Guide

How to read a QCM specification

Parameters to keep an eye on, what they mean and why they are important

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Introduction

When you are to invest in a new QCM-system, there are several aspects of the instrument to consider. The first aspect that comes to mind is most likely the hardware capabilities. From an experimental setup and execution perspective, the hardware must fulfill the needed requirements.

Another aspect that is important to consider is the quality of the data generated. Because what is the point of running the experiments if the results are ambiguous and the data cannot be trusted? Therefore, the specification of the parameters related to the data quality is equally important to evaluate.

In this guide, you will get the full picture on how to read a QCM specification. In the appendix, you will also find the specification for QSense hardware and data quality parameters. Feel free to add other suppliers' QCM specifications for comparison. There are several ways to express QCM parameters. The guide will help you to match the parameters.

Key parameters to consider

In the specification of a QCM instrument

When you are to invest in a new QCM-system, there are several aspects of the instrument to consider. The first aspect that comes to mind is most likely the hardware capabilities. From an experimental setup and execution perspective, the hardware must fulfill the needed requirements. For example, if a flow-mode experiment is planned, the setup must be equipped with flow capabilities, and if the experiment will be run in harsh solvents, the setup must withstand those chemicals. Another aspect that is important to consider is the quality of the data generated. Because what is the point of running the experiments if the results are ambiguous and the data cannot be trusted? Therefore, the specification of the parameters related to the data quality is equally important to evaluate. Here, we present an overview of the key parameters to consider in the specification of a QCM instrument, what the respective parameter means and how they matter in the end use.

Keep an eye on the parameters related to data quality – but which are they?

The key parameter measured by a QCM instrument is the resonance frequency change of the oscillator. Extended QCM setups will in addition to the frequency change, measure one or more parameters related to the energy losses in the system. The parameters included in an instrument specification can, however, both vary and be described with different terminology.

Which of all the parameters specified are relevant and will have an impact on the end measurement, and how can they be compared between different instrument suppliers?

Some parameters are more important than others

The relevance of a certain parameter may, to some extent, be determined by the actual measurement situation. For example, high time resolution may not be critical if very slow surface interaction processes are studied, and a high measurement sensitivity may not be important if large changes are to be measured. An aspect which is critical irrespective of the end use, however, is the assurance that the measurement reflects the process being studied. For example, a measured decrease in frequency should reflect mass uptake (or change in solvent properties) and not be induced by an uncontrolled drift in temperature. The temperature has a large impact on the resonance frequency, and therefore it is important to assure a good temperature control that keeps the temperature stable throughout the measurement. There are also other factors that will influence the information quality of the measured signal, such as noise and drift. The magnitude of these and other parameters, listed in the table on page 3, will significantly impact the measurement result.

Theoretical values vs actual ones

Some parameters mentioned in the context of QCM are purely theoretical, see table on page 3. These parameters are true but most often irrelevant in the actual measurement situation.

Measurement resolution

One example of such a parameter is the measurement resolution. The instrument electronics may fulfill a certain precision and be able to deliver a certain number of decimals in the measured signal, but this number doesn't mean that all the decimals have any meaning. Noise and drift will ultimately determine the data quality and determine how many of the measured decimals that in the end are significant.

Mass sensitivity

Another example of a theoretical parameter often specified is the theoretical mass sensitivity. The theoretical mass sensitivity is a value that depends purely on the fundamental resonant frequency of the crystal[1]. The higher the fundamental mode, the higher the theoretical mass sensitivity. A 5 MHz crystal will have a mass sensitivity of 17.7 ng/(cm^2·Hz), and a 10MHz crystal will have a theoretical mass sensitivity of 4.4 ng/cm^2·Hz). However, it must be considered that the noise level also increases with higher fundamental resonant frequency, which means that a higher theoretical sensitivity does not necessarily correlate with a better mass detection limit (the useful mass sensitivity) in the actual measurement situation. When assessing the specified sensitivity, it is therefore not sufficient to only look at the theoretical number relating to the crystal. To get the useful mass sensitivity which is relevant in a measurement situation, the measurement sensitivity, which determines how many significant decimals that can be resolved, must be considered. So, even if there is a theoretically high mass sensitivity inherent in the high-fundamental mode crystal, this can be significantly impaired by limitations of the hardware and electronics, which reduces how much of the crystal capacity that can be utilized in the actual measurement output.

