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Simulation of Absorption Cross Section: A Preliminary Study of Infrared Absorption Spectroscopy for Sulfur Dioxide Gas Measurement

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Abstract

Sulfur dioxide (SO_2), an unpleasant-smelling toxic gas, is among the six common air pollutants. These gases, particularly Sulfur Dioxide, are released through the combustion of fossil fuels or other materials containing sulfur. This gas can react with other substances in the atmosphere, forming tiny particles that may enter the lungs and lead to similar adverse health effects. Previously, it has been reported that the development of sulfur dioxide gas sensor such as semiconductor, electrochemical, and others show a long response time compared to absorption spectroscopy-based sensor. Thus, the aim of this project is detection of sulfur dioxide using absorption spectroscopy technique in the infrared region. Initially, the infrared region's absorption cross-section of sulfur dioxide was simulated using the Spectralcalc.com® simulator. The validity of the simulation results was established by comparing them to previous research. The deviation of less than 1% was obtained for the value of absorption cross section. Thus, it indicates the suitability of the Spectralcalc.com® simulator for obtaining the value of absorption cross section in the infrared region. Then, simulations were conducted to analyze the effects of pressure on the absorption cross-section, ranging from 800 mbar to 1200 mbar. According to the simulation, the wavelength at 1412 cm^{-1} exhibited minimal pressure effect, making it conducive for accurate sulfur dioxide concentration calculation.

1. Introduction

During 1733–1804, sulfur dioxide (SO_2) was first studied in detail by English physicist and chemist Joseph Priestly. Also, the ancient Greeks and Romans disinfected their homes by burning sulfur [5]. Disease-causing and rotting microorganisms were eradicated by the sulfur dioxide. Nowadays, Sulfur Dioxide (SO_2) is known as a major source of air pollution in Malaysia. Malaysia's air pollution issues are also significantly exacerbated by the country's rapid urbanisation, economic growth, and other socioeconomic activities. The data provided by the Acid Deposition Monitoring Network in East Asia states that power plants generated 41% of the sulfur dioxide emissions, followed by industry (23%), transportation (16%), and other sources (2%) [3]. In terms of the Air Quality Index, the majority of the time, air quality in Malaysia is good to moderate, with the exception of seasonal pollution episodes influenced by meteorology and transboundary impacts. Sulfur dioxide (SO_2) is an inorganic compound and a heavy, colourless, poisonous gas [7]. Natural volcanic activity and the combustion of fossil fuels are the primary sources of sulfur dioxide emissions. Human, animal, and plant health are all at risk from this gas. The chemical compound of sulfur dioxide is SO_2, formed by the formation of one atom of sulfur and two atoms of oxygen. The common element sulfur (S) is burned to produce sulfur dioxide (SO_2). Furthermore, sulfur dioxide is used as a bleach, disinfectant, refrigerant, reducing agent, and food preservative, especially in the preservation of dried fruits. Exposure to sulfur dioxide can occur through skin contact or inhalation of ambient air. Individuals residing in proximity to industrial sources may encounter sulfur dioxide on a daily basis. Occupations in industries involved in the generation of sulfur dioxide, such as copper smelting, power plants, and facilities producing sulfuric acid, paper, food preservatives, and fertilizers, are more likely to result in exposure of sulfur dioxide. Prolonged exposure to sulfur dioxide is linked to higher overall mortality rates and increase hospitalization rates for cardiac diseases.

2. Principle of Measurement

According to the Beer-Lambert law, the properties of the medium through which light is travelling affect how much light is attenuated. In spectroscopy, the Beer-Lambert law is a principle that explains the absorption of radiant energy by an absorbing substance. Beer's Law asserts that the absorbance of light in a sample or solution is directly proportional to the concentration of the solution through which the light passes [6].The formula of absorption cross section, (σ) [4]:

$$\sigma = -\frac{1000000RT}{c_{(ppm)}N_A Pl}\ln\left(\frac{I}{I_0}\right) \tag{1}$$

Rearranging equation (1), the equation for gas concentration in ppm is:

$$c_{(ppm)} = -\frac{1000000RT}{\sigma N_A Pl}\ln\left(\frac{I}{I_0}\right) \tag{2}$$

$c_{(ppm)}$ is concentration of gas in ppm
R is gas constant, 8.205746 x 10^{-5} atm m^3 $mol^{-1}K^{-1}$
T is temperature in K
σ is absorption cross section of sample in m^2 $molecule^{-1}$
N_A is Avogadro number, 6.023 x 1023 molecule mol^{-1}
P is pressure of gas in atm
l is path length in m
I is intensity after the light passed through the sample
I_o is intensity before the light passed through the sample

