

## Computation of Equivalent Circuit Parameters of QCM and Evaluation of the Measurement Uncertainties

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**Abstract.** This paper presents an approach of computing the parameters of quartz crystal microbalance (QCM) equivalent circuit model using the least squares algorithm in MATLAB. Modification of the measured data's order in the least squares algorithm was implemented so that the precision was improved. Compared with nonlinear least squares algorithm, the computation method in this paper was faster and simpler with little lower accuracy. Moreover, Monte Carlo Method was utilized to evaluate the measurement uncertainties. An experiment on the temperature response of QCM's equivalent circuit parameters was performed to show that the proposed approach was accurate and fast. The measurement errors are less than 0.6%.

### Introduction

QCM has been used as a gravimetric sensor in many sensing applications for its high sensitivity. Since Kanazawa demonstrated that QCM could be applied in liquid phase<sup>[1]</sup>, applications of QCM have extended to numerous fields like physics, electrochemistry and biology. In some applications resonant frequency is not the only parameter of interest, for properties of the added loading on the quartz sometimes are simply related to the parameters of the crystal's equivalent circuit model. Each parameter of the QCM's Butterworth-Van-Dyke (BVD) equivalent circuit model (shown in Fig. 1) represents a physical property of the quartz and its coating<sup>[2]</sup>. On the other hand, oscillators are always a good choice for QCM sensors with the merits of low cost, continuous measurement and integration capability<sup>[3]</sup>. The resonant frequency of oscillators is mainly determined by the equivalent circuit parameters. When loadings, especially in liquid occur on the surface of QCM, the oscillator's resonant frequency may have a big difference with the fundamental resonant frequency of QCM. Hence, the exact measurement of the equivalent circuit parameters can make a big difference in improving the precision of oscillators. Impedance analysis or network analysis are the most common means to obtain QCM's equivalent circuit parameters. Responses of QCM in a small range of spectrum near the resonant frequency are usually measured through a high precision instrument. With the conductance and admittance spectra, the parameters can be estimated. A highly accurate and reliable non-linear Levenberg-Marquadt least squares fitting algorithm has been used for estimating the parameters, however the algorithm suffers from the defects of requiring large space and time<sup>[2, 4]</sup>.

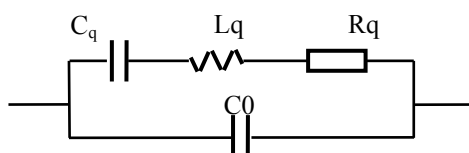


Fig. 1 Equivalent circuit model of QCM

In this paper, an algorithm for computing the equivalent circuit parameters of QCM based on least squares in MATLAB is described. Aimed at a high precision, the order of the measured data in least squares algorithm is modified. And such a computing method's uncertainty is evaluated through Monte Carlo mathematical simulation. An experiment about the temperature effects on the QCM

equivalent circuit parameters is performed and the results were compared with the algorithm of computing resonant frequency demonstrated in [5].

## Experimental Method

The sensing element consisted of an AT-cut quartz crystal vibrating at 4MHz. The quartz was stuck directly on a Peltier element by a PTFE gasket, which ensured heat transfer meanwhile maintained the fundamental resonant frequency of the quartz. The radiator underneath the Peltier element was employed to play a better cooling effect. A platinum resistance thermometer was placed on the quartz surface in order to follow the quartz temperature. The admittance spectra of QCM was measured by an impedance analyzer (Agilent 4294A) connected to a computer via GPIB interface. The measurement system is given in Fig. 2.

