

An Ultraviolet Halitosis Detection Using An Open-Path Optical Fibre Based Sensor

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Abstract: This paper provides an overview of the development of the optical fibre based sensor to detect halitosis (bad breath) using an open-path technique. The unique characteristic of each compound which corresponds to their identification allows the open-path technique to be best suited method in measuring gaseous compounds. In this study, the technique is designed to analyze the absorption spectral lines of Methyl Mercaptan gas within the ultraviolet wavelength region. Then, the developed sensor was used in cross sensitivity evaluation between Methyl Mercaptan and other breathing gases such as Oxygen, Carbon Dioxide, and water vapor to confirm the reliability of the sensor. The absorption cross section spectrum of the Methyl Mercaptan which generated from the study almost match up the theory with the potential peak selection at 203.5 nm. The cross sensitivity analysis carried out shows that there are no distinctive interference effects within the wavelength region of 200 nm to 250 nm especially at 203.5 nm absorption peak. Experimental results validate the use of the open-path fibre technique in a halitosis sensor within the selected ultraviolet region.

Keywords: Fibre optics, Halitosis, Methyl Mercaptan, Sensor

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I INTRODUCTION

Halitosis or bad breath, which is one type of oral malodor indicate foul smells emanating from the mouth. Halitosis comes from the Latin word halitus, meaning breath or exhalation, combined with the Greek suffix, -osis, referring to the state of disease [1]. Originally, the word "halitosis" itself was created as the scientific name of malodor in 1874 by Joseph William Howe [2].

Having halitosis frequently causes embarrassment and affects interpersonal social communication [3]. The so called disease has increasingly come to the forefront of public and dental professional awareness in the early 1990s. The continuous concern of halitosis for both genders and for all age groups acquires them to seek for consultation from dental professionals. Approximately more than 50% of the general populations have halitosis with varying degrees of severity [4].

It was confirmed that 89.8 percent out of 1,687 patients of the cases were due to oral causes. The dorsum of the tongue easily accumulates food debris and dental bacterial plaque [5]. The large surface area of the tongue with its microscopic uneven and papillary structure allows it to become an excellent putrefactive habitat for gram-negative anaerobic bacteria that metabolise proteins as an energy source. The process produce Volatile Sulfur Compounds (VSCs) which are key identifiable gases in bad breath [5]–[8]. In addition, Methyl Mercaptan (CH₃SH) is one of the major odorous VSCs, which are known to be involved in halitosis, periodontal diseases [5], and the predominant causative factor of noticeable oral malodor [9].

Self-diagnosis of halitosis is possible but it is not easy because of the familiarity with the smell from one's own breath [10]. Therefore, certain protocols of assessments and development of sensors were introduced for further detection and evaluation of the halitosis. Halimeter which used the conventional CH₃SH monitoring methods was established but known as an expensive device in the dental field [11], [12]. Following that, biosensors to monitor CH₃SH have been described by Minamide et al., [13], [14]. Then, CH₃SH biosensor coupled with sensitive hydrogen peroxide was developed to get the most sensitive and optimal detection method of H₂O₂ for a CH₃SH amperometric biosensor [15].

However, many breath sensors have been investigated and developed via optics method for they are more stable and better for various kind of breath analysis usage. A simple breathing condition sensor to measure humidity in breathing gases has been introduced by Morisawa et al. [16]. Few years later, Lewicki et al. [17] has developed breath sensor to detect ammonia due to the presence of bacteria in the stomach. Optical breath sensors designed for halitosis are also reported and developed previously using technique of integration between Micro Electro Mechanical System (MEMS) and Complementary Metal-Oxide Semiconductor (CMOS) [18].

The CMOS-MEMS fabrication technology is a relatively low in cost but the primary drawback of CMOS-MEMS is the inability to optimize the mechanical properties of the micro-structures, which can limit the

performance of certain devices. Therefore, development of this new optical breath sensor which is low in cost and more sensitive could be an interesting option to halitosis monitoring methods in the dental field.

