GAS CONCENTRATION MEASUREMENTS OF C_2H_2 USING A CALIBRATION RELATION OF TDLS SPECTROMETER

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ABSTRACT

The work has been demonstrated by varying the wavelength of a tunable DFB laser diode, a Tunable Diode Laser Spectroscopy (TDLS) simulation method employing a sinusoidal signal to enhances the sensitivity of the spectrometer. Since the laser drive current is tuned, altering the current will cause the laser diode's wavelength to shift within the Near Infrared (NIR) tuning range of around 0.02 nm. A set focus value of 0.5 ppm and a fixed open path length (distance between laser source and back reflector) of 100 m were used to evaluate the TDLS's sensitivity. A MATLAB code was written to change the exact wavelength of the near infrared region, and the frequency domain evaluations were taken to extract the value of the second harmonic, which is an indication of the presence of the gas to be detected. The value of wavelength has been found in NIR region of the acetylene was about 1530. 47 nm. It should be noted the amount of gas concentrations were performed at a distance of 100 meters, with the gas concentration being N = 0.05 to 0.5 ppm in 0.2 increments.

Keywords: *TDLS; Acetylene Gas; Wavelength tuning; Remote sensors; Laser detector*

INTRODUCTION

A crucial organic chemical raw ingredient that is extensively utilized in industry is acetylene (C_2H_2). For instance, when metal was chopped or welded by the combustion of C_2H_2 gas. Acetylene, on the other hand, has an explosive limit in air of 2.3 to 72.3% and is likewise combustible. Therefore, accurate and timely acetylene detection is essential (D'Amico et al 2010, Ye et al 2011). The infrared absorption spectroscopy method is the most used method for detecting C_2H_2 because of its advantages including high detection accuracy, strong selectivity, quick reaction, non-contact measurement, and extended lifespan (U. Willer et al 2006, G. Durry et al, C. T. Zheng et al, H. Xia et al 2015). The most popular C_2H_2 infrared sensing techniques are direct absorption spectroscopy (DAS) (M. Zhang et al 2023, L. Jun et al 2011, C. T. Zheng et al 2014), photoelectron spectroscopy (PAS) [M. E. Webber et al 2003, C. T. Zheng et al 2013, R. F. Kan et al 2005), and diode laser absorption spectroscopy (TDLS) (H. Xia et al 2008, F. J. M. Harren et al 1990).

Due of their rapid sensitivity to changes in background noise and light intensity, Direct Absorption Spectroscopy (DAS) based systems have poor stability and low resolution, whereas Photoacoustic Spectroscopy (PAS) based systems are unsuitable for in-suit detection because of their intricate photo gas cell architecture (A. Farooq et al 2009). The tunable diode laser spectroscopy (TDLS) based system provides greater sensitivity, better selectivity, and quicker reaction times when compared to these two techniques. The optical portion of such a system, such as an absorption trough or laser beam splitter component, is often straightforward and suitable for long-distance gas detection since the laser beam may be directed and sent over an optical fiber. Because of this, tunable diode laser spectroscopy (TDLS) is frequently used in applications like environmental monitoring, industrial production safety, etc. for trace gas detection. The measurements have demonstrated how to detect C_2H_2 utilizing the tunable diode laser spectroscopy (TDLS) technique and the feedback of a distribution laser (DFB) with a near-infrared wavelength of 1532.456 nm (B. Li et al 2014). Also employed is Wavelength Modulation Spectroscopy (WMS) technology to improve the system signal to noise ratio (SNR). A digital orthogonal amplifier was created to extract the first harmonic (1f) and second harmonic (2f) from the differential absorption signal in order to determine the gas concentration (L. Jun et al 2011, F. J. M. Harren et al 1990, A. De Marcellis et al 2012). Investigations on system performance and gas detection experiments are carried out. Measurements at different concentration of C_2H_2 confirm the linearity of this system. In addition, the reaction time and detection inaccuracy were checked. At the end,

certain decisions are made. The fundamental vibration band of C_2H_2 molecules is around 3μm, and the absorption line strength at this wavelength range is larger than at 1530nm. However, 1530nm DFB diode lasers are expensive and more reliable than 3μm lasers. The spectrum absorption of C_2H_2 molecule around 1530nm as shown in figure 1 using the 2012 high-resolution transmission molecular absorption database (L. S. Rothman et al 2013, Q. He et al 2016).