Using Equation (1), the absorption cross-section of sulfur dioxide can be determined by considering various relevant parameters Furthermore, Equation (2) allows for the determination of sulfur dioxide concentration by rearranging the Equation (1). This Equation (2) establishes a relationship among the sulfur dioxide absorption cross-section (σ), temperature (T), pressure (P), gas cell path length (l), and transmittance (I/I_0). Importantly, these parameters can be measured in real-time. Consequently, the real-time calculation of the sulfur dioxide absorption cross-section becomes achievable through the utilization of these parameters.

2.1 Absorption Spectrum

Absorption spectroscopy in the infrared (IR) region, commonly referred to as infrared absorption spectroscopy or IR spectroscopy, is a technique used to analyze the interaction between infrared radiation and matter. It offers valuable insights into the molecular composition, functional groups, and chemical bonds found in a sample. In infrared spectroscopy, a sample is exposed to a beam of infrared light, and the absorption of light at specific wavelengths is subsequently measured. The sample absorbs certain wavelengths of infrared light, resulting in characteristic absorption patterns or spectra. These absorption patterns arise from the excitation of molecular vibrations, such as stretching, bending, and rotational motions of chemical bonds within the sample. The absorption frequencies are commonly expressed in wavenumbers, which are the reciprocal of the wavelength of light (usually in cm^{-1}). Higher wavenumbers correspond to shorter wavelengths and higher

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energy infrared radiation. Light absorption in the infrared (IR) region involves the interaction between infrared radiation and matter. The infrared (IR) region encompasses wavelengths that are longer than those of visible light, typically ranging from around 700 nanometers (nm) to 1 millimeter (mm) [8]. The spectrum provides valuable information about the specific vibrational modes present in the sample and can be used for qualitative and quantitative analysis.

3. Simulation Methodology

This project aims to facilitate research in identifying the wavelength range of sulfur dioxide and designing sulfur dioxide gas sensors within the infrared region. The designed sensors will be implemented in the Spectralcalc.com simulator. Consequently, the project will exclusively undergo development through software simulation, and the details of the results will be elaborated upon.

3.1 Simulation Setting for Determination of Sulfur Dioxide Absorption Cross Section

In the beginning, the gas cell simulator on Spectralcalc.com is employed to simulate sulfur dioxide absorption wavelengths. This initial simulation serves as the main exploration to acquire data on sulfur dioxide absorption cross-section, particularly in the infrared region. Equation (2) emphasizes the importance of the sulfur dioxide absorption cross-section as important parameter for precise sulfur dioxide concentration calculations. In this context, the computation of output transmittance is selected for the wavelength range from 1298 cm^{-1} to 1412 cm^{-1}, which corresponds to the region of interest for sulfur dioxide absorption in the infrared region [1].

Table 1 *List of Inputs to be set in observer tab and gas cell tab to simulate sulfur dioxide spectrum [1]*

Tab	Input parameter	Value
Observer	i. Compute	Transmittance
	ii. Waveband	1298 cm^{-1} - 1412 cm^{-1}
Gas cell	i. No. of gases	1
	ii. Line list	HITRAN2020
	iii. No. of cell	1
	iv. Path length	560cm (5.6m)
	v. Pressure	1013.25 mbar (1 atm)
	vi. Temperature	623.15 K
	vii. Gas type	Sulfur Dioxide (SO_2)
	viii. Concentration	100 ppm (VMM = 0.0001)

3.2 Simulation Setting for Analysis of Pressure Effect

The investigation of how changes in pressure affect the spectroscopic characteristics and behaviors of a sample is termed the analysis of pressure effects in spectroscopy. Equation (1) establishes a relationship between absorption cross section (σ) and pressure, as well as temperature. In this project, the pressure is constrained to the range of 800 to 1200 mbar, specifically relevant to sulfur dioxide gas sensors used for detecting emissions in the industrial sector. Nevertheless, the values of other parameters remain constant, only the pressure range is modified. The goal is to ascertain absorption cross section (σ) at wavelengths with minimal pressure dependence, as obtaining accurate concentration values is important.

4. Results and Discussions

The simulation is performed using the Spectralcalc.com® gas cell simulator, focusing on precisely determining the concentration of sulfur dioxide gas by investigating the effect of temperature and pressure in the infrared region. To expand the scope of sulfur dioxide concentration, the process begins with theoretical calculations and simulations using Beer's law and the Spectralcalc.com® gas cell simulator. This setup enables the accurate simulation of sulfur dioxide gas concentration for the detection of gas emissions.

