Correction of Thermal Deviations in Fabry-Perot Resonator Based Measurements of Specific Gases in Millimeter Wave Bands

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Abstract. Due to the thermal expansivity of the material used in the Fabry-Perot resonator mirrors, the resonator cavity length can change and this might therefore have an impact on the resonant frequency during high-resolution spectroscopy measurements. Based on measurements and simulations, this paper discusses the influences of temperature on the precise determination of gas attenuation measured in a Fabry-Perot resonator. Several measures to mitigate such influence and to correct the measured results were tested. A correction method for the measured data was proposed.

Keywords
Fabry-Perot resonator, gas attenuation measurement, thermal deviation.

1. Introduction

Several gas absorption measurements have been performed using the Fabry-Perot resonator at the Department of Electromagnetic Field at CTU in Prague [1] [2], starting with a first rare experiment in the nineteen seventies [3]. The great sensitivity of the Fabry-Perot resonant cavity is the result of its very high quality factor. The gas absorption measurements in this case come to measurement and consequential evaluation of quality factor of the empty and gas-filled resonator [4].

It would hardly be feasible to maintain all the instruments at a constant temperature while measurements are being taken, both because human assistance is required and because the whole workplace is too extensive to be thermally stable. What is more, thermal stability would have to be maintained over a long period, since the resonator must be mechanically retuned on many occasions during measurement in order to set the resonant frequencies.

Temporal graduations of the environment may strongly influence measurement precision since each measurement is relatively time consuming. Several hundred mirror positions have to be set up one by one in order to obtain the frequency dependence of gas absorption around only one particular spectral line (e.g. the measurement of 316 resonant curves takes approximately 16 minutes). Given this requirement, it is impossible to retune every individual resonance peak, while simultaneously evaluating deviations and the correct temporal and other influences by re-setting the mirror position.

In this paper specific result deviations of Fabry-Perot resonator-based microwave measurements are discussed. The paper is organized according to the following pattern: First, thermal errors are experimentally determined and compared to the theoretical assumptions. In the following subsection, a correction method for obtaining measured data is proposed. Then examples of the results achieved, as well as their processing and correction, are discussed based on whether individual absorption measurements of specific gases have either high narrow absorption peaks or low absorption levels. After this, the gas attenuation measurement error is expressed. The paper concludes with a brief summary including our main suggestions for Fabry-Perot microwave measurements.

2. Measurement of Temperature Deviations

From a basic physical perspective, thermal expansion is a feature of any substance. This property causes a change in volume as a result of temperature change. This effect can be described by the following expression [5]

\[ \Delta L = \alpha L \Delta T \] (1)

where \( \Delta L \) and \( \Delta T \) stand for changes in the length and temperature of the sample, \( \alpha \) introduces the cubic expansion coefficient and \( L \) is the original length of a measured sample.

The resonator tube used for our measurements has a length of 0.55 m and a diameter of 0.17 m and was fabricated from stainless steel whose temperature coefficient of expansion is relatively high (\( \alpha = 17 \cdot 10^{-6} \, \text{K}^{-1} \) [6].
The resonator consists of two positioned spherical mirrors, a dielectric coupling foil placed inside a cavity, and specially designed input and output windows with dielectric lenses. The mirrors have a 0.455 m radius of curvature, a diameter of 0.15 m and are made of bronze with a gold layer with a thickness of 5 µm.

The resonator has to fulfill the following resonant condition (derived from theoretical expression for resonators [7]):

\[
\frac{2d}{\lambda} = q + (2p+l+1) \cdot \frac{1}{\pi} \arccos \left( \sqrt{\left(1 - \frac{d}{R_1}\right) \left(1 - \frac{d}{R_2}\right)} \right) - \frac{3.31r(\sqrt{\varepsilon_r} - 1)}{\lambda_0}
\]

(2)

where \( p, q, l \) are indexes of TEM modes, \( q \) means the number of half-wavelengths in the \( d \) distance between mirrors (the mirror spacing is tunable from 0.495 to 0.510 m), \( R_{1,2} \) stand for the radii of the curvature of mirrors, \( t \) stands for thickness of the dielectric coupling foil and \( \varepsilon_r \) is its relative permittivity. The second part of the right side of (2) introduces the correction from the plane to the spherical wave and the last part of (2) represents an approximate correction of the dielectric foil.