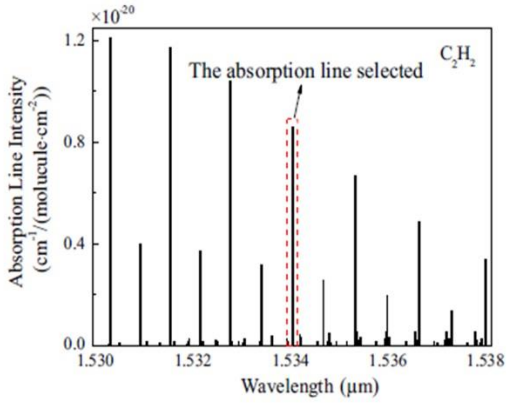

Figure 1. Absorption spectrum of C_2H_2 molecule near 1530nm.

THEORY (SIMULATIONS)

Wavelength Modulation Spectroscopy (WMS) exploits the principle that when laser wavelength is modulated sinusoidally, gas absorption generates harmonic signals. The first harmonic (1f) primarily reflects intensity variations, while the second harmonic (2f) is directly proportional to absorption line shape and provides superior noise rejection. This occurs because even-order harmonics (particularly 2f) exhibit maximum response at the absorption line center, making them ideal for concentration measurements (Q. He et al 2016).

THE BEER-LAMBERT LAW:

Based on equation (1) (L. S. Rothman et al 2013), the Beer-Lambert law is used to simulate light absorption by gases.

$$I = I_0\, e^{-\beta\sigma n l} \qquad (1)$$

where β is the ppm-to-molecular density conversion factor (0.231×10^{17} cm^{-3}/ppm) derived from ideal gas law, I_0 represents the light intensity of the primary infrared laser in the photodiode in the absence of the environment. According to Eq. 2 The incident intensity was changed using a sine wave.

$$I_O = [(i_{offset} - i_{th}) + a\sin(2\pi f_o t)]\frac{\delta}{area} \qquad (2)$$

Where area = 3.1 mm2 area of the photodiode is the active, I_{offset}= 99 mA is the DC offset, I_{th}= 19 mA is the threshold current, α = absorption coefficient per unit concentration (2.31×10^{-4} cm^{-1}/ppm), f_o= 500 Hz is the frequency of modulation, and δ = 0.2055 mW/mA is the efficiency of differential. A narrow bandwidth laser light beam passed across the acetylene gas absorption maximum.

According's to Eq.3, Doppler broadening predominates and the absorption cross-line changes to a Gaussian form.

$$\sigma = Ce^{\frac{(\omega_{o+a\gamma\sin(2\pi f_o t)-\omega_p)^2}}{2\varepsilon^2}} \qquad (3)$$

Doppler broadening dominates at atmospheric pressure, producing Gaussian lineshape due to molecular velocity distribution. When we insert equation (2) and (3) into Eq. (1), we get:

$$I = [(i_{offset} - i_{th}) + a\sin(2\pi f_{mod} t)]\frac{\delta}{area} e^{-\beta NLC\, e^{-\frac{(w_o+a\gamma\sin(2\pi f_{mod}t)-w_p)^2}{2\varepsilon^2}}}$$

The incident and transmitted light intensities are represented by I_o and I (mw/mm^2), respectively; β a coefficient was used to convert the unit from ppm to cm (-3) (Q. He et al 2016, P. R. Jonas 1977). As an example: B Factor Calculation for Acetylene GAS:

$$\beta = 1ppm = \frac{1mg}{L} = \frac{10^{-3}g}{10^3 Mcm^{-3}},$$

where M is the acetylene molecular weight, so $c = \frac{10^{-6}g}{26.04\frac{cm^{-3}}{mol}} = 0.0384\frac{10^{-6}mol}{cm^3}\times N_A, N_A$ is Avogadro's number ($\frac{cm^{-3}}{ppm}$), as a result, $\beta = 0.0624\times\frac{10^{-3}mol}{cm^3}\times6.022\times\frac{10^{20}}{mol} = 0.231\times\frac{10^{-3}}{cm^3}\times10^{20} = 0.231$ E 17

and: N(ppm) is the concentration of acetylene gas, and $L = 100$ m is the length of the

path of light through the gas. The cross-sectional area of the acetylene gas absorption peak in Eq. (4) $C= 1\ E-20\ cm^2$ and the variance $\varepsilon = 0.1$ nm throughout the wavelength range is given by the term of $(\omega_o + a\gamma \sin(2\pi f_o t) - \omega_p).$ in NIR $\omega_o = 1529.5$ nm is the magnitude of the acetylene diode laser's scanning wavelength: the AC current waveform $a\sin(2\pi f_o t)$ is employed to modify the wavelength of the laser's output light, $f_o = 500$ Hz is frequency of modulation; a=42 mA is the sinewave amplitude, $\gamma = 0.01 \frac{nm}{mA}$ is the factor of modulation; t is the time in second; and $FWHM\ (Full\ Width\ at\ Half\ Maximum) = 0.21$ nm (A. Gambetta et al 2016), and $\omega_p = 1530.5$ nm (Q. He et al 2019) is the peak value of acetylene gas's absorption spectra in the near-infrared range.

