



THE NEXT GENERATION OF OPEN SOURCE QUARTZ CRYSTAL MICROBALANCE

SOFTWARE USER GUIDE VERSION 0.1.5 ©openQCM by Novaetech Srl

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openQCM NEXT Software Application

The openQCM Next software user interface is designed to utilize all the functionalities of the device. Developed using the Python programming language, it ensures an open-source approach for scientific applications.



openQCM NEXT python software application version 0.1.5

The openQCM NEXT software application is developed using the Python programming language, which is open-source, object-oriented, and well-suited for scientific applications. Python makes the software program easy to modify and develop for custom applications.

The new openQCM NEXT software is capable of leveraging all the main functionalities of the device, including real-time monitoring of frequency and dissipation on the fundamental mode and overtones. It can acquire nearly 5 sweep signals simultaneously and process frequency and dissipation measurements in approximately 7 seconds. Additionally, the application enables real-time control and monitoring of the sensor module temperature.

Software GUI General Description



Connection and Measurement Setting

Serial COM Port	Drop-down menu for selecting the COM port connected to the openQCM Next device
Operation Mode	Calibration: record the quartz resonator calibration signal for resonance peak detection
	Single Measurement: real-time monitoring of frequency and dissipation at a single frequency in the quartz resonator spectrum.
	Multiscan Measurement: real time monitoring of frequency and dissipation on fundamental and overtone harmonics of the quartz resonator
Frequency / Quartz Resonators	Calibration operation mode: Select 10 MHz or 5 MHz quartz resonator fundamental frequency
	Single Measurement mode: Select the quartz resonator frequency to monitor

Temperature setting and indicator

Temperature Ctrl ON	Enable the temperature control
Temperature Ctrl OFF	Disable the temperature control
TEC Controller Reset	Press the button to reset the temperature controller after an error status event. Disabled by default
PID Set	Press the button to change the PID parameters of the TEC control
P Share	Proportional parameter. Default value 1000 mA/K Range: (0 to 100000 mA/K)
I Share	Intergral parameter. Default value 200 mA/(K*sec) Range: (0 to 100000 mA/(K*sec))
D Share	Proportional parameter. Default value 100 (mA*s)/K Range: (0 to 100000 (mA*s)/K)
Temperature Set	Press the button to change the set temperature in real time. Default value: 25°C. (Nominal Temperature range: 5°C to 45°C).
Temperature (°C)	Current temperature value

Temperature Real Time Graph

Real Time Plot: Temperature	Real time plot of temperature data measured in °C
•	

Amplitude and Phase Real Time Graph

Real Time Plot: Amplitude / Phase	Calibration: plot of amplitude and phase signals over all frequencies ranging from 1 MHz to 51 MHz
	Single Measurement: plot of amplitude and phase sweep signals around the selected single resonance frequency (fundamental or harmonic overtones)
	Multiscan measurement: Plot of amplitude sweep signals for all detected resonance frequencies, including both fundamental and harmonic overtones.

Frequency and Dissipation Real Time Graph

Real-Time Plot: Resonance Frequency Real-Time Plot: Dissipation	Single Measurement: real-time plot of frequency and dissipation of a selected vibration mode (fundamental or harmonic overtones)
	Multiscan measurement: Real-time plot of the frequency and dissipation for all detected vibration modes, including both fundamental and harmonic overtones.

Control and graphic buttons

Start	Start a measurement session for each operation mode.
Stop	Stop a measurement session for both single and multiscan operation modes.
Set Reference	Press the button to set the current values of frequency and dissipation as the reference value to measure variations, applicable for both single and multiscan operation modes
Reset Reference	Press the button to reset the current frequency and dissipation values to their actual values, applicable for both single and multiscan operation modes."
Clear Plots	Clear the history of each real-time graph
Progress bar	Calibration: indicator showing the progress of the frequency scan across all frequencies ranging from 1 MHz to 51 MHz
	Single and multiscan measurement: Indicator showing the accumulation of initial raw data before processing the frequency and dissipation data.