Following (1) and (2), it is obvious that with thermal variation undesirable detuning of the Fabry-Perot resonator inevitably occurs. It can subsequently result in a declination of accuracy when evaluating the attenuation coefficient. The theoretically determined dependence of resonant frequency deviation on temperature is depicted in Fig. 1 (dashed line). The change in the temperature by 1 Kelvin causes detuning of the Fabry-Perot resonator by 1.044 MHz. If the Fabry-Perot resonator is heated, the resonant frequency decreases while cooling down the Fabry-Perot resonator results in an increase of the resonant frequency.

Assuming the spectral line has a narrow shape within the measured frequency band (e.g. the acetonitrile spectral line has a half-depth of peak with a width of 2.3 MHz at a frequency of 55.1925 GHz and pressure of 7 µbar), one has to re-measure resonant curve over the band of 20 MHz for each mirror setting of the resonators. This has to be done twice – first for the evacuated resonator to measure the unloaded quality factor and afterwards for the resonator filled with the sample gas. As found during our investigation, the temperature in the resonator’s close vicinity may fluctuate in the range of tenths of a Kelvin. Above all, computers or measurement equipment (microwave generator and spectral analyzer) heat up the ambient air and if they are placed near the resonator, (e.g. due to the short lengths of the microwave cables required), they may cause heating of the resonator body. These issues were verified by long term measurements. Temperature variation was measured every second by four thermal sensors TQS3 (ranging from -55 °C to +125 °C with a resolution of 0.1 °C) placed evenly along the resonator body. First, the resonator was heated and temperature variations as well as the resonant frequency deviations were observed. Then the heater was switched off and the measurement was repeated for a gradual temperature fall. Results of measurement in terms of the influence of frequency deviations on the temperature gradient are depicted in Fig. 1. The dashed line represents an approximation given by the analytical model. The gray solid line introduces the measured data when the Fabry-Perot resonator was heating up. In this case, resonant frequency decreased by 0.979 MHz for 1 K of heating. Contrary to that, resonant frequency increased by 1.04 MHz for 1 K during the cooling of the Fabry-Perot resonator (black solid line).

Since the Fabry-Perot resonator contains mechanical parts and it is impossible to guarantee its constant ambient temperature, the measured characteristics of gas absorption have to be precisely corrected. Therefore, the next part of the paper proposes particular correction schemes based on these measurements.

### 3. Correction of Measured Data

As discussed above, due to the possible thermal influences and mechanical inaccuracies of mirror settings in the Fabry-Perot resonator, resonant frequency deviations can be observed even for the same mirror distances set by remote control for both measurements, with and without gas. In order to reduce this error, the following correction method was proposed. The correction method is primarily based on a determination of the resonant frequency and unloaded quality factor by fitting the theoretical expression of transmission coefficient [4] into the measured data. The theoretical transmission coefficient of radial excited Fabry-Perot resonator can be determined from the following equation
\[ T(\omega) = \frac{1 + Q_0^2 \left( \frac{\omega_0}{\omega} - \frac{\omega}{\omega_0} \right)^2}{(1 + \kappa)^2 + Q_0^2 \left( \frac{\omega_0}{\omega} - \frac{\omega}{\omega_0} \right)^2} \] (3)

where \( Q_0 \) stands for the unloaded quality factor, \( \kappa \) means the coefficient of coupling and \( \omega_0 \) stands for angular frequency.

Afterwards, precise values of coupling coefficients are determined from measured transmission coefficients at the resonant frequencies obtained by the previous step.