Ask about noise and long-term stability

When evaluating the data quality that the instrument will deliver, noise and drift are two important parameters to consider. The noise will, in the end, determine the useful measurement sensitivity, i.e. how many of the displayed decimals that will be significant. The long-term drift will determine if the information collected can be trusted, or if the results are ambiguous due to influence from other sources such as temperature drift or mechanical stresses. If not specified, it can be relevant to request information on noise and stability from the supplier. Comparing specifications, it is also worth paying attention to the unit of the specified parameter. Knowing how parameters are extracted or calculated, the unit can sometimes reveal whether the specified parameter is a theoretical or an actual one. This also allows for recalculation of specified parameters to compare between instruments, where the parameters sometimes can be specified in a different way.

How are the parameters measured, and under what conditions are they valid?

The conditions at which a parameter is measured and how calculations are made are important information and should be specified by the supplier. For example, at what temperature has the specified drift been captured? How long was the measurement and in what temperature range is the specification valid? Is it valid in gas phase or in liquid phase (and in that case which liquid)? The specified numbers may only be valid under certain conditions, which is important to be aware of when considering and comparing instrument specifications.

PARAMETER	EXPLANATION AND SIGNIFICANCE	UNIT
RESOLUTION		
Time	The time resolution, or **sampling rate**, describes how many data points that are collected per second. The higher the sampling rate, the faster kinetic processes can be resolved in an experiment.	Hz
Frequency	The **frequency resolution** is basically the number of decimals the instrument can display. A high resolution does not necessarily mean that small frequency changes can be detected; the extent to which the displayed numbers are significant depends on the noise level. As long as the frequency resolution is better than the noise level, which means that it is possible to resolve the changes taking place, it is not relevant for a real measurement situation. Example: If, for example, only two decimals are significant (above the noise level), it does not matter if the resolution is 10 decimals or 15.	Hz
Dissipation	Same as above	unitless
Mass	The **mass resolution** correlates with the frequency resolution (see above) by a multiplication of the constant sensitivity factor (for a 5 MHz sensor, this is 17.7 $ng/(cm^2 \cdot Hz)$). As long as the resolution is better than the noise level, i.e., you are able to resolve the changes taking place, this parameter is not relevant for a real measurement situation.	ng/cm^2
Temperature	The **temperature resolution** describes how exact the actual temperature can be measured. As long as the temperature resolution is better than the stability level, i.e., that it is possible to measure the temperature changes taking place, it has no relevance for a real measurement situation.	˚C
SENSITIVITY		
Frequency	The useful frequency sensitivity is the smallest significant change that can be resolved in the frequency signal. The sensitivity almost always depends more on the noise level than on how many decimals that can be displayed. I.e. it is the noise level, which in the end will determine how many of the displayed decimals of the frequency parameter that are significant. Example: the instrument has a specified signal resolution of 0.001 Hz, and a noise level of 0.05 Hz. Assuming you accept a signal-to-noise ratio of 2, the useful frequency sensitivity will be 0.1 Hz	Hz
Mass (theoretical)	The theoretical mass sensitivity depends on the crystal fundamental mode [1]. Example: For a 5 MHz crystal it is 17.7 $ng/(cm^2 \cdot Hz)$ The extent to which the theoretical mass sensitivity is useful is determined by the useful frequency sensitivity, i.e. the smallest significant change in frequency signal that can be resolved.	$ng/(cm^2 \cdot Hz)$
Mass (useful)	The **useful mass sensitivity**, i.e. the sensitivity which can be achieved in an experimental situation, equals the theoretical mass sensitivity multiplied by the useful frequency sensitivity. Example: With a 5 MHz crystal, the theoretical sensitivity is 17.7 $ng/(cm^2 \cdot Hz)$. With a useful frequency sensitivity of 0.1 Hz, the useful mass sensitivity will be 1.8 ng/cm^2.	ng/cm^2
Dissipation	The useful dissipation sensitivity is the smallest significant change that can be resolved in the Dissipation signal. The useful sensitivity almost always depends more on the noise level than on how many decimals that can be displayed.	unitless
NOISE		
Frequency	The noise describes uncontrolled, short-term variations, of the signal. The noise will determine how much of the measured signal that can be utilized and determine how many of the displayed decimals that are significant.	Hz
Dissipation	Same as above	unitless
Temperature	Same as above	˚C
LONG-TERM STABILITY		
Frequency	Frequency stability, or drift, describes long-term variations of the signal. A stable signal is important, especially for longer measurements. High drift will make the results ambiguous and it will be unclear whether the measured frequency response reflects mass changes or if it is due to undefined instrument variations.	Hz/h
Dissipation	Same as above	1/h
Temperature	The temperature stability describes the temperature drift per time unit. Since the temperature affects the QCM signals, a good temperature control and stability is essential for reliable measurement results.	˚C/h

