Spectra Comparison For An Optical Breathing Gas Sensor Development

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Abstract. This paper describes a preliminary study of the possibility for inhaled and exhaled gases interference during Methyl Mercaptan measurement in the 200 *nm* - 250 *nm* region. An absorption spectrum for Methyl Mercaptan was compared with the breathing system gases absorption lines to theoretically justify that there are no discernible interference effects during the Methyl Mercaptan concentration measurements. It was theoretically found that the primary breathing gases namely nitrogen, oxygen, carbon dioxide and water vapor have no significant interference for Methyl Mercaptan sensing in the 200 *nm* - 250 *nm* region.

INTRODUCTION

Inhaled and exhaled gases are a mixture of gaseous chemical elements and compounds involved in a respiration process (Breathing gases). A research studies toward a breathing gas sensor development can give significant contribution especially in many industries such as medical and health sector. One of the main medical applications for breathing gas sensor development is to detect halitosis. Halitosis or bad breath is normally measured to diagnose dental hygiene in clinical dentistry. The main chemical constituents of oral odorous chemicals are volatile organic compounds such as Methyl Mercaptan CH_3SH [1, 2]. Human beings are sensitive to halitosis in others but unable to assess the halitosis in their own breath. There are many breathing sensors that have been investigated and developed but they are for different kinds of breathing analysis usage. Morisawa and Muto [3] has developed a simple breathing condition sensor to measure humidity in breathing gases. Lewicki et al [4] has developed a breath sensor to detect ammonia due to the presence of bacteria in the stomach.

In this initial investigation of the breathing gases sensor, it is focused on halitosis detection. Breathing sensors for halitosis are also reported and developed previously but they are using different technology such as MEMs and MOS sensor which have their own drawbacks as discussed in previous paper [5]. One of the main disadvantages is that they are not selective to single gas detection alone especially when measuring the gas in the presence of water vapor [6]. Therefore a development of a new breathing sensor that is selective to single gas detection is necessary and can be a great alternative to the current existing commercial sensors. In order to develop a selective breathing sensor, a preliminary study on the gas interference must be carried out. In this paper, the absorption spectrum of the Methyl Mercaptan gas is theoretically compared with a few common inhaled and exhaled gases.

THEORY

Different gas species absorb light at different characteristic wavelengths and for Methyl Mercaptan gas, it has its own specific gas absorption spectrum. A comprehensive collection of absorption cross sections for most common atmospheric gases molecules can be accessed from the Max Planck Institute, MPI Mainz UV-VIS database [7]. The data from this database [6] vary from source to source and they depend on

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temperature and wavelength range. Two examples of Methyl Mercaptan gas absorption spectra reported by McMillan (1996) [7] and Vaghjiani (1993) [8] are shown in Figure 1.

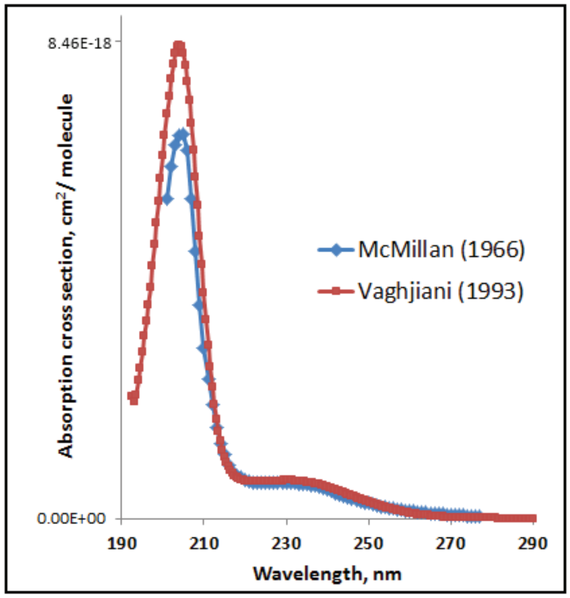

FIGURE 1: Absorption cross section for CH_3SH in the UV region

As can be seen from Figure 1, the general shape of Methyl Mercaptan gas absorption spectra are the same except for the peak values located at around 203 nm which have different height. This is a normal phenomenon and has been explained earlier in a PhD thesis [9]. Furthermore, the small difference in theoretical peak height does not offer major contribution in cross sensitivity effect within the tested gases as demonstrated in previous report [10].