Further, the attenuation coefficient is enumerated by

\[ \alpha = \frac{27288}{\lambda Q_0} \left( \frac{\kappa}{\kappa'} - 1 \right) \text{ (dB/km)} \] (4)

where \( \lambda \) is wavelength and, \( \kappa \) and \( \kappa' \) are coupling coefficients without (evacuated) and with the sample gas.

In cases where gases with very low absorption properties were measured (e.g. dibromomethane \( \text{CH}_2\text{Br}_2 \) at 71.856 GHz), a scatter of attenuation coefficient of \( \pm0.2 \text{ dB/km} \) was achieved using this correction method. In this case, the accuracy of the resonator tuning had to be, at most, \( \pm30 \text{ kHz} \). The frequency dependence of the coupling coefficient and the frequency deviation of both measurements under vacuum and with gas (\( \text{CH}_2\text{Br}_2 \)) are depicted in Fig. 2 and Fig. 3, respectively.

The above-mentioned steps of the correction method allow us to find the resonant frequency under both Fabry-Perot resonator states – with gas and without gas. This approach eliminates the error of resonant frequency determination by thermal deviation but only for gases with low attenuation. When the peak of resonant curve is distorted by gas absorption higher than approximately 3 dB/km, a simple measurement of the lowest transmission coefficient cannot be properly utilized to determine the resonant frequency. In the case of high gas absorption rates, when resonant curves with a narrow spectral line have to be measured, the next step follows where resonance curves are reconstructed. This is done by generic fitting of the outer 80 % (obtained from experimental parametric study) of the width of the resonance curve. An illustrative example of such measured characteristics of specific gas (Carbonyl sulfide, OCS) having a high absorption rate at a frequency of 60.814 GHz is demonstrated in Fig. 4. One can clearly distinguish a distortion from the difference between resonances of both measurements – the evacuated and gas-filled resonator.

Measured frequency offset of tuned resonant frequencies (under equally set resonator mirrors) of an OCS gas-filled resonator (pressure of 15 µbar) and evacuated resonator is then shown in Fig. 5.
As can be seen, frequency offsets of up to 300 kHz arose during measurement. These were mainly initiated by variations in the ambient temperature and were fully suppressed by the proposed correction method.

4. Expression of Gas Attenuation Error

When determining the reflection coefficient from measured curves, the frequency deviation $\Delta \omega$ causes an error of the calculated attenuation coefficient by

$$\Delta \alpha = \frac{27288}{\lambda Q_0} \left( \sqrt{\frac{T(\omega_0 - \Delta \omega)}{T(\omega_0)}} - 1 \right). \text{ (dB/km)} \quad (5)$$

This relation is based on a modification of (4), where the coupling coefficients $\kappa$ and $\kappa'$ have been transformed to a deviation of the transmission coefficient $T(\omega_0)$ according to (3). The attenuation error is then given by measured frequency offset $\Delta \omega$. For the sake of precision, the dependence of the attenuation coefficient error (with an unloaded quality factor $Q_0 = 10^5$ and the coupling coefficient $\kappa = 1$) at different resonant frequencies is depicted in Fig. 6. The unloaded quality factor varies in the frequency band 26–80 GHz between $6 \cdot 10^4$ and $1.5 \cdot 10^5$. The attenuation error reaches almost the same range when analyzed in dependence on resonant frequency as well as the unloaded quality factor determined according to (5).

5. Conclusion

Thermal deviations of Fabry-Perot resonator based measurements were investigated in the paper and possible measurement errors were discussed. In cases where the Fabry-Perot resonator is heated or cooled, the resonant frequency drifts towards smaller or higher frequencies, respectively. As was observed, the drift of the resonant frequency of the Fabry-Perot resonator can reach around 1 MHz per 1 K of thermal deviation. This causes substantial errors in the evaluation of the results. The correction method based on fitting a theoretical shape to measured resonant curves has been proposed. As new error determination for gas attenuation measurements dependent on the error of the resonant tuning was derived.

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References


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