4.1 Validation of Simulation Result for Sulfur Dioxide Absorption Cross Section in Infrared Region

The assessed wavelength range for the absorption cross-section of sulfur dioxide in the infrared region is from 1298 cm^{-1} to 1412 cm^{-1}. The simulation results are compared with previous experimental work to evaluate the effectiveness of the Spectralcalc.com® gas cell simulator in determining the absorption cross-section for sulfur dioxide. Figure 1 exhibits a pattern that closely resembles the experimental results, consistent with previous research conducted by previous research [1]. The alignment in patterns between simulation and experimentation suggests a high degree of accuracy and reliability in the simulated data.

The simulation results for sulfur dioxide are presented in Figure 1, depicting (1-transmittance) vs. wavelength (cm^{-1}). Comparison the sulfur dioxide absorption cross-section results obtained with the Spectralcalc.com® gas cell simulator to those of earlier research [1] reveals a similar trend. This comparison is important because the wavelength at which sulfur dioxide absorbs plays a vital role in accurately determining its concentration. The concentration of sulfur dioxide is dependent on transmittance (I/I_o), as defined by Equation (2). Hence, the subsequent analysis will utilize the transmittance graph in Figure 2. Table 2 shows how a comparison is conducted at three wavelengths. The data was provided in previous work [1] at another website [2] that was mention in the original article.

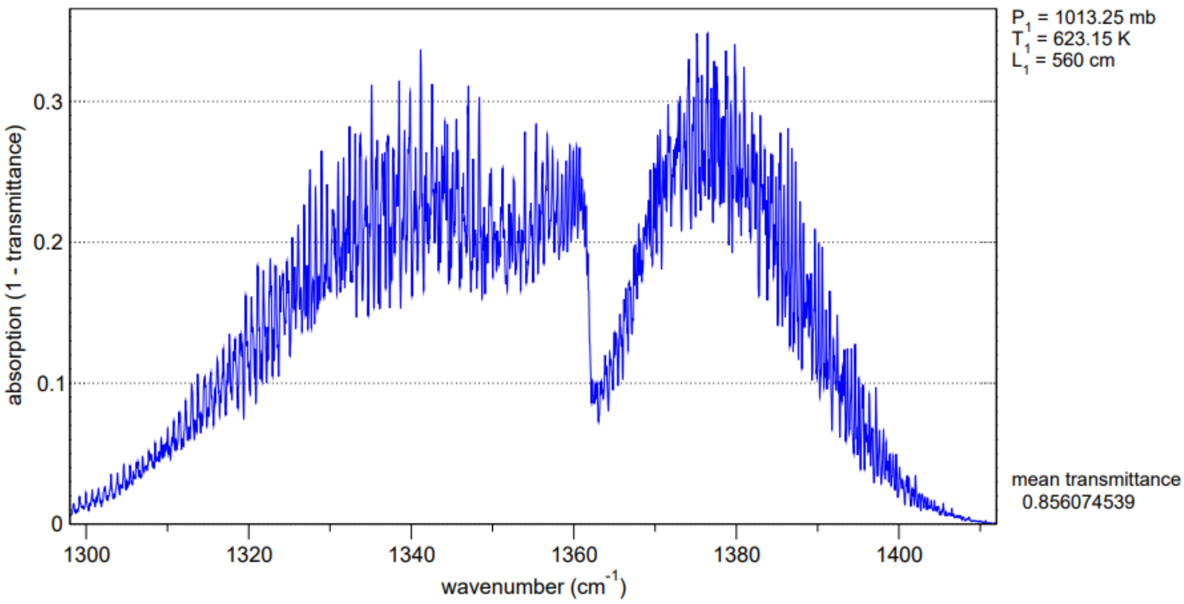

Fig. 1 *Simulation result of absorption sulfur dioxide from 1298 cm^{-1} to 1412 cm^{-1}*

