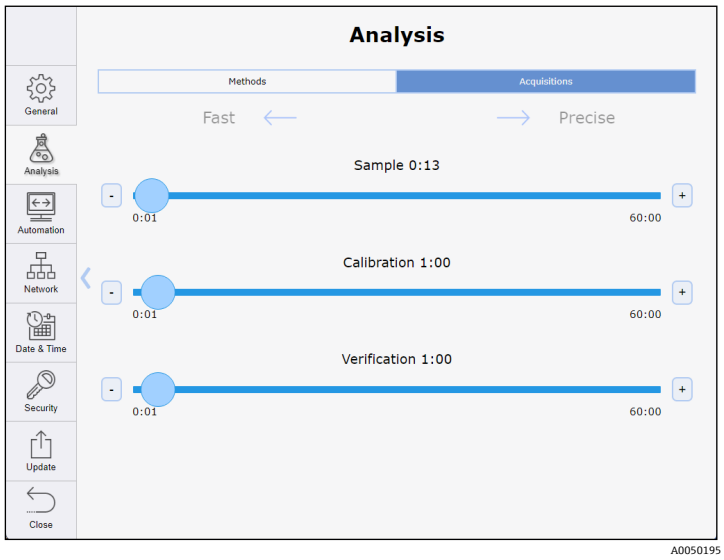


Figure 59. System analysis – acquisitions page

6.5 Viewing model and method results

During active experiments, process values are automatically displayed on the dashboard instead of the current spectra.

On the dashboard, click the quadrant display to toggle between viewing the most recent spectrum or the process values.

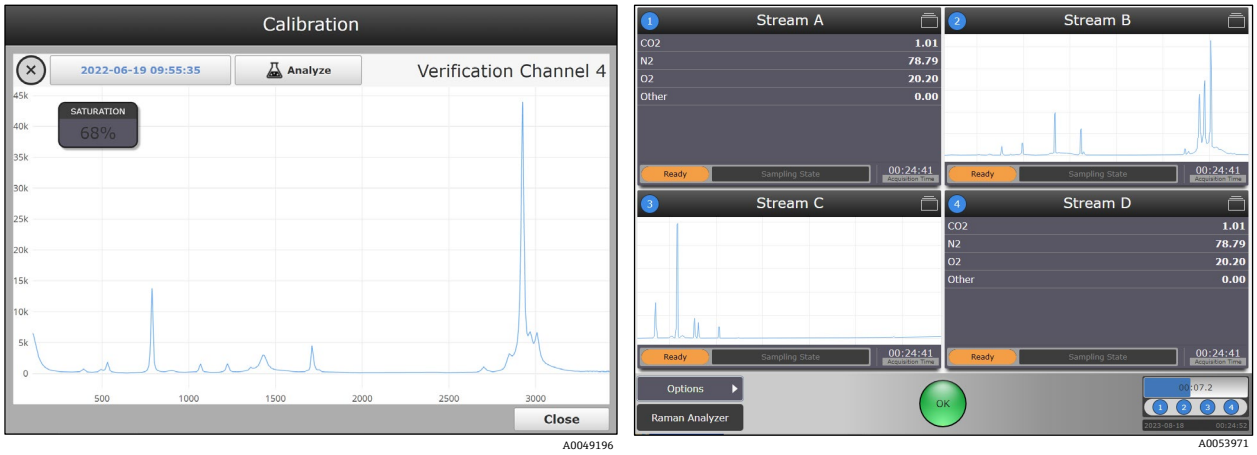


Figure 60. View of spectrum for Raman Rxn2, Raman Rxn4 probe 1 (left) and Raman Rxn5 stream (right)

- For hybrid analyzer configurations, the current spectrum and process values are both automatically displayed, there is no need to click the window to change views.
- For single-channel analyzers, there is no quadrant view. Process values display under the Analysis tab.
- Model and method results update each time a new spectrum is complete, or after each buffer cycle in continuous mode.
- If models are not active for a probe/batch, then “No Analysis” appears when the spectral plot is clicked.

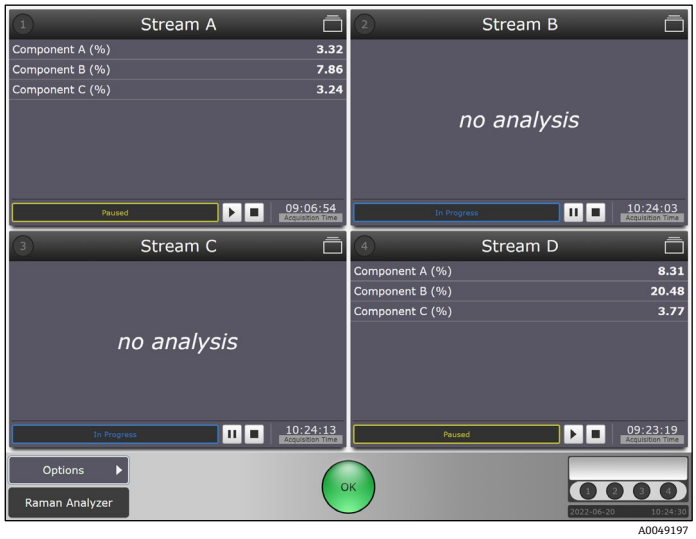


Figure 61. Results for a Raman Rxn2 four-channel analyzer with models active for probe 1 and probe 4

To access additional model result information

The following instructions are also the only way to view model results for single-channel analyzers.

1. From a probe details view, click the **Analysis** tab.
2. Click **Expand** and **Collapse** to show or hide model details.

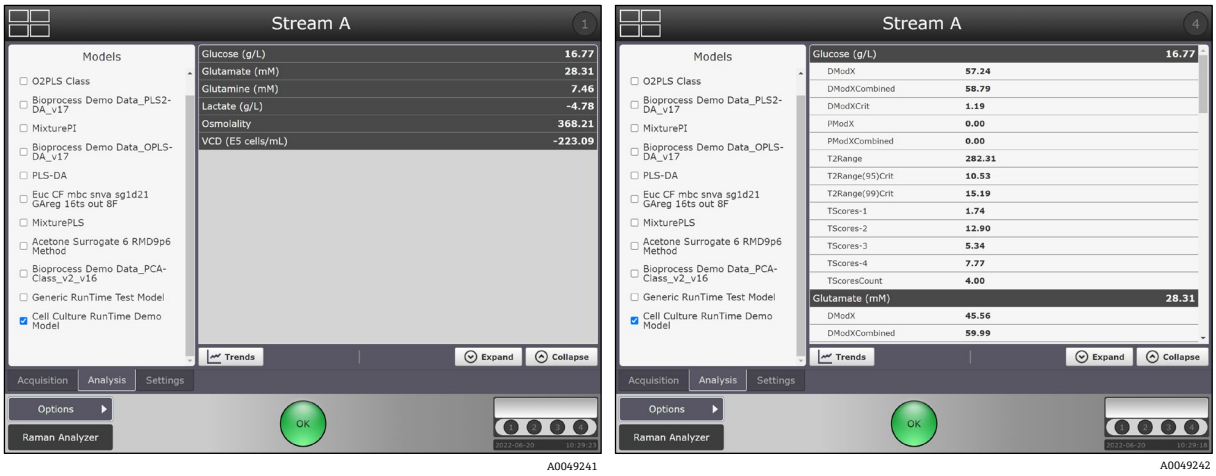


Figure 62. Probe details view of model process values and properties

3. Click **Trends** to enter the trend viewer.
4. Select a Principal Trend and, if desired, a Comparison Trend.

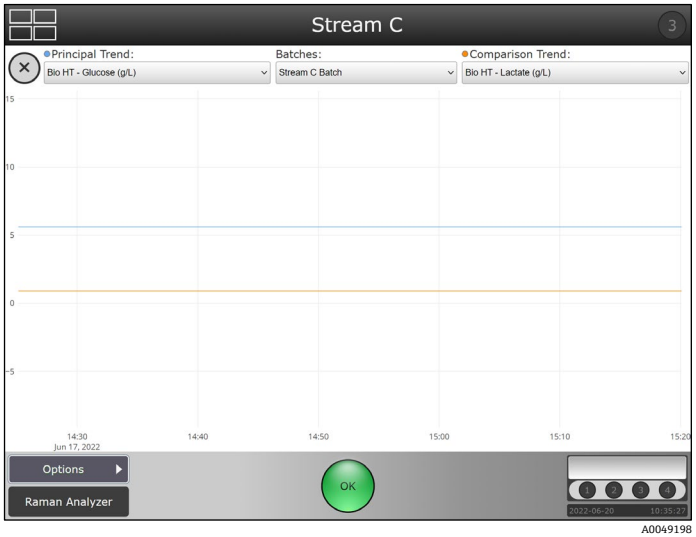


Figure 63. Model results in the trend view

6.6 Saving model results

Stored model results are included when exporting spectral batch data as a *.csv file. Real-time prediction results are also available via OPC or Modbus if client connections are established.