II METHODOLOGY

Open-path technique is one of the most common methods in gas detection using the spectroscopic principles for the optical fibre sensor. This technique is widely used because it allows a significant proportion of the light sensed by the detector interacted with the test gas and it is capable to simultaneously detect different gas substances in mixture at real time. Open-path technique for this optical sensor is the open-path absorption sensor that is designed to monitor the absorption spectral lines of CH_3SH and then evaluate the cross sensitivity of CH_3SH with other breathing gases such as oxygen (O_2), carbon dioxide (CO_2) and water vapor (H_2O). The technique is best suited to measure gaseous compounds because of the unique characteristic of each compound that allowed their identification.

In the development of the sensor, the optical fibre is one of the main players. Theoretically, light travels in straight lines and reflecting off headed obstacles. But, optical fibres allow light to travel in any direction and bending around corners. Optical fibres are capable of carrying more information over longer distances. A single mode optical fibre can transmit trillions of bits per second when the signals are wavelength multiplexed.

The experimental setup is shown in Fig. 1. Ultraviolet (UV) light source used was the DH-2000 from Ocean Optics which was a Deuterium-Halogen lamp. Type of fibre used to transmit the light from the light source was a 600 μm core size Optran UVNS, UV Non Solarising. Two collimating lens were placed at both ends of the gas cell which approximately 1 cm in diameter and 54 cm long. The lenses were used to focus the incident and transmitted light. Next, the transmitted light was then passed through another optical fibre at the other end of the gas cell to the light detector. Maya2000 spectrometer from Ocean Optics was used as the light detector. The spectrometer which provides resolution to 0.65 nm (FWHM) has from 190 to 1100 nm range was connected to the computer with Spectrasuite software installed. Ocean Optics developed the software for the benefit of the users to have data acquisition from the spectrometer and able to perform data processing of the initial and transmitted intensity of the analysed gas.

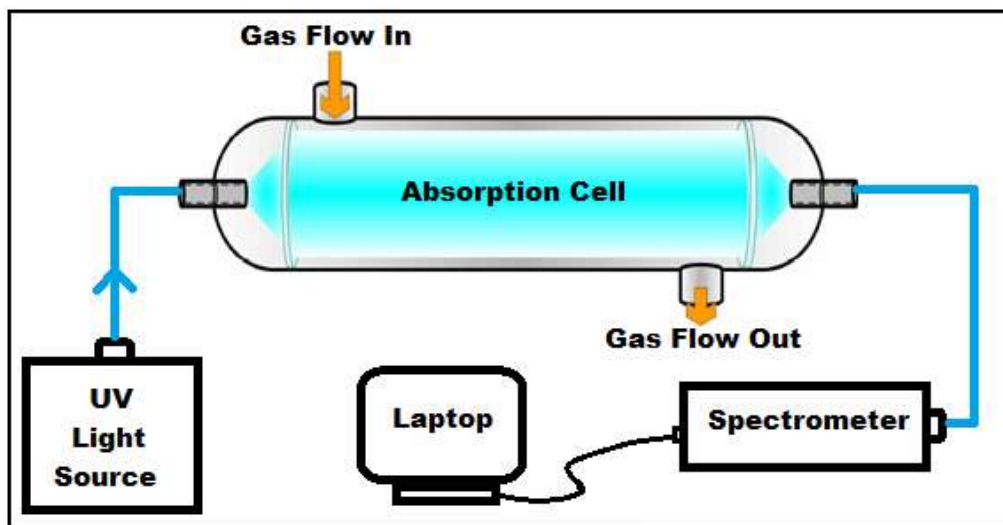


Figure 1: Generic design of the halitosis sensor.

The experimental setup was used to obtain the CH_3SH absorption spectrum. The absorption spectrum is unique for each gas because different gas species absorb light at different characteristic wavelength. In order to calculate the absorption cross section for CH_3SH , the Beer-Lambert Law has been utilized. It described the linear relationship between absorbance and concentration of an absorbing species and featured a general equation as shown in (1) below:

$$\frac{I}{I_o} = e^{(-\sigma.N.I)} \quad (1)$$

Where I is the transmitted intensity, I_0 is the incident intensity, l (cm) is the distance that light travels through the gas, σ ($cm^2/Molecule$) is the absorption cross section and N ($Molecules/cm^3$) is the gas concentration. Equation (1) then derived as been reported in previous paper [19] to get equation (2) as shown below:

$$\sigma = \frac{-[\ln \frac{I}{I_0}][24.4]}{ppm \times N_A \times l \times 10^{-9}} \quad (2)$$

Following the setup, nitrogen (N_2) gas was released to neutralize the absorption cell and initial intensity recorded as reference. Then, 100 ppm CH_3SH gas was released and the data recorded as transmitted intensity. Using (2), we can accurately calculate the absorption cross section of CH_3SH from both readings.