In cross sensitivity studies, the absorption spectra observation is focused on the spectra wavelength overlapping. If any gas spectrum overlaps to another gas spectrum at certain wavelength range, it shows that these two gases absorb the light within the same particular wavelength range. Hence cross sensitivity among these two gases is said to be occurred at that specific wavelength range. The overlapping spectrum comparison method for interference study in this investigation is a common method and used in many research projects [11-13]. Apparently this initial cross sensitivity studies method is important and useful to determine absorption wavelength in the development of a new optical breathing sensor. This is to avoid any cross sensitivity issue with surrounding gases existing within the system.

The theoretical absorption cross section reported by McMillan (1996) [7] and Vaghjiani (1993) [8] shows that Methyl Mercaptan gas absorbs light within the wavelength range of 190 nm to 250 nm. However the interference study for the Methyl Mercaptan gas with a few relevant inhaled and exhaled gases is restricted to 200 nm - 210 nm wavelength range as the gas absorption spectrum has an excellent peak at 203.5 nm. Hence this peak wavelength is a potential point and will be selected for detection of Methyl Mercaptan gas in the UV region for this breathing sensor development. Therefore the cross sensitivity studies must focus on this wavelength range of (200 nm - 210 nm) for any gas interference observation and testing.

ANALYSIS

In this preliminary research, the cross sensitivity study is made between Methyl Mercaptan gas and the main composition of breathing (inhaled and exhaled) gases. The main components of breathing gases are nitrogen, oxygen, carbon dioxide and water vapor and their percentage are shown in Figure 2. Human breath also contains volatile organic compounds (VOCs) and their percentage varies depending on situations and human activities. These compounds consist of methanol, isoprene, acetone, ethanol and other alcohols. Since there are many types of VOCs and the amount of these gases vary and are relatively small, their impact on cross sensitivity can be ignored. Therefore, this investigation is limited to the cross-sensitivity assessment of Methyl Mercaptan gas with nitrogen, oxygen, carbon dioxide and water vapor.

	Inhaled (%)	Exhaled (%)
Nitrogen	**78**	**78**
Oxygen	**20.9**	**16**
Carbon Dioxide	**0.04**	**4**
Water Vapor	**0.1**	**1.04**
Others	**0.96**	**0.96**

FIGURE 2: Composition of breathing gases [14]

Interference with unrelated measurand in a rich environment when performing a gas concentration measurement can reduce the reliability of the developed sensor. Since the interference problems can affect the accuracy of the measurement, different approaches have been employed to overcome this problem, such as using gas separation techniques [15-16] or a ratio calculation [17]. In this paper, the interference possibility with the three main components of breathing gas which are oxygen, carbon dioxide and water vapor is investigated and discussed. The absorption data for these three breathing gases and Methyl Mercaptan gas absorption spectra are obtained from the MPI Mainz UV-VIS database [18]. However there is no data available for nitrogen in the wavelength range of 190 nm - 250 nm in the database 018] and therefore it is assumed that this gas does not absorb any UV light in the wavelength range (190 nm - 250 nm).

The absorption spectra for oxygen, carbon dioxide and water vapor are plotted and compared with the Methyl Mercaptan gas spectrum in the 190 nm - 250 nm region. Based on the absorption spectra comparison shown in Figure 3, the absorption amount for oxygen is relatively small compared to Methyl Mercaptan spectrum in the 190 nm - 250 nm region and it can be considered as zero and negligible. This means that oxygen does not absorb light relative to Methyl Mercaptan in this wavelength region. Hence, this will be a good potential band to select an absorption point for Methyl Mercaptan measurement in the UV region since there will be no interference effect with oxygen.

On top of that, carbon dioxide and water vapor also display the same results as the absorption at that particular band is relatively small compared to Methyl Mercaptan. Based on Figure 3 it is difficult to see the absorption amount for oxygen, carbon dioxide and water vapor because these three lines are overlapping to each other. Therefore, for absorption spectra comparison purpose, logarithmic value (log10 X) has been introduced to the vertical axis of the graph as shown in Figure 4. Subsequently the curves for all absorption spectra have transformed and the degree of absorption for oxygen, carbon dioxide and water vapor can be easily distinguished.