Frequency and Dissipation Indicator

Frequency and Dissipation Indicator	Single measurement: real-time indicator of the current frequency (in Hz) and dissipation (in ppm "parts per million") values of the selected vibration mode (fundamental or harmonic overtones)
	Multiscan measurement: Real-time indicator of the current frequency (in Hz) and dissipation (in ppm "parts per million") values for all detected vibration modes, fundamental and harmonic overtones

Vibration Mode Selector

Fundamental and harmonic overtones	Multiscan Measurement: Select radio buttons to display real-time plots of frequency, dissipation, and amplitude for
	the corresponding vibration mode.

Datalog Sampling Time

Datalog Sampling time	Multiscan Measurement: select the datalog sampling time using the drop - down menu. The default value is the hardware minimum sampling time
Time elapsed	Time elapsed between consecutive datalog samples

Add-on Features (BETA)

LOG DATA VIEW	Under development
RAW DATA VIEW	Under development

Calibration Mode of Measurement



Calibration measurement of a 5 MHz quartz resonator in contact with air. The real-time amplitude graph shows the detection of the resonance frequencies up to the 9th overtone

The calibration mode of measurement performs a frequency sweep across the available range from 1 MHz to 51 MHz, acquiring the amplitude and phase spectrum of the quartz resonator. The primary goal is to detect the resonance frequencies, including both the fundamental mode and harmonic overtones, of the quartz resonators. It is also necessary to remove the baseline signal in the wide frequency range for frequency and dissipation post-processing.

It is necessary to select the fundamental mode of the quartz resonator under test using the Frequency/ Quartz Resonators drop-down menu, 5 MHz or 10 MHz option. It is suggested to perform the calibration on a new and clean quartz resonator in contact with air. The calibration measurement must be started each time the quartz resonator is changed.

Single Mode of Measurement



Single-mode measurement of a 5 MHz quartz resonator in contact with air, measuring its fundamental mode of vibration, with active temperature control set to T = 25.0 °C.

The single-mode of measurement performs a frequency sweep around a selected single vibration mode, whether it's the fundamental frequency or a harmonic overtone, and retrieves the frequency and dissipation data in real-time.

The vibration mode is selected using the Frequency/Quartz Resonators drop-down menu.

The thermal control can be activated on the fly by pressing the Temperature Ctrl ON button. The temperature set point can be changed on the fly by adjusting the Temperature Set value and pressing the Temperature Set button.

A new measurement session begins by pressing the Start button.

Multiscan Mode of Measurement



Multiscan mode of measurement of a 5 MHz quartz resonator in contact with air, measuring from fundamental to 9th overtone mode of vibration, with active temperature control set to T = 25.0 °C. Frequency and dissipation variations are referred to the initial reference values

The Multiscan mode of measurement performs a frequency sweep around each mode of vibration, including both fundamental and harmonic overtones, one after another. It retrieves the frequency and dissipation data in real-time for all harmonics almost simultaneously.

The thermal control can be activated on the fly by pressing the Temperature Ctrl ON button. Temperature set point can be changed on the fly by adjusting the Temperature Set value and pressing the Temperature Set button.

The visualisation of the frequency and dissipation multi-plot graph can be enhanced by pressing the 'Set Reference' button, which sets the current frequency and dissipation values as the reference values to measure variations. Additionally, by selecting the radio buttons in the vibration mode selector, it is possible to visualise only the desired harmonics of interest.

TEC Controller Reset



Pop-up window of TEC controller status error alert.

ress the button to reset the temperature controller after an error status event. Disabled by default.

The software decodes the MTD415T internal 16 bit error register, which identifies the reason why the module enters in error state. More information available at paragraph 6.3 "Error Register and Safety Bitmask" of MTD415T Data Sheet Rev. 1.2.

Data File

The data file is automatically saved every time a new measurement session is started, whether it's in single-mode or multiscan mode.