In this study, cross sensitivity testing method is significantly crucial in deciding the choice of absorption wavelength region for the sensor. It is to ensure that the developed halitosis sensor is sturdy and reliable for usage [20]. For that reason, the same experimental setup was used to further investigate the possibility of any interference between CH_3SH and the breathing gases. N_2 , O_2 , CO_2 and H_2O are the main players of the air that we breathe in and out as the gas composition is shown in Fig. 2.

| Breathing Gas | Inhaled (%) | Exhaled (%) |
|------------------------|-------------|-------------|
| Nitrogen, N_2 | 78 | 78 |
| Oxygen, O_2 | 20.9 | 16 |
| Carbon Dioxide, CO_2 | 0.04 | 4 |
| Water Vapor, H_2O | 0.1 | 1.04 |
| Others | 0.96 | 0.96 |

Figure 2: The composition of Breathing Gases [21].

Cross sensitivity with N_2 is not an issue as reports [22], [23] shows that there is no absorption due to N_2 in the UV region. Thus, the investigation is focus towards the cross sensitivity assessment of CH_3SH with O_2 and CO_2 . Subsequently, the two main breathing gases O_2 and CO_2 were chosen for the cross sensitivity testing using the developed sensor.

Additionally, cross sensitivity issue with H_2O is negligible because from previous studies based on the Max Planck Institute, MPI Mainz UV-VIS [24] as featured in Fig. 3, shown non-existence of absorption spectra for H_2O in the wavelength region of 200 nm to 250 nm for selected temperature of 298K. The absorption spectra of H_2O featured are for the wavelength region of 180 nm to 200 nm. Furthermore, it has been reported that H_2O absorption cross section in the UV region is only appreciable for wavelength range which is lower than 190 nm [25].

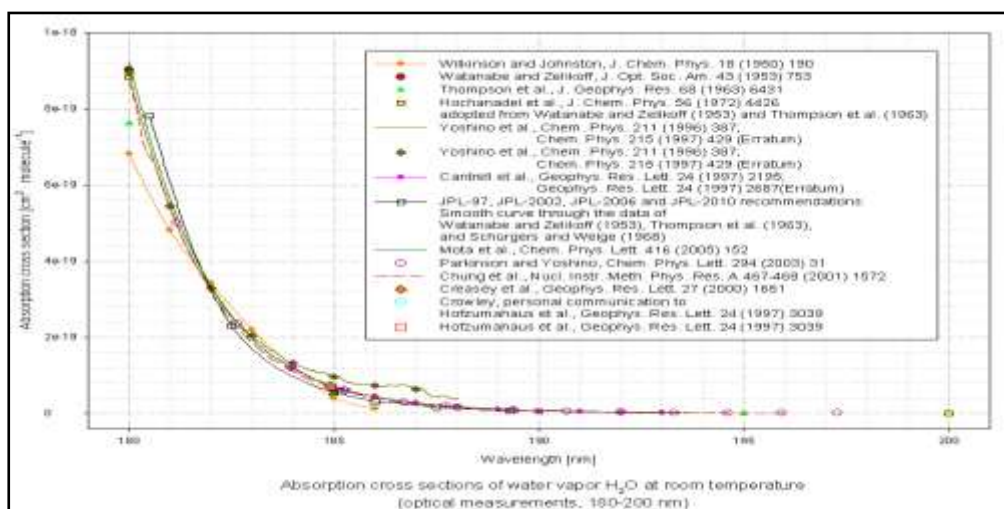


Figure 3: Absorption cross sections of water vapor, H_2O for various studies

III RESULTS AND DISCUSSIONS

The spectrum of the CH_3SH gas graph was plotted using a spreadsheet and compared with the theory as shown in Figure 4. The database of Max Planck Institute, MPI Mainz UV-VIS [24] used to get examples of

CH₃SH gas absorption spectra for comparison purpose thus used them as the theoretical data. The database comprises of data sets from different sources and each of them depends on different choice of temperature and wavelength range [26]. Two data sets of CH₃SH gas absorption spectra [27], [28] which have almost similar temperature and wavelength range as the experiment are taken from the database and plotted as shown in Fig. 4. McMillan's reported data used temperature of 298 K within wavelength region of 201 nm to 277 nm and Vaghjiani's work covered broader wavelength range of 192.5 nm to 309.5 nm with gas temperature of 296 K.