7 System integration

This chapter provides essential information for integrating Raman RunTime. This includes network configuration as well as automations for OPC and Modbus connections.

7.1 Network configuration

7.1.1 Network configuration for Raman Rxn2 and Raman Rxn4

The table below summarizes the ports relevant to specific features. Ports for OPC Classic are assigned dynamically in the indicated range; fixed-port behavior is only available for OPC UA.

It is only necessary to open firewall ports for the features intended for use.

Protocol	Ports
OPC UA	TCP 4840, 4843, 52601, and **62886**
OPC Classic	TCP **135** and **49152-65535**
Modbus	TCP **502**
File Sharing	TCP **139** and **445**
Remote Access	TCP **3594** and **4526** for Secure connection; TCP **3593**, **4525**, and 5674 for Standard connection; UDP 3702

Ports in bold should be regarded as mandatory for the associated protocol; other ports are recommended for full functionality (e.g. discovery services).

7.1.2 Network configuration for Raman Rxn5

The Network tab in System Settings configures communication options between the analyzer and a host network. Both dynamic host configuration protocol (DHCP) and static options ae provided.

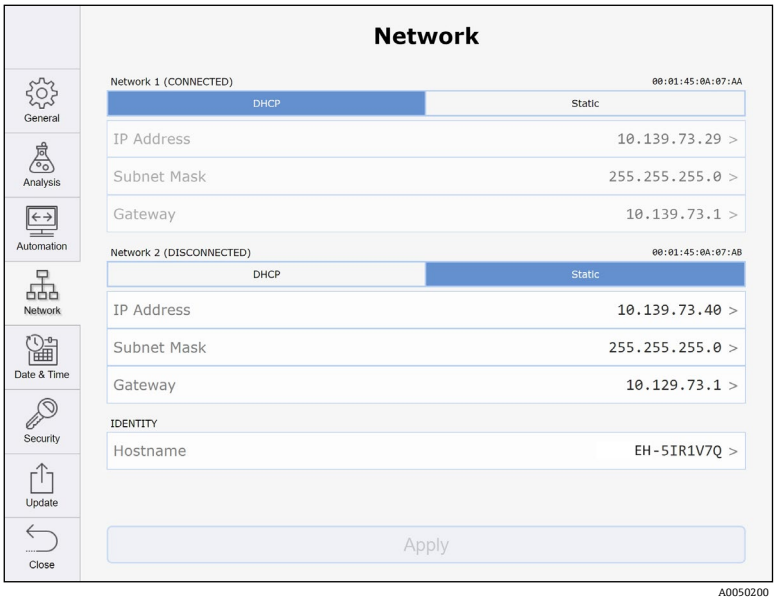


Figure 64. System settings – network tab – DHCP

7.2 Automation connection for Raman Rxn2, Raman Rxn4, and hybrid configurations

Raman RunTime provides network-connected clients with analyzer data as well as analyzer control functions. OPC UA is the recommended protocol because it allows transfer of large data comprised of full spectral data and diagnostics and is a more reliable connection than OPC Classic. However, legacy support for OPC Classic (DCOM, also called OPC DA) clients is included.

The Raman Rxn system must be connected to a network for OPC functionality. Network settings can be viewed and configured in **Options > System > Network**.

7.2.1 Basic OPC connectivity

The Raman RunTime OPC server can connect to Raman data library through an OPC unified automation (UA) client connection. The OPC connection allows users to view, control, and collect spectra from Endress+Hauser Raman Rxn analyzer systems within Raman data library.

A minimum of Raman RunTime v6.4 is required for an OPC connection between Raman RunTime and Raman data library. Raman Rxn analyzers running Raman RunTime versions lower than v6.4 can use an SPC spectral source as described below.

To access the OPC server, all clients must authenticate with the username and password of an authorized user.

To update OPC server settings

1. From the RunTime dashboard, navigate to **Options**, then click **System**.
2. Select the **Automation** tab.
   - The built-in user with the name 'kaiser-opc' is always authorized for OPC access. The password for 'kaiser-opc' is 'opc' by default; this password can be changed under **Options > System > Automation**.
   - The OPC server can be accessed with user credentials created and managed under **Options > System > Security**.
3. Set the **OPC UA (recommended).** OPC UA clients access the OPC server using UA's binary protocol to connect to opc.tcp://<computer-name>, providing the name and password of an authorized user. The "computer name" can be viewed or changed under **Options > System > Network**.

   The Basic128Rsa15, Basic256, and Basic256Sha256 algorithm suites are supported for signing and optionally encrypting OPC communications.

UA Certificates

The first time that a given UA client connects to a Raman RunTime system, it is necessary for that client to accept or "trust" the certificate that the OPC server provides to identify itself. The mechanisms for accepting the server's certificate vary by client.

The OPC server provides a self-signed certificate; accordingly, it is common for the client to display a warning that the server's identity cannot be verified. Such a warning is normal, and the server's certificate must be accepted to enable the client to connect.

The OPC server's certificate is tied to the hostname of the Raman RunTime system. Any time the hostname is changed, a new certificate is generated automatically, and UA clients need to accept the new certificate before they can connect again.

OPC Classic (deprecated)

Full OPC functionality is available to OPC Classic clients. However, OPC Classic entails additional set-up requirements, and many opportunities exist for client-side configuration to interfere with successful communication, often in ways that are challenging to diagnose. Also, the underlying technology of OPC Classic can limit installation flexibility. For these reasons, it is recommended to use OPC UA instead of OPC Classic whenever possible.

The OPC Classic client program must be executed using credentials that exactly match (name and password) an authorized user on the Raman RunTime system. This implies that a Windows user account must be created on the client workstation with a name matching that of a Raman RunTime user, and that their passwords must be kept in sync.

Asynchronous updates for OPC classic

In addition to responding to polling requests from clients, the OPC server can provide asynchronous updates in which the server notifies clients of changes in the values of subscribed tags without the need for clients to continually poll the server.

When using OPC classic, clients may fail to connect unless asynchronous updates are enabled. To enable asynchronous updates, the 'kaiser-opc' user must exist on the client workstation with a password that matches the Raman RunTime system, regardless of whether the client program accesses the server using the 'kaiser-opc' user credentials.

Client workstations must reside in the same TCP/IP subnet as the analyzer, with no intervening network address translation (NAT).

If the 'kaiser-opc' password is changed under **Options > System > Automation**, the Raman RunTime system must be restarted under **Options > System > General** for the new password to take effect.

OPC tags

See *Raman RunTime Automation OPC v6.6 (p/n 4005856)* to view the current list and history of OPC Tags for Raman RunTime.

7.2.2 Modbus map

The Raman Rxn2, Raman Rxn4, and Rxn5 analyzers provide automation data via Modbus TCP (Ethernet) or Modbus RTU (RS-485 serial). If models are running on the instrument, the prediction values available over Modbus may be configured at **Options > System > Automation > Modbus**. In addition to prediction values, other instrument diagnostic values are available over Modbus.

See *Raman RunTime Automation Modbus v6.6 (p/n 4005855)* to view the current Modbus Map for Raman RunTime.

7.2.3 HTTPS automation

See *HTTPS Automation Interface v6.6 (p/n 4005857*) to view details on using HTTPS protocol to transfer supported file types to Raman RunTime.

7.3 Automation connections for Raman Rxn5

The Automation tab in the System Settings screen allows the user to configure the interface between the analyzer and an external computer. The OPC page provides configuration options for an OPC interface. The Modbus page provides configuration options for a Modbus interface.

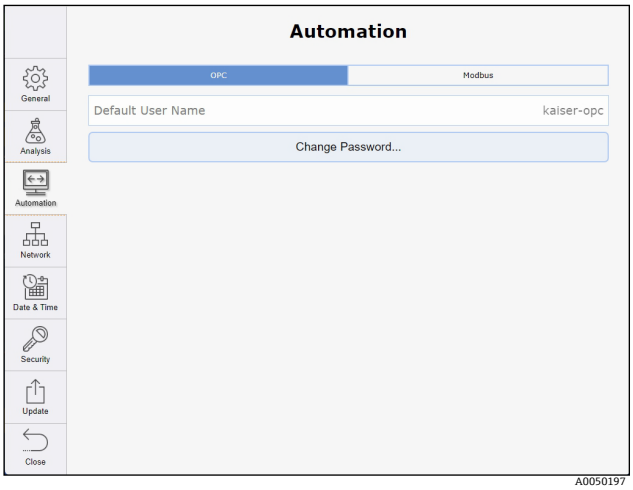


Figure 65. System settings – automation tab – OPC

Modbus output can be configured independently for each channel of the analyzer. Once the components and derived values for a channel have been selected, the channel map provides the details of the assigned Modbus registers for each component.