Concluding remarks

When about to invest in a new QCM-setup, there are several aspects that will be considered such as price, hardware design and experimental capabilities. As the overall objective of any experiment is to be able to answer a predefined question with certainty, the data quality is also essential to assess. For example, it is not only of utmost importance to be able to resolve, via the measured signal, what happens, but it is also crucial that the information collected can be trusted. Key parameters relating to the data quality, and which should be kept an eye on, are the resolution, sensitivity, noise, and drift[2]. When reading and comparing the specification of QCM instruments, it should be noted which of the specified values are theoretical and which are useful. Also, under what conditions the specified numbers are valid should be considered.

References

Reference

1. G. Sauerbrey; Z. Phys., 155:206-222, 1959

Footnotes

1. The mass sensitivity, C, is $C = t_q \cdot \rho_q / f$ [1], where f is the fundamental frequency, $\rho_q = 2648\ kg/m^3$ is the density of quartz, and t_q is the thickness of the crystal. The thickness of a crystal of fundamental frequency, f, is obtained via $f = \upsilon_q/(2 \cdot t_q)$, where $\upsilon_q = 3340\ m/s$ is the velocity of sound in AT-cut quartz.
2. Both the electronic capabilities and the mechanical design will impact these parameters. The mechanical design is important since it can result in both mechanical- and temperature fluctuations, which both affect the crystal oscillation.

Appendix

Measurement characteristics QSense Explorer, Analyzer and Pro

PARAMETER	SPECIFICATION	COMMENT		
TECHNOLOGY	**QCM-D**			
Parameters measured	frequency (f), Dissipation (D)			
Frequency range (MHz)	1-72			
Sensor fundamental frequency (MHz)	5	Standard QSensor, 5MHz		
Measured sensor harmonics	7	5 MHz QSensor		
RESOLUTION				
Maximum time resolution (sampling rate, Hz)	> 100	One sensor and one harmonic		
Frequency resolution (Hz) (mass resolution)	< 1 μ (< 17,7·10^{-6} ng/cm^2)	As long as this number is smaller than the noise level, it has no relevance for a real measurement situation		
Dissipation resolution (1)	< 10^{-12}	As long as this number is smaller than the noise level, it has no relevance for a real measurement situation		
Temperature resolution (˚C)	0.001	As long as this number is smaller than the noise level, it has no relevance for a real measurement situation		
SENSITIVITY				
Maximum mass sensitivity in liquid (ng/cm^2)	0.5	Data from single frequency mode. One data point is collected every 5 seconds. The Sauerbrey relation is assumed to be valid.		
Standard mass sensitivity in liquid (ng/cm^2)	1.8	Data from single frequency mode. One data point is collected every 5 seconds. The Sauerbrey relation is assumed to be valid.		
Maximum Dissipation sensitivity in liquid (1)	0.04·10^{-6}	Data from single frequency mode. One data point is collected every 5 seconds. The Sauerbrey relation is assumed to be valid.		
Standard Dissipation sensitivity in liquid (1)	0.1·10^{-6}	Data from multiple frequency mode (7 harmonics); 4 data points are collected within 1 second.		
NOICE				
Frequency (Hz) (mass)	0.06 (1 ng/cm^2)	Typical frequency (mass) noise std in water at RT, measured within a period of two minutes.		
Dissipation (1)	20·10^{-9}	Typical Dissipation noise std in water at RT, measured within a period of two minutes.		
Temperature (˚C)	0.01	Typical Temperature noise std in water at RT, measured within a period of two minutes.		
LONG-TERM STABILITY				
Frequency (Hz/h)	< 2	Standard Au QSensor (QSX 301) in water at RT. In air, the drifts are usually larger, due to slower changes in e.g. humidity.		
Dissipation (1/h)	< 0.2·10^{-6}	Standard Au QSensor (QSX 301) in water at RT. In air, the drifts are usually larger, due to slower changes in e.g. humidity.		
Temperature ˚C/h	0.02	The temperature stability depends on variations in how the ambient affects the warming or cooling of the chamber. The specified temperature stability may not be reached if the room temperature changes more than +/- 1° C, if there is a draft or a heat source nearby. The temperature of the sample solutions outside the chamber should preferably be within +/- 2K from the working temperature of the chamber.		