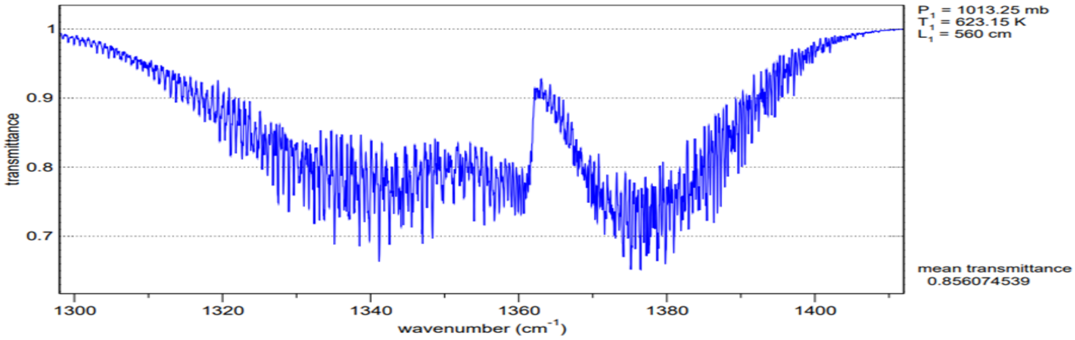

Fig. 2 *Simulation result of transmittance for sulfur dioxide absorption cross section from 1298 cm^{-1} to 1412 cm^{-1}*

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Table 2 *Comparison of sulfur dioxide absorption cross section (σ), Between previous experiment and this simulation work (in unit of cm^2 $moleculce^{-1}$)*

Wavelength previous work (cm^{-1})	Wavelength simulation (cm^{-1})	Previous work [2]	This simulation work
1409.84613	1409.84716	2.12424 x 10^{-25}	2.26036 x 10^{-25}
1409.88673	1409.889477	2.35527 x 10^{-25}	2.47502x 10^{-25}
1411.1007	1411.106069	1.07069 x 10^{-25}	1.12163x 10^{-25}

Table 3 provides a comparative analysis based on differences derived from the data in Table 2. The slight disparities between the values obtained from previous research [1] and the current simulations underscore the promising capabilities of the Spectralcalc.com® gas cell simulator. The Spectralcalc.com® gas cell simulator is well-suited for acquiring the absorption cross-section of sulfur dioxide in the infrared region and for performing additional analysis on spectroscopy gas sensors designed for sulfur dioxide. Since the variation remains below 1%, proceed to the next step, investigating how pressure affects the sulfur dioxide absorption cross-section using the Spectralcalc.com® gas cell simulator. Ensuring accuracy in calculating sulfur dioxide concentration is crucial, and it requires utilizing the exact value for the sulfur dioxide absorption cross-section.

Table 3 *The difference in sulfur dioxide absorption cross section (σ), Between previous experiment and this simulation work*

Wavelength (cm^{-1})	Difference
1409.84	0.06
1409.88	0.04
1411.10	0.04

4.2 Analysis of Pressure Effect

The analysis begins by configuring the simulator's input using the settings outlined in Table 1. However, the pressure is adjusted from 800 mbar to 1200 mbar based on actual gas sensor values. The primary objective of this section is to examine the effect of pressure on the absorption cross-section of sulfur dioxide. In order to achieve this goal, an investigation into the pressure variation from 800 mbar to 1200 mbar is implemented.

Figure 2 illustrates the absorption cross-sectional area for a 100 ppm sulfur dioxide concentration at various pressures, depicting three sensitivity conditions: very sensitive, moderate, and less sensitive to pressure effects. Computed using transmittance output from the simulator at pressures spanning from 800 mbar to 1200 mbar, the graph showcases significant fluctuations in absorption cross section within the 1298 cm^{-1} to 1412 cm^{-1} wavelength range in response to pressure variations. Wavelengths exhibiting high pressure dependence should be avoided in real-world applications, as they may lead to inaccurate predictions of sulfur dioxide gas concentration.

Fig. 2 *Value of absorption cross section due to 100 ppm of sulfur dioxide at various pressure.*