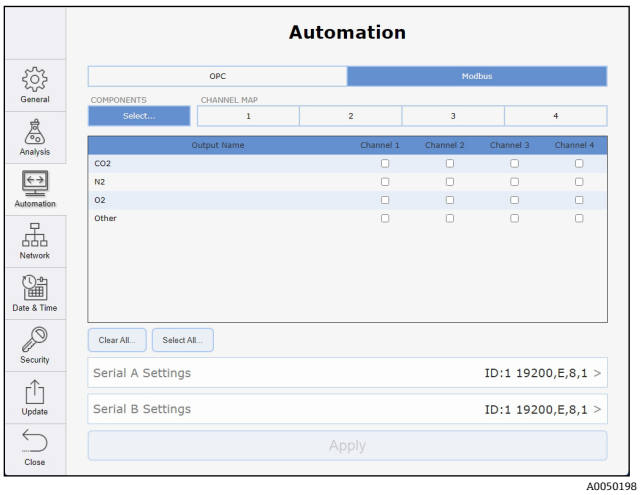


Figure 66. System settings – automation tab – Modbus

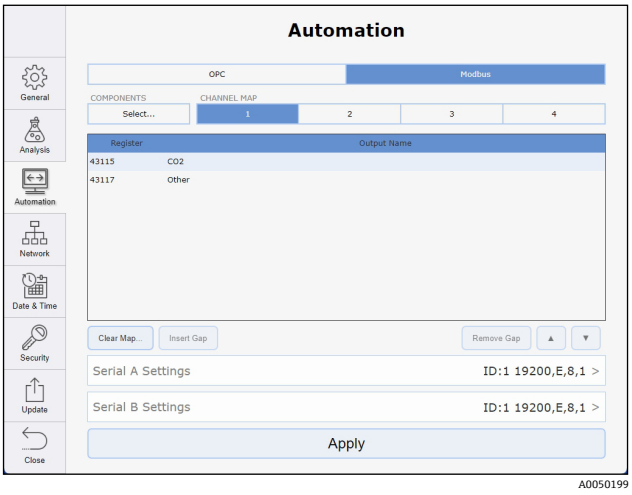


Figure 67. System settings – automation tab – Modbus channel map

7.4 SPC spectral sources

Raman Rxn analyzers running Raman RunTime versions lower than v6.4 can automatically export spectra to Raman data library through the SPC spectral source feature. The SPC spectral source requires an input path, in which Raman data library watches for new files and imports them, and an output path, to which Raman data library moves the SPC files after they are imported.

Refer to *SPC file network export* → for instructions on exporting .spc files from Raman RunTime.

7.4.1 SPC file network export

If the Raman Rxn is connected to a network, spectral (*.spc) files are automatically saved in network-accessible folders. A common file share is available on the Raman Rxn at *<computer-name>\DataLibraryBatchExport*. This directory contains distinct subfolders corresponding to each acquisition batch:

1. Batch folder names are of the form *Probe <#>_<batch>_<YYYYmmdd-HHmmss>*, where *<#>* is the instrument collection channel, *<batch>* is a user-specified batch name, and *<YYYYmmdd-HHmmss>* encodes the date and time the batch was started.
2. Spectrum file names are of the form *<batch>_<YYYYmmdd-HHmmss>*, which encodes the time the individual acquisition completed.

When security in Raman RunTime is enabled, only authenticated users have access to the SPC file network export as well as read and delete privileges within the network folder.

7.5 Batch data management

Each stream or probe channel can display the amount of storage that different spectral batches are occupying on the system. It is recommended that data be exported periodically to avoid filling up analyzer storage. Raman analyzers are not configured for long-term data storage.

If you find that the storage use affects the analyzers ability to collect data, RunTime can be configured to not store spectra locally and only transmit it, encrypted, over OPC-UA protocol and in conjunction with a PAT platform. If your organization does not utilize OPC-UA and PAT, data offloading every couple years is required.

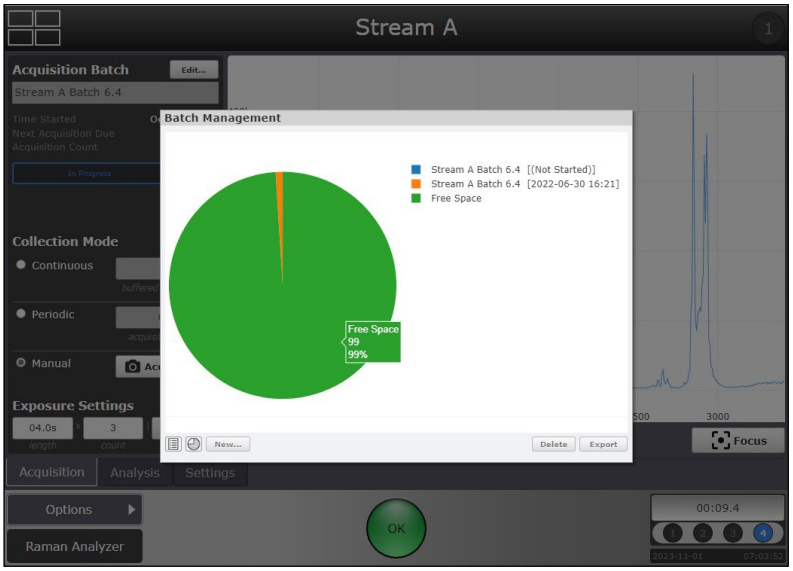
To view batch space use

1. From the stream details screen, select **Edit**.

   The Batch Management screen appears.

2. Click the **Pie Chart** A0057891 .

   The batch management pie chart shows the amount of memory available on the analyzer and the amount of space each batch is utilizing, as a percentage value. You can export batch data from this screen. See *Batch data export* → 🗎, below.



A0054363

Figure 68. Batch management screen showing batch data storage used and available

7.5.1 Batch data export

Spectral batch data (*.spc format) and model results (*.csv format) for collected batches can be exported locally from the Raman Rxn2 or Raman Rxn4 onto a USB memory stick or downloaded via remote access. When models are active and predicting during collection, two *.csv files (processvalues.csv and allproperties.csv) containing model results are included in the export.

To export batch data

1. Connect a USB memory stick to the USB port on the front of the Raman analyzer.
2. From the probe detail view, click **Edit**, check the batches to export, then click **Copy**.
3. Browse to the USB memory stick and desired folder and click **Select Folder**.

7.6 Data storage

Raman RunTime stores spectral (*.spc) files locally. With Raman Rxn2 and Raman Rxn4 analyzers, these files can be accessed over network. Spectral batch data can be transferred or exported onto a USB memory stick or, with Raman Rxn2 and Raman Rxn4 analyzers, over the local network.

The General tab in System Settings displays the amount of system memory (RAM) available on the analyzer in the lower right corner of the screen.

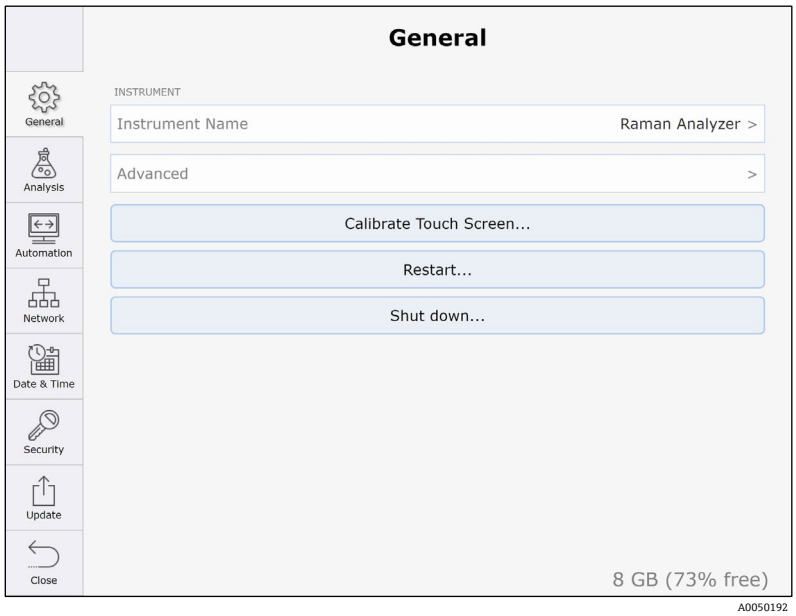


Figure 69. General settings window for the Raman Rxn2 analyzer showing free memory (RAM) available (8 GB–73 % free)

8 Troubleshooting and maintenance

8.1 OPC connection troubleshooting

Endress+Hauser cannot support connection to user-specific OPC clients. Endress+Hauser uses a free OPC Client, UaExpert, for testing server-to-client connections. An Endress+Hauser service engineer can provide instructions for the UaExpert Client to run Raman RunTime OPC Server tests. If problems persist, check the following items:

- Confirm whether the current version of Raman RunTime is operating.
- Verify the **Status** of “Connected” under **Options > System > Network**.