As observed in Figure 4, both plotted data sets from the database showed the same formation as the experimental result. There is similarity in the general shape of all three CH₃SH gas absorption spectra but have different height for the peak. The peaks which located at around 203 nm to 204 nm showed three different values. The value from the experimental data is lower than both theoretical data sets from the database. This condition is acceptable and considered normal. There were quite a number of reasons for this to happen. Firstly, the slight difference of the peaks values might resulted from the difference in gas temperature [29]. It was observed that there was a significant temperature effect for the UV absorption particularly at the peaks. Another reason would be the usage of different light sources [30], [31].

Nevertheless, the result showed that the experimental CH₃SH absorption spectral is uniquely in good agreement with the theoretical data sets for the selected wavelength region of 200 nm to 250 nm. Accordingly, the open-path fibre based sensor developed earlier is appropriate to be used for the test gas detection.

In this experiment where cross sensitivity is concern, the absorption spectrum of CH₃SH is observed to determine whether or not the spectra wavelength is overlapping with other breathing gases. Since, in the case of any gases show the overlapping pattern with each other, these gases actually absorb lights within that certain wavelength region and the cross sensitivity occurs. Therefore, the assessment of possible cross sensitivity among the gases was carried out as plotted in Fig. 5. In order to validate the negligible cross sensitivity issue with H₂O, data from one of the studies [32] were taken from the MPI Mainz UV-VIS, plotted and used for the comprehensive interference investigation.

