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Research paper

A potential development of breathing gas sensor using an open path fibre technique

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ABSTRACT

This paper describes a potential development of methyl mercaptan or bad breathing gas measurement in the 200 nm–250 nm region. Methyl mercaptan shows a potential peak selection at 204 nm and the absorption cross section spectrum display a similar pattern with the theory. A cross sensitivity analysis is also reported and it shows that there are no discernible interference effects between the methyl mercaptan gas with other breathing gases such as carbon dioxide, oxygen and water vapor at 204 nm.

1. Introduction

Breathing gas is a mixture of gaseous chemical elements and compounds involved in a respiration process (inhaled and exhaled gases). A research and development of breathing gas sensor can give a significant contribution especially in medical industry. 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 CH3SH [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] have developed a simple breathing condition sensor to measure humidity in breathing gases. Lewicki et al. [4] have developed a breath sensor to detect ammonia due to the presence of bacteria in the stomach.

In this initial investigation of the breathing gas sensor, it is focused on methyl mercaptan detection. Breathing sensors for halitosis are also reported and developed previously but they are using different technologies such as MEMs and MOS sensor which have their own drawbacks as discussed in a 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 methyl mercaptan gas must be carried out. In this paper, the absorption cross section spectrum of the methyl mercaptan gas in the ultraviolet region is reported.

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 [7–8] or a ratio calculation [9]. In this paper, the interference possibility with the main components of breathing gas which are oxygen, carbon dioxide and water vapor is investigated and discussed.

2. 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 gas molecules can be accessed from the Max Planck Institute, MPI Mainz UV–VIS database [10]. The data from this database vary from source to source and they depend on temperature and wavelength range. Two examples of methyl mercaptan gas absorption spectra as reported by McMillan [11] and Vaghjiani [12] are shown in Fig. 3.

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For absorption spectrum comparison with the theoretical data is shown in Fig. 3, the Beer-Lambert Law has been utilised. The Beer-Lambert law described the linear relationship between absorbance and concentration of an absorbing species and its general form is shown in Eq. (1).

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

where I is the transmitted intensity, I_o 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.

In order to calculate the absorption cross section for methyl mercaptan, Eq. (1) is derived and a variation of the Beer-Lambert Law is given by Eq. (2). The details of the derivation have been reported in a previous paper [13].

$$\sigma = \frac{-\left[\ln \frac{I}{I_o}\right][24.4]}{\text{ppm} \times N_A \times l \times 10^{-9}} \tag{2}$$

Using Eq. (2), we can accurately calculate that the absorption cross section with gas concentration (ppm) is known. This method of gas absorption cross section calculation was similarly described in [14–15].

In cross sensitivity studies, the absorption spectraum observations are focused on the spectra wavelength overlapping. If any gas spectrum overlaps to another gas spectrum at a 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 have 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 [16–18]. Apparently this initial cross sensitivity study 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.

In this 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 Fig. 1.

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 amounts 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

Fig. 1. Composition of breathing gases [19].

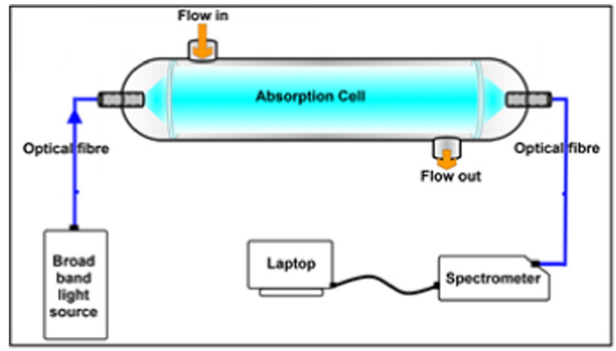

Fig. 2. Generic design of an optical breathing sensor.

3. Experimental setup

The schematic experimental arrangement is shown in Fig. 2. A Deuterium-Halogen lamp (DH-2000 from Ocean Optics) was used as a light source. The light was transmitted through a fibre (Optran UVNS, Ultra Violet Non-Solarising) with 600 μm core size. Two collimating lens were placed at both ends of the gas cell and were used to focus the incident and transmitted light. The diameter and the length of the gas cell are approximately 1 cm and 54 cm respectively. The transmitted light then travel through another optical fibre at the other end of the test gas cell to the light detector. The light detector used in this experiment was *Maya2000* spectrometer from Ocean Optics. The spectrometer has a range from 190 to 1100 nm and it provides resolution to 0.65 nm (FWHM). The spectrometer was connected to the computer with Spectrasuite software installed. This is a specifically designed program developed by Ocean Optics in order to have data acquisition from the spectrometer. It also can perform some data processing so that the initial and transmitted intensity of the analysed gas present can be output to the user.

4. Results and analysis

Initially, nitrogen gas was released in the gas cell to clear any present gases and initial intensity was recorded. It was followed by releasing 100 ppm methyl mercaptan gas and the data was captured as transmitted intensity. The carrier for methyl mercaptan gas is nitrogen which has no effect on cross sensitivity. Furthermore, the absorption value is negated when initial intensity was recorded where the test cell was filled by nitrogen gas. The flowrate for both gases is not a major concern in this setup since this is not a concentration measurement process. Moreover, it has been reported that the gas flowrate does not give any effect in absorption cross section measurement. [20]. Based on both reading, the absorption cross section of methyl mercaptan can be calculated using an Eq. (2). The spectrum of the methyl mercaptan gas graph

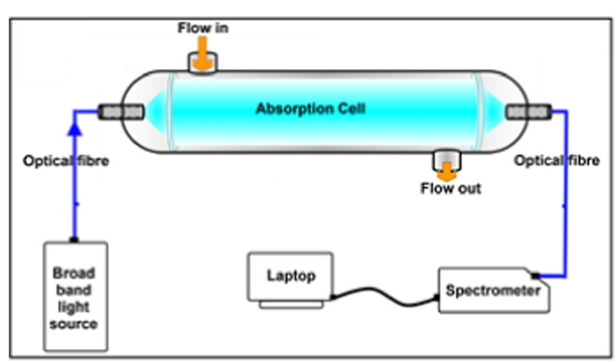

Fig. 3. Comparison between measured and theoretical absorption spectrum of methyl mercaptan.