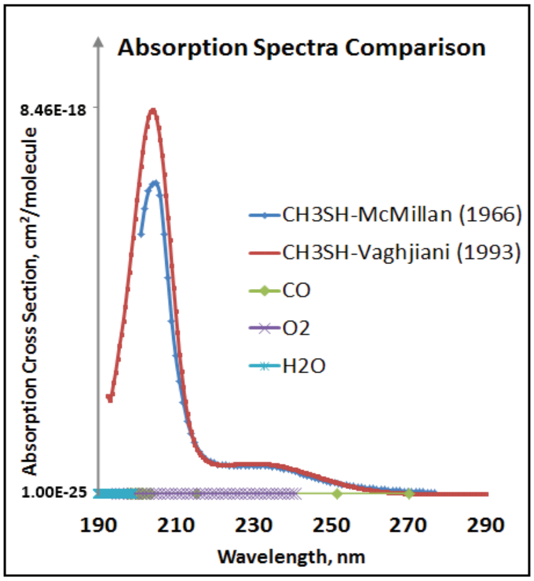

FIGURE 3: Absorption comparison with CO_2, O_2 and H_2O gas

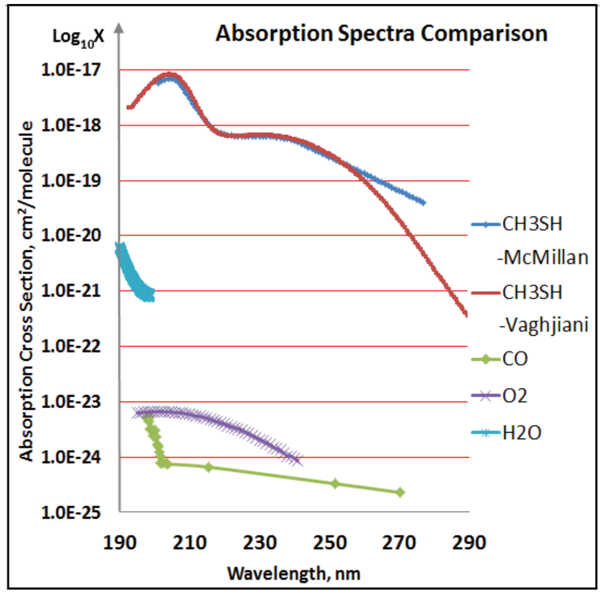

FIGURE 4: Logarithmic values for absorption cross section

Based on the clearly seen curves in Figure 5, the absorption line for water vapor only exists from 190 nm – 199 nm. This is because absorption data is not available for water vapor from 200 nm – 250 nm particularly at the same temperature (298K). To the best of our knowledge, there is no previous works to measure water vapor absorption cross section in the region of 200 nm to 250 nm. Although research [19] has been done to determine the spectrum for water molecule in the region of 190 nm to 250 nm, it is only for high temperature which is from 1000 to 3700 K.

It has been reported by H. Okabe et al [20], water vapor absorption cross section becomes appreciable only in the UV region lower than 190 nm. It is also reported in the UVACS database, that water vapor spectrum only exists in the range 120-189 nm and 260-330 nm [21]. This justifies our assumption above that water does not absorb the UV light (relative to Methyl Mercaptan) within 200-250 nm region. Therefore by measuring Methyl Mercaptan gas in the UV region mainly around this band can overcome interference with water vapor. Hence the future developed sensor is expected to carry out better measurement accuracy and provide more advantages relative to the sensor with different absorption bands such as infrared.

Based on Figure 4, it can be clearly seen that these three main breathing gases do not significantly absorb any UV light relative to Methyl Mercaptan in the wavelength region of 190 nm to 250 nm. Therefore it is a clear advantage to measure Methyl Mercaptan absorption cross section within the wavelength region especially at 203 nm, as the peak for Methyl Mercaption absorption is at this point and there are no possible interference issues with the surrounding breathing gases.

CONCLUSIONS AND FUTURE WORK

A preliminary study of the primary human inhaled and exhaled gases interference for Methyl Mercaptan measurement in the wavelength of 200 nm -250 nm range has been described. It is clear that there is no potential interference for Methyl Mercaptan measurement in the presence of the nitrogen, oxygen, carbon dioxide and water vapor. Therefore it is recommended that the Methyl Mercaptan absorption measurement is made at this selected wavelength band to avoid any possible interferences with other elements of breathing gas. Future work will focus on the experimental tests to verify this theoretical breathing gas interference with the Methyl Mercaptan absorption measurement. Subsequently it will be possible to produce a good Methyl Mercaptan sensor with no interference issue with the surrounding breathing gases.

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