The data file is saved in the folder "logged_data", which is located in the main directory of the application, as indicated below:

.../openQCM_Next_py_0.1.5/logged_data/

The data file name is automatically generated, with the prefix of the file name matching to the date - time of the measurement session start, as in the example below for a data file acquired on April 18, 2023, at 15:16:03 in multiscan mode of measurement

2023-Apr-18_15-16-03_multi_.csv

The data file format is in CSV (Comma Separated Values) format. The columns of the data file are shown below

Date,Time,Relative_time,Temperature,Frequency_n,Dissipation_n, ...

where:

- Date: the date of acquisition of the data file, format YYYY-MM-DD
- Time: the current time of acquisition, hh:mm:ss
- Relative_time: the elapsed time since the beginning of the acquisition, measured in seconds
- Temperature: the current value of temperature, measured in °C
- Frequency_n: the current value of the QCM frequency corresponding to the n-th overtone, measured in Hz.
- Dissipation_n: the current value of the QCM dissipation corresponding to the n-th overtone, measured in ppm ("parts per million").

Firmware Update

F irmware update for openQCM Next Software version 0.1.5. Firmware update is necessary for integration and compatibility with the latest version of the openQCM Next Python software version 0.1.5.

Info			
Serial COM Port	COM18 ~		
Operation mode	Calibration 🔻	Real-Time Plot: Resonance Frequency	
Frequency - Quartz Sensors	@5MHz_QCM ~		
Temperature Control			
Temperature Ctrl ON	Temperature Crtl OFF		
TEC Contr	oller RESET		
PID Set	Default #1		
Cycling Time [msec]	50		
P Share [mA/K]	500 🗘	00;00:00 00:00:00 00:00:00 00:00:00	00:00
I Share [mA/(K+sec)]	50	Time (s)	
D Share [(mA*s)/K]	300 🗘	Raal-Time Dist: Discination	
Temperature Set	25		
Temperature (° C)	0	■ FIRMWARE UPDATE ×	
Frequency (Hz)		Please update firmware version 0.1.4. Press Yes button to continue the firmware	
F0	0	원 /! update procedure	
F3 —	0		
F 5	0		
F7	0		
F 9	0	00:00:00 00:00:00 00:00:00 00:00:00	00:00
Dissipation (ppm)		Time (s)	
D0	0		
D 3 —	0	Real-Time Plot: Amplitude / Phase Real-Time Plot: Temperature	
D 5	0		
D7 —	0	0.8 Q 0.8	
D 9	0		
○ 0th ○ 3rd ○ 5	ith 🔿 7th 🔿 9th	itude	
Datalog Sampling Time (sec)	Default 👻		
Time elapsed (sec)	0	0.2 - 0.2 - 0.2	
ADD-ON FEATORES (DETA)	VIEW (BETA)		
DAVIDUT		U U U U U U U U U U 1 00:00:00 Franuency (Hz)	00:00
RAW DATA	VIEW (DETA)	incluency (ris)	
Program status		Start Stop Set Reference Reset Reference Clear Plots 0%	

- Launch the openQCM Next Software version 0.1.5 to check the firmware compatibility. If your openQCM Next device needs a firmware update, a pop-up window will appear at software startup
- Press Yes button to continue the firmware update procedure
- The Firmware update application will open. Press the Upload button
- Select and upload the binary file openQCM_Next_py_0.1.5_BETA_teensy.ino.TEENSY40.hex



Add-On Features (BETA)

The openQCM Next software has been upgraded with additional features that provide real-time visualization of both raw and processed data. Users can now simultaneously operate these newly integrated applications in parallel with the main software. This concurrent usage allows ongoing data collection while facilitating the review of previously acquired data. These updates aim to enhance the user experience, providing researchers with a streamlined workflow for more efficient monitoring of their experiments and facilitating quick, data-driven decision-making.

Log Data View (Beta)



openQCM Next Log Data View GUI

Software add-on for the openQCM Next offers the capability to view and analyse data recorded during experiments. It presents a visual display of the recorded data, and aids in recognizing long-term trends, patterns, and potential areas of interest. This feature is designed for detailed post-experimental evaluation, supporting the refinement of future experiments and the extraction of comprehensive insights.