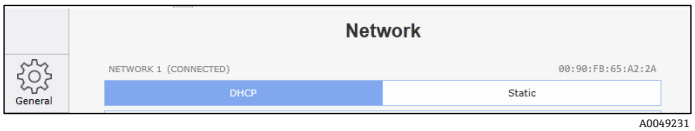


Figure 70. Network screen showing connected

- Make sure the correct Ethernet port is used.
- Check whether the Ethernet port is active with link/activity lights.
- Make sure a valid IP Address is shown.
- Test the ping from a direct connected laptop and ensure both are configured properly.
- Validate the OPC UA communication by using a test client such as UaExpert.
- Check port configuration on client.

8.2 Diagnostic environment data

System diagnostics can be viewed from **Options > Diagnostics > Environment** tab. From the Diagnostics screen, you can view system environment data, trend historical environment data, save an export file to perform a system restore, if necessary. System exports should be done regularly to ensure the system configurations and calibrations are backed up for future use.

System exports are intended for Endress+Hauser Support to investigate problems or restore analyzers. The contents are subject to change with new RunTime versions and should not be treated as user-accessible files.

A full export is recommended for regular archival of system info and logs and is required for a system restore. Full exports can be large.

8.2.1 Trends

To display trends of diagnostic values

1. Navigate to **Options > Diagnostics** from the main Raman RunTime menu.

   The Environment tab within the Systems Diagnostics dialog box appears. System data displays here.

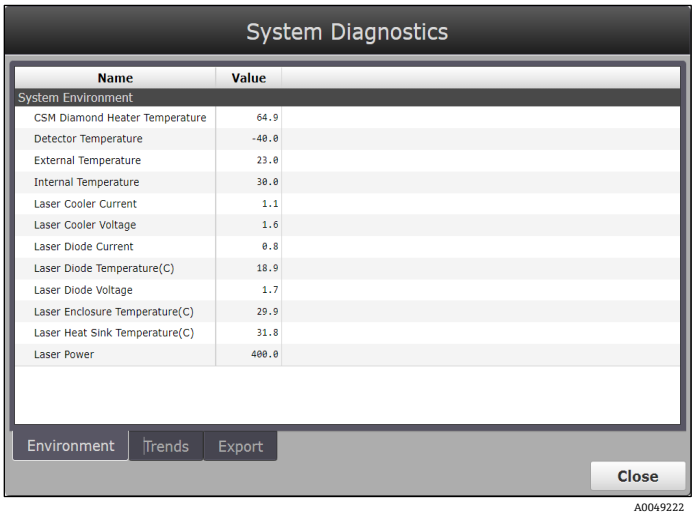


Figure 71. Environment tab to view system data

2. Click the **Trends** tab.

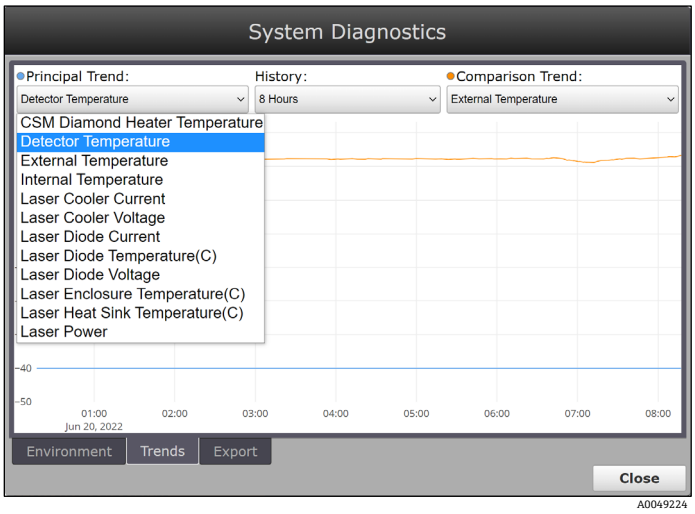


Figure 72. Principal trend options

3. In the Trends tab, select the **Principal Trend**, **History**, or **Comparison Trend** as shown below.

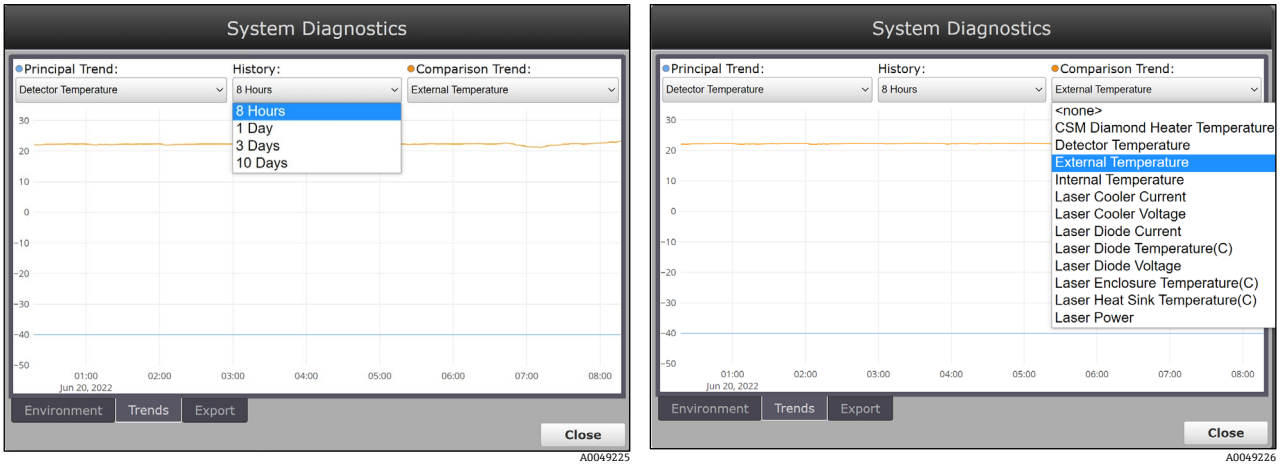


Figure 73. History and comparison trend options

8.3 System Export

Endress+Hauser recommends exporting user data, spectral data, custom settings, and configurations frequently through a full system export. A full system export that is saved onto external media is also recommended. These exports should be considered for inclusion in the local site standard operating procedure (SOP).

To create a new export file

1. From the RunTime dashboard, go to **Options > Diagnostics > Export** tab.
2. Click **New**.
3. Select between **Basic**, **Diagnostic**, and **Full** exports:
   - **Basic**. A Basic export contains the configuration and calibration information.
   - **Diagnostic**. A Diagnostic export provides logs to assist in troubleshooting with Endress+Hauser.
   - **Full**. The Full export contains all comprehensive acquisition and analysis information in addition to information available in the Basic and Diagnostic options. Full exports are large files, often several gigabytes (GB) in size. A Full export is recommended for regular archival of system information and logs. A Full export may be requested when working with Endress+Hauser Support.
4. Click **Export** to create the file.

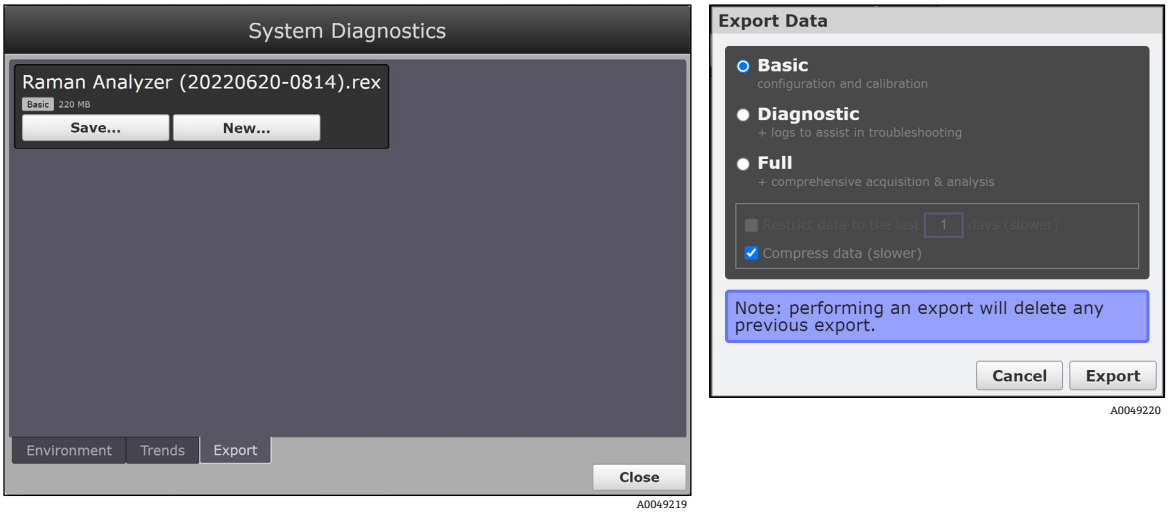


Figure 74. Steps to create a new export file

5. Once the export archive has been generated, click **Save** to save the created export file to a USB drive or download it to the network computer accessing the remote interface of the Raman RunTime software.

While the last generated export file is saved onto the onboard analyzer storage, it is only saved there until a newer export file is generated, which overwrites the old one. As such, the generated export files should be periodically backed up onto a USB drive for backup and restore purposes.