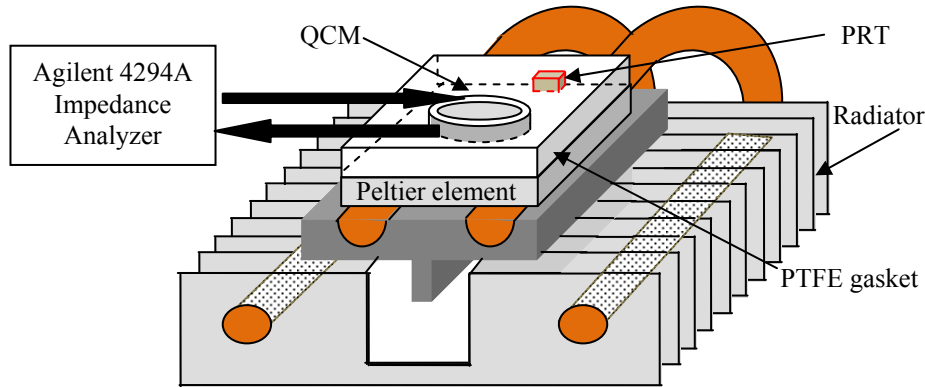


Fig. 2 Schematic diagram of the measurement system

The temperature of QCM was determined by the cooling power for the Peltier element. In this experiment, we set three different values of cooling power to get the QCM temperature response at 24°C, 26 °C and 29°C. When the temperature stabilized at the desired value, the measurement began. The spectrum was configured around the resonant frequency of 2 KHz here. The measuring points were set at 501 so that the resolution reached 4Hz.

## Result and Analyses

**Computing the equivalent circuit parameters of QCM in impedance analysis method.** As shown in Fig. 1, the QCM equivalent circuit model consists of the motional branch  $R_q$ ,  $L_q$ ,  $C_q$  and the static capacitor  $C_0$ . The motional series resonant frequency  $f_s$  is usually regarded as the response of QCM sensors in many applications. And  $f_s$  can be obtained through  $L_q$  and  $C_q$  as follows:

$$f_s = 1/2\pi\sqrt{L_q C_q} . \quad (1)$$

The admittance spectra of the quartz generated from the BVD model can be expressed as:

$$Y_Q(\omega) = G + jB = 1/(R_q + j\omega L_q + 1/j\omega C_q) + j\omega C_0, \quad (2)$$

where G and B can be expressed respectively as:

$$G = R_q / [R_q^2 + (\omega L_q - 1/\omega C_q)^2], B = \omega C_0 - (\omega L_q - 1/\omega C_q) / [R_q^2 + (\omega L_q - 1/\omega C_q)^2]. \quad (3)$$

Firstly, the motional branch parameters were computed through the expression of G in Eq. 3 by least-square fitting and the expression were transferred to the general form as:

$$Y = f(\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3; \beta_1, \beta_2, \beta_3) = f(\mathbf{X}, \boldsymbol{\beta}), \quad (4)$$

where the measured points denoted as  $\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3$  and  $\mathbf{Y}$  were:

$$x_{1i} = \omega_i^2, x_{2i} = G_i \omega_i^2, x_{3i} = -G_i \omega_i^4, y_i = G_i, i = 1, 2, \dots, n, \quad (5)$$

where  $n$  equaled to 501 in this experiment. And the three parameters to be estimated were  $\boldsymbol{\beta}$  :

$$\beta_1 = R_q C_q^2, \beta_2 = 2C_q L_q - R_q^2 C_q^2, \beta_3 = C_q^2 L_q^2. \quad (6)$$

The problem was to compute the estimates of  $\boldsymbol{\beta}$  which would minimize

$$\Phi = \sum_{i=1}^n |y_i - \hat{y}_i| = \|\mathbf{Y} - \hat{\mathbf{Y}}\|^2, \quad (7)$$

where  $\hat{y}_i$  was the value of  $y_i$  predicted by Eq. 4 at the  $i$  th data point.

While measuring the QCM with resonant frequency at approximate 4 MHz, the range of the spectra was too narrow so that  $\mathbf{X}_2$  and  $\mathbf{X}_3$  were linear, in other words,  $\mathbf{X}$  was not column full rank. In order to improve the accuracy of the computation,  $\mathbf{X}$ 's order was modified as follow:

$$x_{1i} = 10^{-14} \omega_i^2, x_{2i} = 10^{-11} G_i \omega_i^2, x_{3i} = -10^{-25} G_i \omega_i^4, y_i = G_i, i = 1, 2, \dots, n \quad (8)$$

and the order of  $\boldsymbol{\beta}$  changed accordingly:

$$\beta_1 = 10^{14} R_q C_q^2, \beta_2 = 10^{11} (2C_q L_q - R_q^2 C_q^2), \beta_3 = 10^{25} C_q^2 L_q^2 \quad (9)$$

Then we would obtain the estimation of  $\boldsymbol{\beta}$  with a higher accuracy:

$$\hat{\boldsymbol{\beta}} = \mathbf{X}^+ \mathbf{Y} \quad (10)$$

Secondly, we computed the values of  $R_q, L_q$  and  $C_q$  through solving Eq. 9.