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Setup, Sample handling system and Sensors

FEATURE	QSENSE EXPLORER	QSENSE ANALYZER	QSENSE PRO		
Channels	1	4	8		
Possibility to expand to higher throughput channels	Upgrade option to 4 channels	NA	NA		
Volume over sensor	40 ul	40 ul	15 ul		
Minimum sample volume, stagnant	40 ul (10 ul in QOM)	40 ul (10 ul in QOM)	15 ul		
Minimum sample volume, flow mode	200 ul	200 ul	50 ul		
Minimum dispense volume	NA	NA	1 ul		
Working Temperature range ˚C	15˚C - 65˚C (4˚C - 150˚C)	15˚C - 65˚C	4˚C - 70˚C		
Sensor coatings	> 50 standard	> 50 standard	> 50 standard		
Sensor coatings customized	Yes	Yes	Yes		
Possibility to coat sensors ex-situ	Yes	Yes	Yes		
Instrument integration	No	Yes, can be integrated with QSense Explorer chamber for access to extended capability modules	Yes, can be integrated with QSense Explorer chamber for access to extended capability modules		
Ellipsometry	Yes	No	No		
EXTENDED CAPABILITY MODULES					
QOM - direct access to sensor surface	Yes	Yes	No		
QTM - PTFE flow channels	Yes	Yes	No		
QHM - humidity measurements	Yes	Yes	No		
QEM - simultaneous combination with electrochemistry	Yes	Yes	No		
QVM - ALD holder for measurement in gas phase at variable pressure	Yes	Yes	No		
QWM - window access to sensor surface for simultaneous combination with microscopy, optical characterization or irradiation	Yes	Yes (optical characterization or irradiation only)	No		
QELM - simultaneous combination with ellipsometry	Yes	No	No		
QWEM - simultaneous combination with both microscopy and electrochemistry	Yes	No	No		
SIMULTANEOUS TECHNOLOGY COMBINATIONS					
Electrochemistry	Yes	Yes	No		
Microscopy	Yes	No	No		
Ellipsometry	Yes	No	No		
Chemical compatibility	Extended (harsh chemicals)	Extended (harsh chemicals)	Standard		
ANALYSIS SOFTWARE					
Automatic data plotting	Yes	Yes	Yes		
Automated viscoelastic modelling	Yes	Yes	Yes		
Smart tools - analysis method toolbox	Yes, >10 pre-defined methods for data extraction	Yes, >10 pre-defined methods for data extraction	Yes, >10 pre-defined methods for data extraction		
Batch mode - simultaneous analysis of multiple data files	Yes, >100 data files	Yes, >100 data files	Yes, >100 data files		
Template tool - templates can be reused and shared with other users	Yes	Yes	Yes		
Automatic report tool	Yes	Yes	Yes		
OUTPUT DATA					
Raw data	* time-resolved frequency and Dissipation at multiple harmonics	* time-resolved frequency and Dissipation at multiple harmonics	* time-resolved frequency and Dissipation at multiple harmonics		
Modelled data	* time-resolved mass, thickness, viscosity, and elasticity	* time-resolved mass, thickness, viscosity, and elasticity	* time-resolved mass, thickness, viscosity, and elasticity		
Dynamic behavior	* kinetics, slope, rise time and more	* kinetics, slope, rise time and more	* kinetics, slope, rise time and more		

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