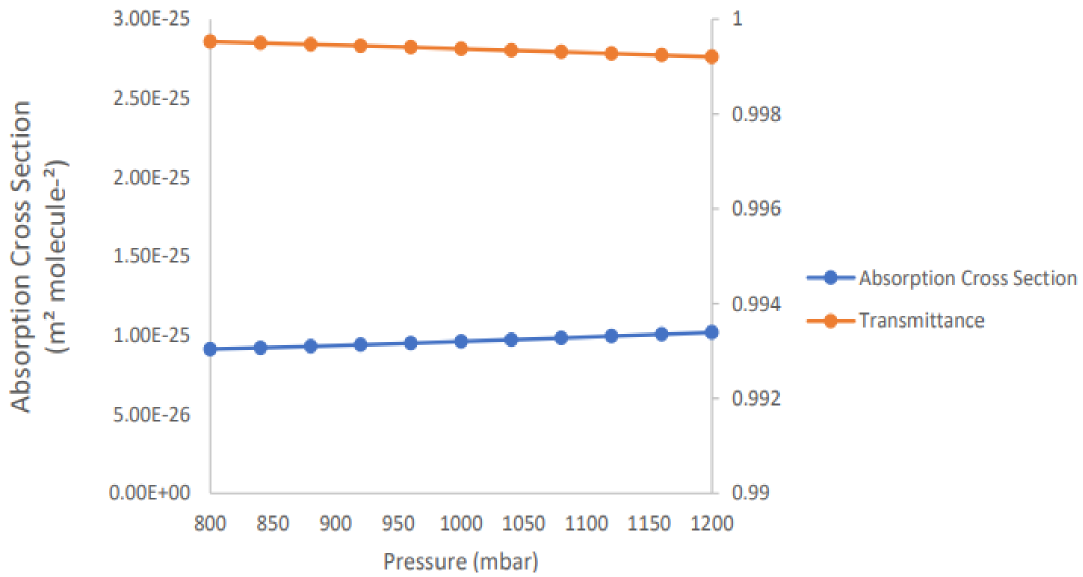

Fig. 3 *Analysis of pressure effect toward sulfur dioxide absorption cross section at 1412 cm^{-1} with output transmittance from Spectralcalc.Com® Gas cell simulator*

Figure 3 illustrates the sulfur dioxide absorption cross-section at a wavelength of 1412 cm^{-1}. Starting at a pressure of 840 mbar, the sulfur dioxide absorption cross-section begins at 9.20 x 10^{-26} m^2 molecule^{-1}, showing a slight decrease as the pressure increases to 1120 mbar at the same wavelength. Simultaneously, an increase in pressure leads to a reduction in transmittance. This observation aligns with Beer's Law, as defined in Equation (1), which assert that higher pressure corresponds to lower transmittance. This may explain the minimal impact on the sulfur dioxide absorption cross-section with the change in pressure from 800 mbar to 323 mbar at the wavelength 1412 cm^{-1}. Therefore, for accurate measurement of sulfur dioxide concentration, it is strongly recommended to consider wavelengths that exhibit less pressure dependence, especially within the pressure range of 800 mbar to 323 mbar, corresponding to the pressure range used by gas sensors. Prioritizing wavelength 1412 cm^{-1} enables precise determination of sulfur dioxide concentration.

5. Conclusion

The majority of sulfur dioxide in the environment is primarily emitted by large industrial facilities such as power plants and oil refineries. Additionally, fires, residential boilers, and automobiles contribute to sulfur dioxide gas emissions in the environment. Sulfur dioxide poisoning can lead to severe health issues and, in rare cases, even death. Numerous industries, including the workplace, are concerned about the risk of sulfur dioxide exposure. Employees may also be exposed to this harmful gas outside the workplace, especially when working in manufacturing. Preventive methods can be applied to control sulfur dioxide exposure. Various control measures can be implemented to reduce people's exposure to sulfur dioxide, but danger may not always be evident. As a result, the absorption spectroscopy method based on the infrared region was successfully utilize to analyse sulfur dioxide concentrations. The goal of this analysis was to ensure worker safety and prevent sulfur dioxide exposure within various industry sectors. The results obtained from the simulation were successfully validated by comparing with previous work [1] shows that the deviation is less than 1%. The validation process demonstrates the Spectralcalc.com® gas cell simulator potential to produce accurate results in determining sulfur dioxide absorption wavelengths in the infrared region. The analysis was extended to investigate how temperature and pressure influence the absorption cross-section of sulfur dioxide. To conduct this experiment, the Spectralcalc.com® gas cell simulator was employed to simulate the effects of temperature and pressure. According to the simulation results, the absorption cross-section of sulfur dioxide at wavelengths of 1412 cm^{-1} exhibited minimal sensitivity to variations in pressure within the ranges of 800 mbar (0.789539 atm) to 1200 mbar (1.18431 atm). These findings suggest that project procedures should consider the specified pressure ranges (800 mbar to 1200 mbar) in light of the observed insensitivity. Including these variables is essential to minimize variations in the absorption cross-section of sulfur dioxide and ensure the accurate measurement of sulfur dioxide concentration in the infrared region.

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Conflict of Interest

The authors declare that there is no conflict of interests regarding the publication of the paper.

Author Contribution

The authors are responsible for the study conception, research design, data collection, data analysis, result interpretation and manuscript drafting.

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