Click the "LOG DATA VIEW (BETA)" button within the main software interface to initiate the openQCM Next Log Data View software add-on.

Press the "GET .CSV DATA FILE" button to navigate to the directory containing data files. Select the data file you want to view and analyze.

Press the "PLOT DATA FILE" button to display the acquired frequency and dissipation data for each overtone on the graph.

Press the "PROCESS" button to measure the variations in frequency and dissipation relative to an initial state (typically when the quartz is in contact with air). To this aim, it is necessary to manually select an initial time interval and a final time interval for measuring these changes. For instance, in the example below, corresponding to the passage from air to water using a 5 MHz quartz crystal, the initial time interval is set from 200 to 400 seconds and the final time interval is set from 1000 to 1200 seconds.

The result of the processing is the measurement of the average values and the standard deviations of the initial and final values, as well as the measurement of the corresponding variations, as shown below.

Frequency average values and standard deviation (Hz), initial state (air) and final state (water)		
Initial state (air)	Final state (water)	
$F_0 = -2.82 \pm 0.34$	$F_0 = -756.54 \pm 0.28$	
$F_3 = 6.22 \pm 0.17$	$F_3 = -1724.07 \pm 0.21$	
$F_5 = 10.44 \pm 0.11$	$F_5 = -2584.35 \pm 1.50$	
$F_7 = 11.34 \pm 0.31$	$F_7 = -3383.32 \pm 1.25$	
$F_9 = 16.86 \pm 0.26$	$F_9 = -3940.88 \pm 9.33$	

Dissipation average values and standard deviation (ppm), initial state (air) and final state (water)

Initial state (air)	Final state (water)
$D_0 = -1.68 \pm 0.18$	$D_0 = 402.18 \pm 0.21$
$D_3 = 1.10 \pm 0.16$	$D_3 = 751.95 \pm 0.54$
$D_5 = -1.34 \pm 0.07$	$D_5 = 1348.77 \pm 1.43$
$D_7 = 1.90 \pm 0.05$	$D_7 = 2460.68 \pm 1.02$
$D_9 = 0.86 \pm 0.12$	$D_9 = 3716.23 \pm 2.46$

Frequency and Dissipation variation caused by the passage from air to pure water.

Frequency variation (Hz):	Dissipation variation (ppm):
Fundamental = -753.71	Fundamental = 403.86
3rd Overtone = -1730.29	3rd Overtone = 750.84
5th Overtone = -2594.78	5th Overtone = 1350.11
7th Overtone = -3394.66	7th Overtone = 2458.78
9th Overtone = -3957.75	9th Overtone = 3715.38



openQCM Next Log Data View, showing a data file corresponding to the passage from air to water using a 5 MHz quartz crystal. The variations in frequency and dissipation are referenced to the value in air.

Raw Data View (Beta)

Software add-on for the openQCM Next is designed to provide real-time visualization of both raw and pre-processed data. It allows researchers to closely monitor the raw data behaviour as they occur during experiments. This enables quick and efficient recognition of patterns, anomalies, and trends, essential for immediate decision-making and adjustments.

Click the "RAW DATA VIEW (BETA)" button within the main software interface to initiate the openQCM Next Log Data View software add-on.

In addition, pre-processed data for noise filtering and elimination are displayed (represented by a continuous black line), along with points of interest on each resonance curve (red crosses) that identify the peak of resonance and bandwidth.



The openQCM Next Raw Data View displays sweep raw data corresponding to air (on the left) and water (on the right) when using a 5 MHz quartz crystal. The continuous black line represents the filtered and smoothed data, while the red crosses indicate the peak and bandwidth of the resonance curves.

Installation Instructions and Usage

Windows OS stand alone application

D ownload the stand alone executable version developed for Windows operating system: openQCM NEXT python software application version 0.1.5. The stand alone executable bundles the Python application and all its dependencies into a single package, allowing you to run the software without installing a Python interpreter or any modules.