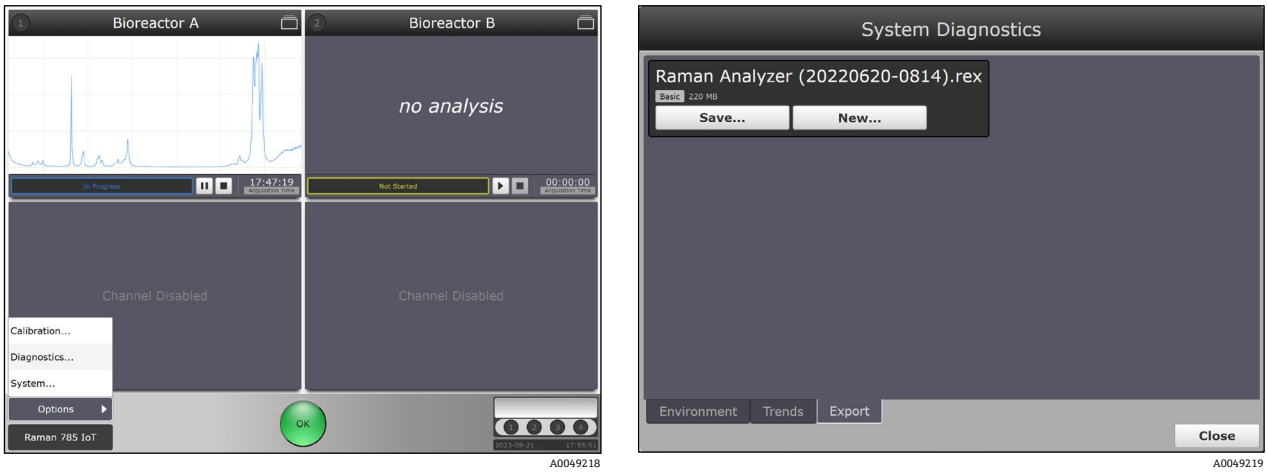


Figure 75. Steps to save an export file

The save option on the same screen allows you to either save the created export file to a USB drive or download it to the network computer accessing the remote interface of the Raman RunTime software.

8.4 System warnings and errors

When the system is fully calibrated and operating as expected, the status button in the bottom middle of the dashboard **Status** bar reads **OK** and appears **Green**.

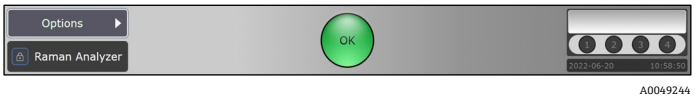
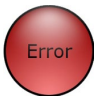


Figure 76. Status bar

Symbol	Description
A0049200	If a system warning is encountered, a **Yellow** warning button displays. Warnings should be acknowledged but immediate action may not be necessary. The button pulses continuously until the problem is resolved. Click **Warning** to view details about the warning.
 A0049202	If a system error is encountered, a **Red** error button displays. An error requires immediate action to restore system performance. Click **Error** to view details about the error.

8.4.1 Resolving system warning and error states

If a system error is encountered, a **Red** error button displays.

To resolve a warning or error state

1. Click the **Yellow** or **Red** status indicator to view details about the warning or error.

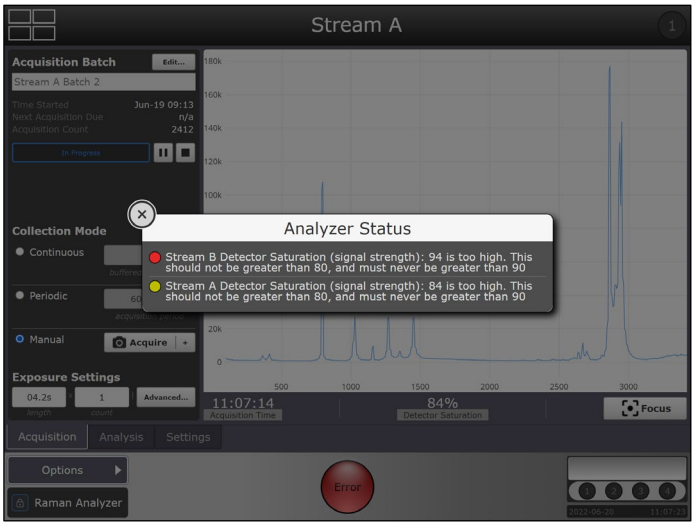
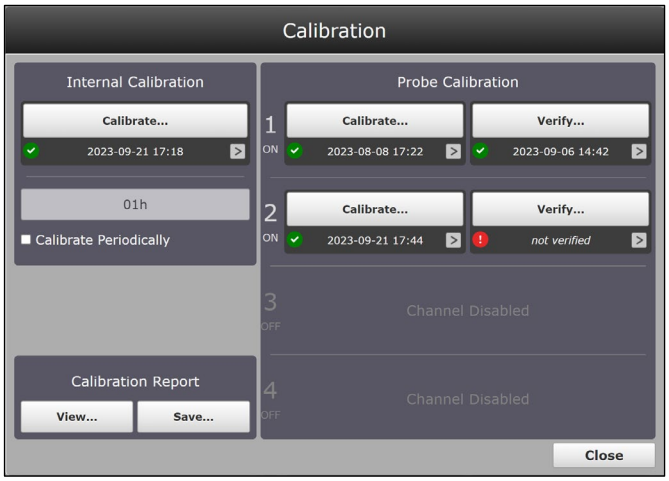
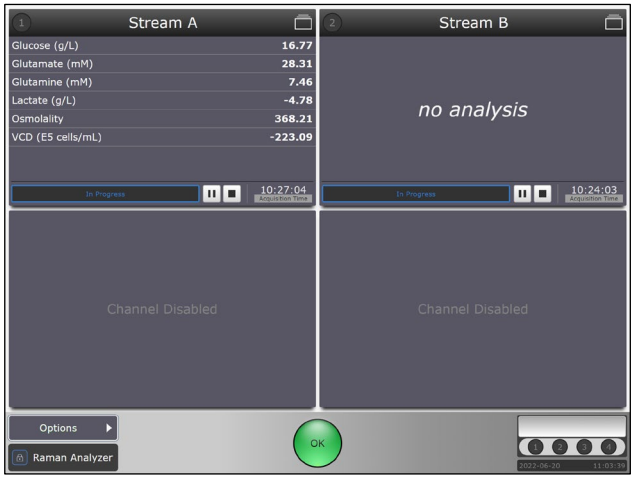


Figure 77. Analyzer status details

2. Correct the error or warning by providing corrective action.



A0049228



A0049246

Figure 78. Channels 3 and 4 shown disabled and warning indicators resolved to green OK state

If the analyzer stops communication with the dashboard, from the dashboard navigate to Options, select System, and choose Restart. The analyzer reboots. This re-establishes communication.

A full list of system warnings and errors is listed in the following tables.

8.4.2 System warnings and errors for Raman Rxn2 and Raman Rxn4 analyzers

Diagnostic Title	Faults when...
Internal Calibration	Internal calibration is missing on a multi-channel instrument.
Wavelength Calibration	Wavelength calibration is missing on a single-channel instrument.
Laser Calibration	Laser calibration is missing on a single-channel instrument.
Intensity Calibration	Intensity calibration is missing on the channel.
Detector Temperature	Camera temperature is out of tolerance.
Detector Locked	Camera temperature is not stable.
Detector Saturation	Camera saturation is < 2 % or > 80 %.
CSM Diamond Heater Temperature	Laser calibration standard temperature is out of tolerance.
CSM Laser Interlock Alarm	Laser interlock was interrupted, e.g. probe cable broken or improperly connected.
Laser Interlock Status	Laser is disabled, e.g. due to being turned off.
Laser Diode Current	Laser diode drive current approaches maximum.
Laser Cooler Open Circuit	An error was received from the laser module.
Laser Diode Current Error	An error was received from the laser module.
Laser Diode Temp Error	An error was received from the laser module.
Laser Diode Temp Startup	An error was received from the laser module.
Laser Diode Temp Warning	An error was received from the laser module.
Laser Power Feedback	An error was received from the laser module.
Laser Power Feedback Error	An error was received from the laser module.
Laser Unit Temp Error	An error was received from the laser module.
Laser Unit Temp Startup	An error was received from the laser module.