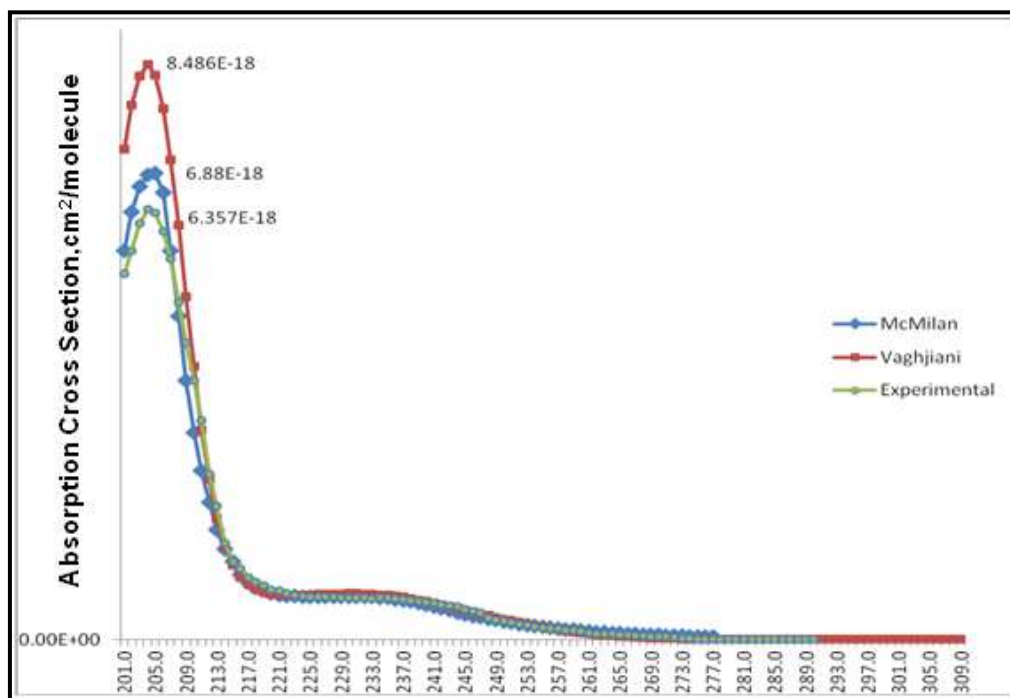


Figure 4: Comparison of absorption cross section for CH₃SH in the UV region

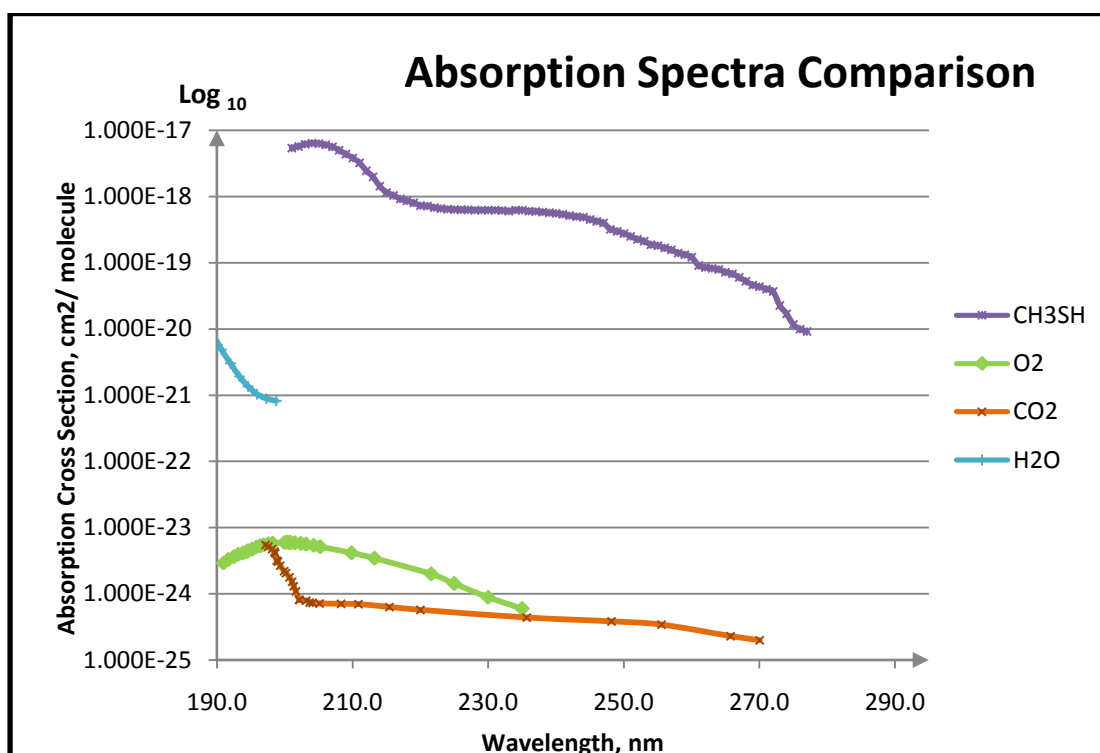


Figure 5: Absorption spectra comparison of CH₃SH with the breathing gases

These so called spectrum comparison method which intended for interference observation was regularly used in several previous studies [33]–[35]. Particularly for absorption spectra comparison purpose, logarithmic value ($\log_{10} X$) has been introduced to the vertical axis of the graph. As a result, the degree of absorption for O₂, CO₂ and H₂O can be clearly distinguished. Obviously from Fig. 5, the absorption amount for O₂, CO₂ and H₂O is comparatively small compared to CH₃SH spectrum and it can be considered as zero and negligible. It means that these breathing gases do not absorb light within the same wavelength region as CH₃SH gas. In addition, this interference study also was restricted to 200 nm to 210 nm wavelength region where the excellent peak of CH₃SH was located at 203.5 nm and as clearly seen, cross sensitivity was not at all an issue. Therefore, this will be a good potential band which was best selected as an absorption point for the development of the halitosis sensor.

IV CONCLUSION

The optical fibre sensor developed using the open-path technique managed to detect the existence of CH₃SH within the selected UV wavelength region. Hence, it was suitable for halitosis detection and be considered as a reliable and sturdy optical breathing sensor. However, CH₃SH is the only VSCs which was evaluated in this study. So, this work can be extended with the usage of other VSCs such as hydrogen sulphide and dimethyl sulphide.

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