- Download the compressed .zip application files here: <u>https://openqcm.com/shared/next/software/openQCM_Next_py_0.1.5_exe.zip</u>
- Unzip the package and browse to the application main directory: .../openQCM_Next_py_0.1.5_exe



• Launch the openQCM-NEXT-0.1.5.exe application shortcut

openQCM NEXT GUI software application version 0.1.5

Python source code

• penQCM Next python source code is intended for users who want to modify and develop the original source code. openQCM is an open science hardware device, and we encourage and support community participation in device and software development. Please visit the openQCM Next software webpage for more info

https://opengcm.com/opengcm-next-software

INSTALLATION GUIDE

Download openQCM Next Python source code latest version 0.1.5 here: https://openqcm.com/shared/next/software/openQCM_Next_py_0.1.5_source.zip

Python environment installation and setup for Windows OS and Mac OS

• Download and install Anaconda open-source Python distribution platform

Windows: Packages for 64-bit Windows with Python 3.9 Anaconda3-2022.05-Windows-x86_64.exe https://repo.anaconda.com/archive/Anaconda3-2022.05-Windows-x86_64.exe

Mac OS: Packages for macOS on x86_64 with Python 3.9 Anaconda3-2022.05-MacOSX-x86_64.pkg https://repo.anaconda.com/archive/Anaconda3-2022.05-MacOSX-x86_64.pkg

installing on macOS anaconda documentation: <u>https://docs.anaconda.com/anaconda/install/mac-os/</u>

• Install the additional python library. Open Anaconda prompt on Windows, or terminal in MacOS and install the additional library package:

conda install pyserial
conda install pyqtgraph
pip install progress bar

Python environment installation and setup on Linux OS (Under verification)

- Download and install Anaconda3 for Python 3.7 version Anaconda3-5.3.0 https://www.anaconda.com/download/
- Type the command below by replacing username with that of your pc to change permission of Anaconda3:

sudo chown -R username:username /home/username/anaconda3

USAGE

Follow the instructions below to run the Python code and launch the application

- Launch Anaconda3 prompt, depending on your operating system
- Navigate to the openQCM Next Python source code main directory on your computer

.../openQCM_Next_py_0.1.5/OPENQCM/

• Launch the python application main GUI by typing the command

python -m openQCM

History changes

Python software

Version: 0.1.5 python version TAG: # VER 0.1.5

General information: Improved the control of MCP9808 TEC error status, using the error register message

Major Update

- Added MCP9808 TEC controller error register table. The MTD415T has an internal 16 bit error register, which identifies the reason why the module enters in error state. More information available at paragraph 6.3 "Error Register and Safety Bitmask" of MTD415T Data Sheet Rev. 1.2
- Change the identification of the COM port connected to Teensy 4.0, by using USB VID:PID=16C0:0483 VID 0 VENDOR_ID and PID = PRODUCT_ID of USB devices to identify hardware, and port[2] = hwid Technical description of serial port

Minor Update

- TEC controller RESET procedure, increased the waiting time to 2 seconds for the transmission of the command enable pin on - enable pin off for module reset.
 The error register can be reset using the "c" command or by setting the Enable pin to Off and On again.
- Improved firmware update procedure. Launch firmware updater also from menu bar, only if a measurement is not running

Teensy Firmware

Version: 0.1.5 version tag // VER 0.1.5

Major Update

- Change the way the MTD415T error status is read by using error register, defined in Error Register and Safety Bitmask (paragraph 6.3 page 18 MTD415T Data Sheet Rev. 1.2)
- Read MTD415T TEC controller error register

Command	Response
E?	return: 16 bit error register
	Reads the Error Register. For responses see section: Error Register and Safety Bitmask (paragraph 6.3 page 18 MTD415T Data Sheet Rev. 1.2)

- Improved MTD415T startup, insert a delay and serial flush in setup()
- Send temperature and error register command in MTD415T status: temperature control active and temperature setpoint ok
- Add a new parameter to the sweep output buffer: error_register_bit

```
amplitude_0;phase_0
amplitude_1;phase_1
. . .
amplitude_n;phase_n
temperature;status_control;error_register_bit;termination_char
```

• Turn the Fan ON if only if the temperature control is active