8.4.3 System warnings and errors for Raman Rxn5 analyzers

Diagnostic	Warning Threshold	Error Threshold	Expected Value
Air Temp External	48 °C (118 °F)	50 °C (122 °F)	-20 °C to 50 °C (-4 °F to 122 °F)
Air Temp Internal	50 °C (122 °F)	55 °C (131 °F)	0 °C to 55 °C (32 °F to 133 °F)

Diagnostic	Warning Threshold	Error Threshold	Expected Value
Grating Temperature	53 °C (127 °F)	55 °C (131 °F)	0 °C to 55 °C (32 °F to 133 °F)
Heatsink HVAC 1 (left) Inside	N/A	N/A	At external > 30 °C (86 °F) Plenum minus 15 °C to 20 °C (59 °F to 68 °F)
Heatsink HVAC 1 (left) Plenum	73 °C (163 °F)	75 °C (167 °F)	At external < 25 °C (77 °F) Inside minus 15 °C to 20 °C (59 °F to 68 °F)
Heatsink HVAC 2 (left) Inside	N/A	N/A	At external > 35 °C (95 °F) Plenum minus 15 °C to 20 °C (59 °F to 68 °F)
Heatsink HVAC 2 (left) Plenum	73 °C (163 °F)	75 °C (167 °F)	At external < 25 °C (77 °F) Inside minus 15 °C to 20 °C (59 °F to 68 °F)
Heatsink Power Supply	73 °C (163 °F)		5 °C to 20 °C (41 °F to 68 °F) over external
Heatsink Spectrograph	58 °C (136 °F)	60 °C (140 °F)	5 °C to 8 °C (41 °F to 46 °F) over external
Relative Humidity	65 %	85 %	–
Channel <ch> Laser Diode Current	2.1 A	N/A	1.0 A to 2.1 A
Channel <ch> Laser Heatsink	63 °C (145 °F)	65 °C (149 °F)	2 °C to 5 °C (36 °F to 41 °F) over external
Channel <ch> Laser Power Out	N/A	N/A	130 mW to 170 mW
Channel <ch> Sample Pressure	N/A	N/A	–
Channel <ch> Sample Temperature	N/A	N/A	–

In addition to diagnostics shown in the **Options > Diagnostics** screen, the software may produce the following diagnostic warnings and alarms during operation.

Diagnostic	Warning Threshold	Error Threshold	Expected Value
Detector Temperature too High	> -40 °C (-40 °F)	> -38 °C (-36 °F)	Not shown unless warning or error
Detector Temperature too Low	< -40 °C (-40 °F)	< -42 °C (-44 °F)	Not shown unless warning or error
Detector Saturation (Signal Strength) too High	> 80 %	> 90 %	30 % – 80 %
Detector Saturation (Signal Strength) too Low	NA	< 2 %	30 % – 80 %
Warnings			
Blower Alarm: The cooling fan is not working properly. The analyzer might overheat.			
Inline Wavelength Calibration Warning. Neon pixel fill below warning level.			
Channel <ch> Inline wavelength calibration failed. Using default wavelength calibration.			
Channel <ch> Inline laser calibration failed. Using default laser wavelength.			
Channel <ch>: <analysis> calibration does not perform within tolerance.			
Channel <ch>: <analysis> calibration has not been verified in more than <x> days.			
System analysis is disabled.			

8.4.4 Diagnostic fault codes for automation

A DCS, control room personnel, or on-site automation teams can have enhanced insight into the Raman analyzer's state. This is achieved through the implementation of OPC tags and Modbus registers that indicate when a system-level diagnostic is in a failing state.

For details on the OPC and Modbus registers that system diagnostics, refer to the following documents:

- See *Raman RunTime Automation OPC v6.6 (p/n 4005856)* to view the current list and history of OPC Tags for Raman RunTime.
- See *Raman RunTime Automation Modbus v6.6 (p/n 4005855)* to view the current Modbus Map for Raman RunTime.
- See *HTTPS Automation Interface v6.6 (p/n 4005857*) to view details on using HTTPS protocol to transfer supported file types to Raman RunTime.

Diagnostic fault codes include the following types.

Code	Description
Sensor (1xx)	
100	Unspecified fault
101	No laser
102	Laser power limit exceeded
103	Signal out of range
104	Component temperature out of specification
Electronic (3xx)	
300	Unspecified fault
301	Service Alert - Laser
302	Service Alert - Neon
303	Malfunction - cooling fan
304	Malfunction - calibration/switching module (CSM)
305	Malfunction - power supply
306	Malfunction - communication
307	Calibration failure
308	Component temperature out of specification
Configuration (5xx)	
500	Unspecified fault
501	System disabled
502	Calibration invalid
503	Configuration invalid
504	Low storage space
Process/Environment (9xx)	
900	Unspecified fault
901	Environmental conditions out of specification

For a detailed matrix of diagnostic fault codes pertaining to specific instrument types, contact Endress+Hauser Support.

8.4.5 Unused channels and probes

In some cases, users may choose not to utilize all available channels on a Raman Rxn analyzer. Unused or uncalibrated channels can issue warnings that place the entire system in a warning state. To resolve erroneous unused channel warnings, you can disable unused probes or channels as shown below.

To disable an unused channel or probe

1. From the dashboard, navigate to **Options > Calibration**.

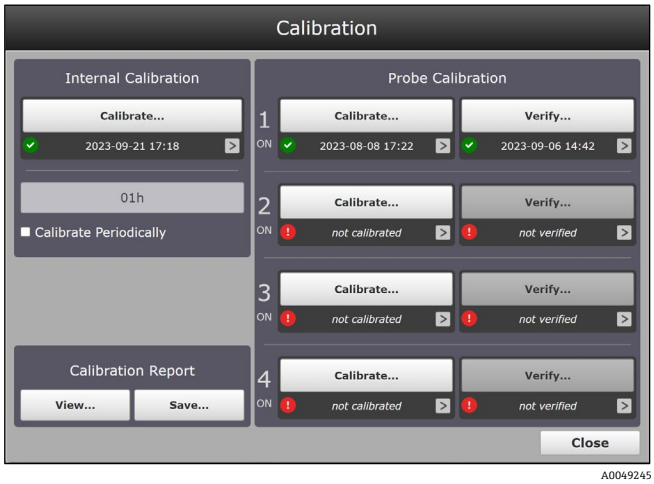


Figure 79. Channels 2, 3 and 4 shown unused/uncalibrated

2. Click the **ON** marker beneath each probe or channel number to toggle it **OFF**.

   A disable channel dialog appears.

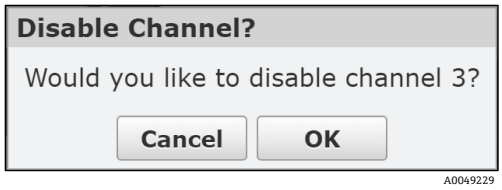
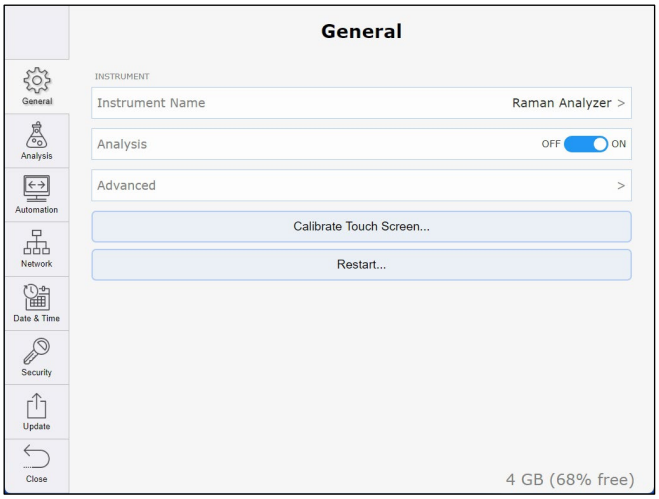


Figure 80. Disable channel 3 prompt

3. Click **OK**.

8.5 Restarting the system

In Raman RunTime, navigate to **Options > System > General** and click **Restart**. Only users with administrative privileges can restart the device if security is enabled.



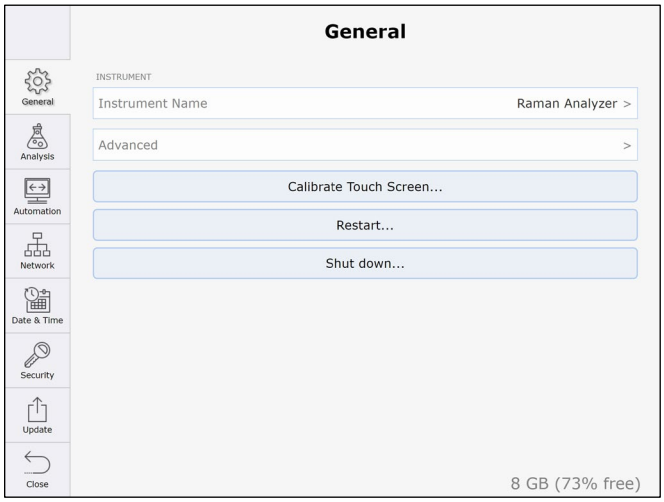


Figure 81. Raman Rxn2 and Raman Rxn4 restart screen (left) Raman Rxn5 restart screen (right)

8.6 Turning off the Raman Rxn2 or Raman Rxn4 analyzer

The following instructions on turning off the system apply only to embedded analyzers. Turning off the system as described in this section is not applicable to non-embedded analyzers used in conjunction with an HMI, the Raman Rxn4 with enclosure, or the Raman Rxn5.