Thirdly, both the measured conductance and admittance data and the estimated  $R_q, L_q$  and  $C_q$  were utilized to estimate  $C_0$ .

From Eq. 3, we got:

$$\omega^2 C_0 = B\omega + G\omega^2 (L_q - 1/C_q) / R_q = Y \quad (11)$$

$C_0$  can be computed through the approach described in the first step, taking  $\mathbf{X}$  as  $\omega^2$  and  $\boldsymbol{\beta}$  as  $C_0$ .

**Evaluation of the measurement uncertainties.** Measurement uncertainties of the system were computed by a Monte Carlo program. In this system, the uncertainties were mainly due to the possible errors in the measured data  $G$  and  $B$ . Errors from the least squares algorithm cannot be ignored either. Referred to the datasheet of Agilent 4294A precision impedance analyzer, the basic impedance accuracy is  $\pm 0.6\%$ . Consequently input errors of  $G$  and  $B$  were set to  $0.6\%$  in a nearly normal distribution. The number of simulated measurement sets  $N_{sim}$  should be large enough to make sure that any further increase in  $N_{sim}$  changes the upper and lower limits of the confidence interval by less than  $1\%$  of their values. Here  $N_{sim}$  equaled to 10000. We performed the least squares algorithm described in 3.1 for  $N_{sim}$  times according to Monte Carlo Method and got the estimations and uncertainties shown in Table 1.

Table 1. Example of fitted values produced on simulated data and their uncertainties

|             | $R_q$ [ $\Omega$ ] | $L_q$ [H] | $C_q$ [fF] | $C_0$ [pF] |
|-------------|--------------------|-----------|------------|------------|
| Actural     | 147.87             | 0.13278   | 11.938     | 3.4501     |
| Fitted      | 148.02             | 0.13285   | 11.931     | 3.4525     |
| Uncertainty | 0.33               | 0.00033   | 0.0030     | 0.0081     |

We find that the measurement uncertainties of  $R_q$ ,  $L_q$  and  $C_q$  are about 0.25%, while the uncertainty of  $C_0$  is less than 3%. As described in 3.1, the computation of  $C_0$  is based on both the admittance and the conductance spectra. And errors from  $R_q$ ,  $L_q$  and  $C_q$  also make contribution to the uncertainty of  $C_0$ . Hence, the uncertainty of  $C_0$  is larger than the others.

**Detailed analysis of the experimental results.** The experimental results are given in Table 2. The values of resonant frequency  $f_s$  are calculated with  $L_q$  and  $C_q$  according to Eq. 1. And  $f_s'$  in the last column refer to the resonant frequency obtained through the method in [5].

Table 2. Example of fitted values produced on simulated data and their uncertainties

| Temperature[°C] | $R_q$ [Ω] | $L_q$ [mH] | $C_q$ [fF] | $C_0$ [pF] | $f_s$ [MHz] | $f_s'$ [MHz] |
|-----------------|-----------|------------|------------|------------|-------------|--------------|
| 24              | 105.18    | 0.12812    | 12.370     | 5.7259     | 3.9978      | 3.9978       |
| 26              | 91.107    | 0.12993    | 12.197     | 3.6704     | 3.9979      | 3.9979       |
| 29              | 82.964    | 0.13148    | 12.053     | 3.9928     | 3.9980      | 3.9980       |

The differences between  $f_s'$  and  $f_s$  are all less than  $10^{-5}$  referring to the results. And the fitted error computed by the MATLAB is about  $10^{-10}$  to  $10^{-11}$ . The averaged measurement uncertainty here is not over 0.6%.

## Conclusions

The parameters of QCM's equivalent circuit model make great sense in studying the sensing theory of QCM sensors and the design of oscillators. A least squares fit method is present in this paper to compute the parameters. The method is implemented through a MATLAB program with a high degree of accuracy. Meanwhile, this method spends less time compared to nonlinear least squares algorithm. The Monte Carlo Method for evaluating uncertainties is performed and the experimental results show that the measurement uncertainties of the motional branch are all less than 0.25% and the uncertainty of  $C_0$  is a little larger. An experiment on the temperature response of the equivalent circuit model is performed as well. Compared with former proposed approaches, its precision is of the same level while the spent time is reduced.

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