The only supported method of turning off a Raman Rxn4 with enclosure is by using the main power switch on the right side of the enclosure. The Raman Rxn5 is hard-wired and the means of removing power can vary by installation. There is a power breaker switch inside Rxn5 which is only accessible when door is open.

There are two ways to properly turn off a Raman Rxn2 or Raman Rxn4 analyzer. One of these two methods should always be used to turn off the analyzer unless it is unresponsive:

- **Turning off the analyzer: method one.** In Raman RunTime, navigate to **Options > System > General** and click **Shut Down**. The analyzer turns off after about 5 seconds.

Figure 82. Shut down

- **Turning off the analyzer: method two (hardware option).** Click and hold the **Push** button power switch until it starts to blink (2 seconds). Release the **Push** button. The analyzer turns off after about 5 seconds.

Performing a hard shut down

To perform a hard shutdown, there are two methods that can be used. Both hard shutdown options involve analyzer hardware and are not options selected from Raman RunTime. They should only be used if Raman RunTime is unresponsive:

- **Performing a hard shut down: method one.** Click and hold the **Push** button power switch for at least 12 seconds until the analyzer powers down. Then release the **Push** button. After 2 seconds, the power switch begins to blink; ignore and continue to hold down the **Power** button until analyzer powers down. Release the button.
- **Performing a hard shut down: method two.** Unplug the analyzer.

8.7 Recovery console

The Recovery console appears if Raman RunTime is unable to initiate. Raman RunTime prompts you to enter recovery console after trying to initiate five times. This section lists options for resolving the problem.

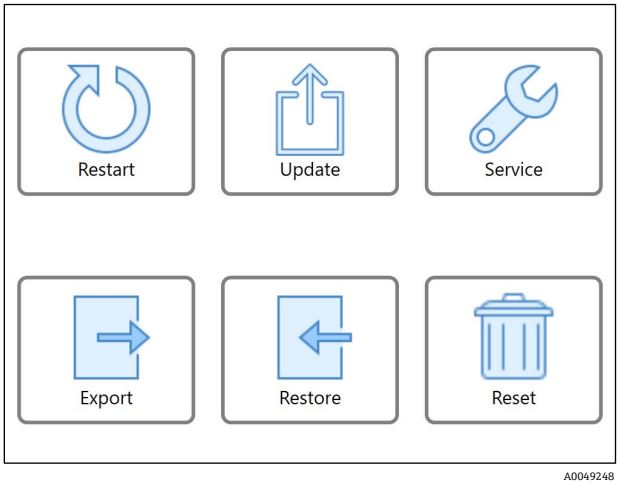


Figure 83. Recovery console menu

The Recovery console consists of the following functions:

- **Restart.** This button restarts the system.
- **Update.** This button is used to update the Raman RunTime embedded software on the analyzer with factory-provided update file(s) that are loaded onto a USB flash drive.
- **Service.** Selecting the Service option will place the analyzer in a service mode. Service mode is only available to qualified service personnel. Contact Endress+Hauser Support for more information about its use.
- **Export.** This button is used to download data, settings, or configurations of the analyzer when it is in an error state.
- **Restore.** This button can restore Raman RunTime to an earlier state. To use this function, there must be a saved file from an earlier time, and that file must be local or on an external USB drive plugged into the analyzer USB port.
- **Reset.** By clicking the **Reset** button, and then **Continue**, the system reboots and deletes all calibrations, models, acquisitions, logs, and other data.

Refer to the following sections for instructions on these features.

8.7.1 Restarting Raman RunTime

The **Restart** button restarts the system. To restart the system, click **Restart**, then click **Yes** on the confirmation dialog.

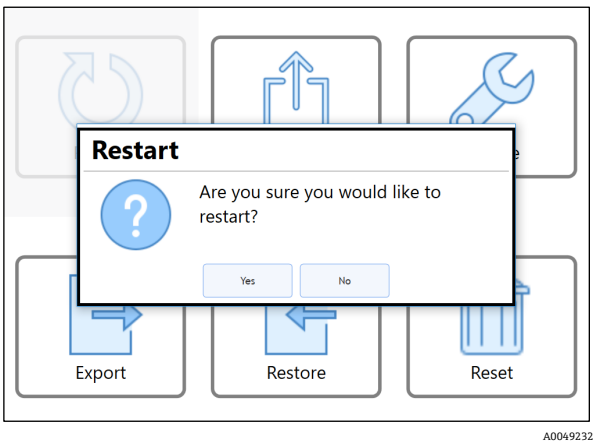


Figure 84. Restart warning

8.7.2 Updating Raman RunTime

The **Update** button is used to update the Raman RunTime embedded software on the analyzer with factory-provided update file(s) that are loaded onto a USB flash drive. Put the USB drive into the USB slot on the front of the analyzer (Raman Rxn2/Raman Rxn4/hybrid) or inside the analyzer (Rxn5) and follow menu prompts to find the file and initiate the update.

Refer to the notice below before attempting an update to Raman RunTime.

NOTICE

- Only Endress+Hauser factory-trained personnel should perform a software upgrade.
- Update files must be installed in a specific order.
- Ensure all prerequisite requirements are met before upgrading Raman RunTime.
- Remote support should be sought through email or phone before an end-user attempting to update.
- Failure to follow this advice may result in the analyzer becoming inoperable. The end-user assumes all responsibility and liability for a self-install option.

To perform a Raman RunTime embedded software update

1. Using factory provided update file(s), go to Options > System > Update.
2. Select the **i** in the bottom right corner to view the current version of the embedded software and a history of installed updates.
3. Click **Choose Update**.

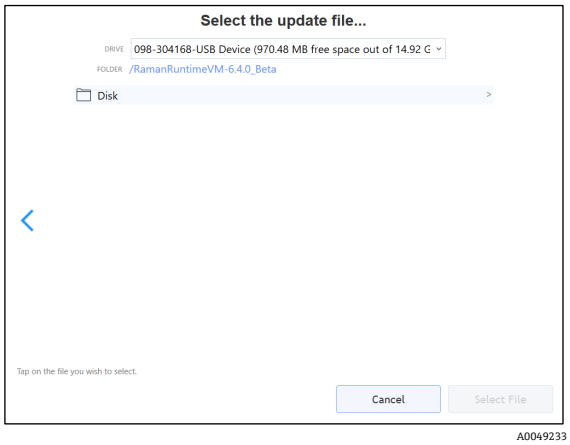


Figure 85. Update mode menu

4. Select the update file to use, one at a time, and in the correct order.

8.7.3 Service

Selecting the Service option will place the analyzer in a service mode. **Service** is only available to qualified service personnel. Contact Endress+Hauser Support for more information about its use.

Figure 86. Service mode menu

8.7.4 Exporting system data

The **Export** button is used to download data, settings, or configurations of the analyzer. The Export function of the Recovery Console is only used when the analyzer is in an error state.

To restore the analyzer, a user can only use an export file previously generated and saved to a USB drive from within Raman RunTime. The last generated and saved export file also resides on the system's onboard memory.

The export generated by the recovery console aids Endress+Hauser Support in investigating problems with the analyzer. This export file cannot be used to restore the analyzer.

Figure 87. Exporting a file

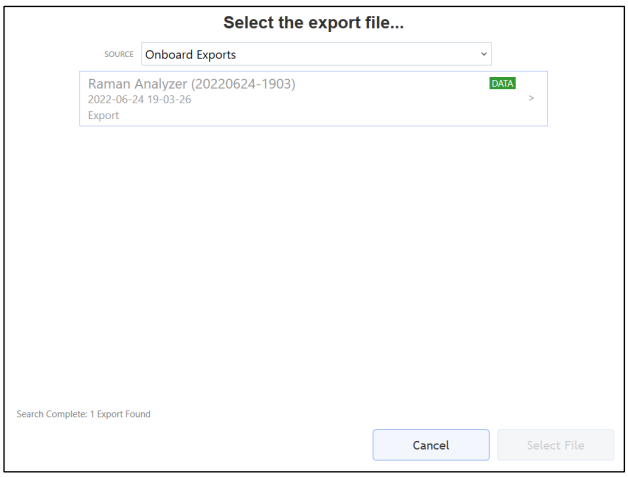
8.7.5 Restoring Raman RunTime

The **Restore** button can restore Raman RunTime to an earlier state of the analyzer that was saved at an earlier time from within Raman RunTime and exists on the onboard storage or on a USB drive. This is the recommended solution to restoring Raman RunTime to an operational mode.

Restore can be done with any level of export (basic, diagnostic, or full). Using a full export adds the option to restore acquisition data and analytic results, in addition to the configuration and calibration information that is restored using any level of export.

To use Restore:

- An earlier export file that was generated from within RunTime must exist, and
- The export file must reside locally or on a USB flash drive inserted into a USB port on the front of the analyzer (Raman Rxn2, Raman Rxn4, hybrid) or inside the analyzer door (Rxn5).



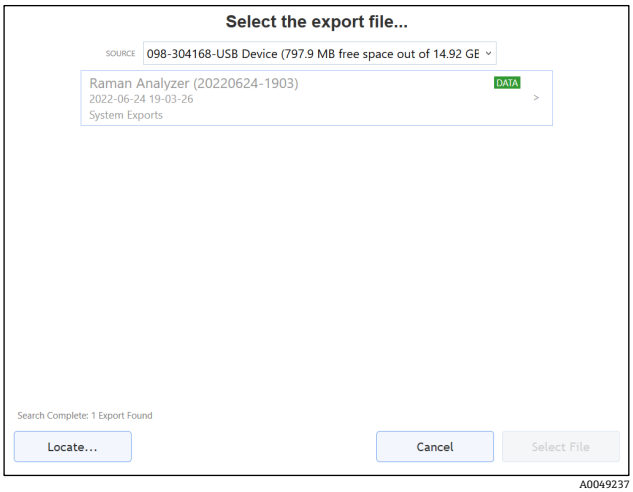
A0049236

Figure 88. Restoring Raman RunTime to an earlier version using export stored on the analyzer storage

To restore Raman RunTime

1. Navigate to the exported system restore file to restore settings and configuration. Choose a Full level export file to restore the settings, configuration, models, and data.

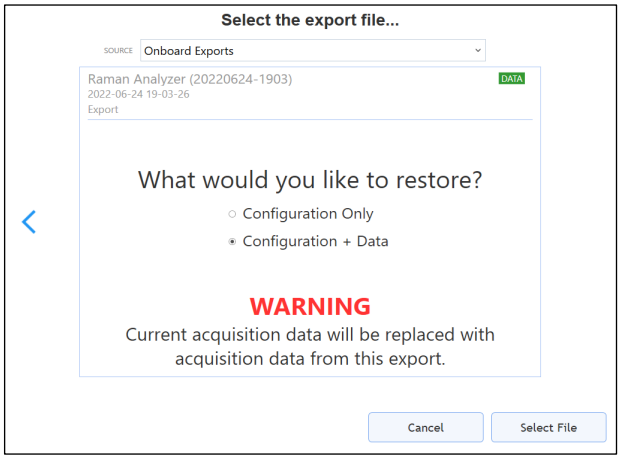
   If an export is Full level and contains the content for a full restore, this is indicated by the Green DATA tag next to the export file as shown below.



A0049237

Figure 89. Restoring Raman RunTime to an earlier version using export stored on a USB drive

While the settings and configuration are always restored, Raman RunTime asks whether the user also wants to restore data as well if a Full export (with a **Green** DATA tag) is available and selected.



A0049238

Figure 90. Warning menu to select level of restore for Raman RunTime

2. Select the file to restore the analyzer.
   Once the file is selected, a dialog displays to confirm the action.

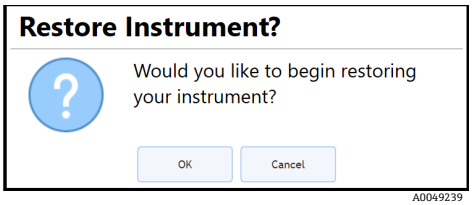


Figure 91. Confirm restore dialog

3. Click **OK**.

   The system now restarts and restores. This can take a while. Do not shut down the analyzer.

The USB drive must remain plugged in while restore is running.

Once the restore is finished, the instrument restarts and Raman RunTime launches.

8.7.6 Resetting Raman RunTime

The **Reset** button forces the system to reboot and delete all calibrations, models, acquisitions, logs, and other data. To reset the system, click the **Reset** button, and then click **Continue**.

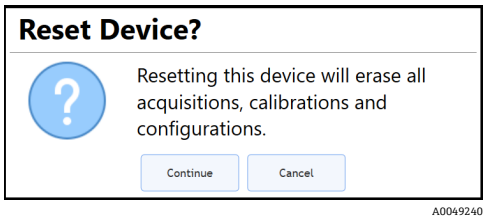


Figure 92. Confirm resetting the device

9 Software updates

9.1 Updating Raman RunTime

From the Update tab in System Settings, you can select and install software updates. Software updates must be either on a flash drive or on the host computer drive or on the workstation computer drive if the system is accessed remotely using a web browser.

Refer to the notice below before attempting an update to Raman RunTime.

NOTICE

Failure to implement the following advice may result in the analyzer becoming inoperable. The end-user assumes all responsibility and liability for a self-install option.

- Only Endress+Hauser factory-trained personnel should perform a software upgrade.
- Update files must be installed in a specific order.
- Ensure all prerequisite requirements are met before upgrading Raman RunTime.
- Remote support should be sought through email or phone before an end-user attempting to update.

Perform a full system export for backup purposes as described in *Export* → 🖹 and save it to an external USB flash drive or an external network before initiating a RunTime update.

To update Raman RunTime software

1. Save the software update file(s) to a USB flash drive or the workstation computer drive.
2. From the dashboard, navigate to **Options**, then **System**.
3. Click the **Update** tab, then click **Choose Update**.

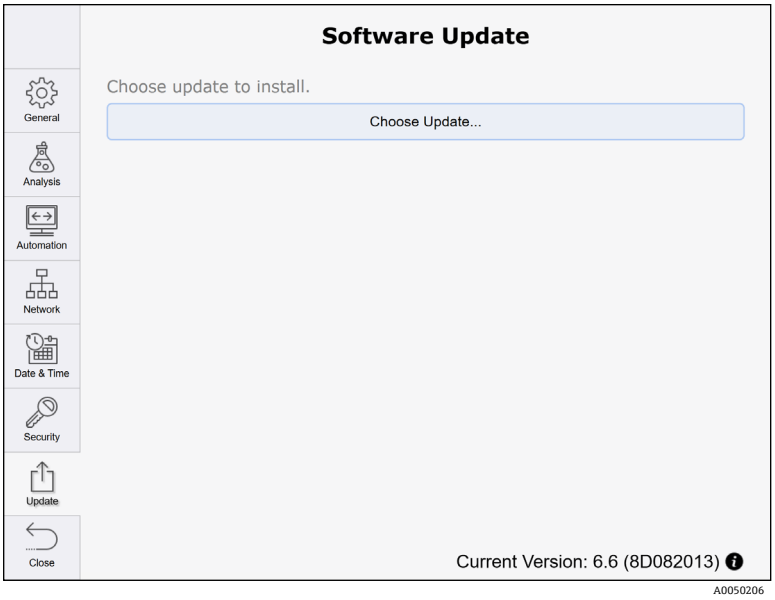


Figure 93. System settings – update tab

4. Navigate to the folder on the USB flash drive or the workstation computer that contains the Raman RunTime update file(s).
5. Select the appropriate update file to install, and in the order as instructed by the E+H trained factory service technician. Click **Select File**.

   The system performs the software update and restarts back the main dashboard when successful. Depending on the amount of data in the system, the update may take up to 20 minutes.
6. Repeat steps 2-5 if the update process involves multiple update files.
7. Select ⓘ in the bottom right corner to view the current version of the RunTime embedded software and a history of installed updates. Confirm the software has update to the desired version.

9.2 Support

Diagnostic exports and the current Raman RunTime version number is needed for Endress+Hauser support. The version can be viewed from **Options > System > Update** and is located on the lower right corner of the screen.

Click **Information** to display additional details about the versions and updates applied.

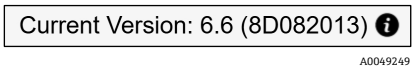


Figure 94. Current version

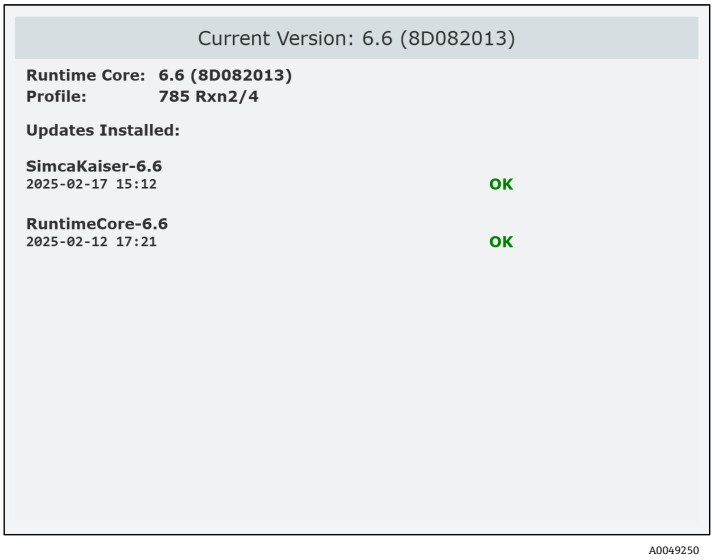


Figure 95. Update history

9.3 Contact information

For Technical Service, refer to our website (https://endress.com/contact) for the list of local sales channels in your area.

10 Copyright information

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