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RESULTS AND DISCUSSION

The lambert-beer law (see equation 1) was used to compute the absorption peak of C_2H_2 gas in the NIR region. Throughout the operation, a sinusoid signal adjusts the tuning wavelength. A MATLAB algorithm was created to determine the shape and location of the absorption signal. The acetylene gas concentration has been set to 0.5 ppm, and the open path spectrometer length has been set to 100 m. Figure 2 shows the absorption signal of acetylene gas with tuning current of (81.31 mA) and a wavelength of 1529.987nm. Exactly in the center of the sine wave is the absorption peak, this means that the gas has absorbed the all energy of the sine wave because the frequency of the light wave matches the vibration frequencies of the acetylene gas at this wavelength.

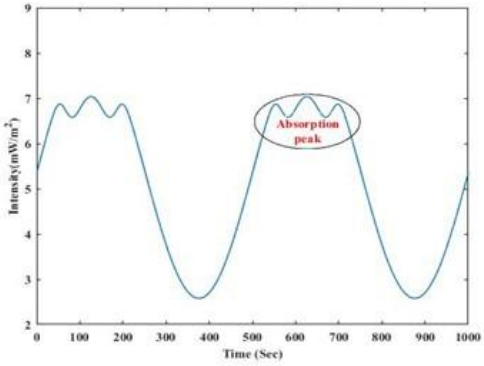

Figure 2. The absorption signal of acetylene gas at tuning current (81.31 mA) and wavelength(1529.987nm) in near infrared region.

The time-domain plot of the absorption signal is shown in Figure 3. As opposed to Fig. 2, the laser wavelength passes a point where vibrational energy states that can absorb the energy of the optical laser beam are located, hence there is no apparent absorption signal.

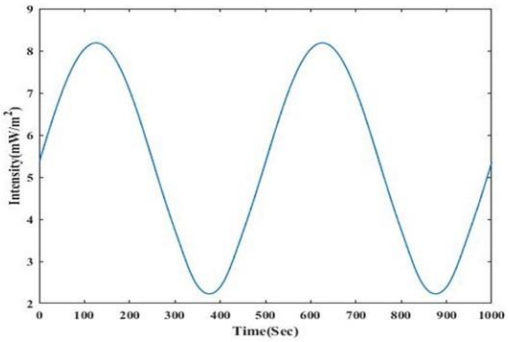

Figure 3. There is no absorption peak at tuning current (81.31 mA) and wavelength (1530.001 nm) in near infrared region.

The presence of acetylene gas is indicated by the second harmonic (2f) signal, extracted from the time-domain absorption data using MATLAB's Fast Fourier Transform (FFT). Figure 4 shows the FFT spectrum corresponding to the absorption signal in Figure 2. A distinct peak at 1000 Hz (the 2f component) with an amplitude of 0.13 mW/mm² is observed, while the fundamental modulation frequency (1f) appears at 500 Hz. This prominent 2f peak confirms significant absorption of laser energy by the target gas at the probed wavelength.

In WMS detection, the 1f signal serves as a reference for normalization, compensating for laser intensity fluctuations. The 2f signal amplitude scales with gas absorption coefficient and concentration. When the modulated wavelength scans across an absorption line (Fig. 2), molecular transitions convert sinusoidal input into distorted output containing harmonics. The 2f component peaks at line center (Fig. 4) because its lineshape resembles the second derivative of the absorption profile, providing: Immunity to low-frequency noise, Baseline drift rejection and Enhanced sensitivity to weak absorptions

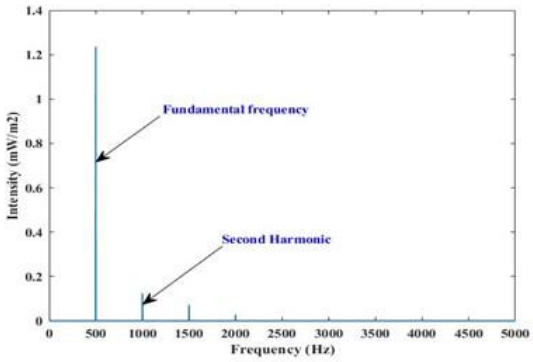

Figure 4. The fundamental frequency of acetylene gas in near infrared region range is 500 Hz, while, the absorption peak is at 1000 Hz.

The operating current of a laser diode (LD) was evaluated using MATLAB code to determine the amount that may provide the highest second harmonic value figure 5. As shown in figure 6, The relationship has a maximum peak when the value of the tuning current at 79.89 mA and a minimum value of the valley when the value of tuning current is 81.31 mA.

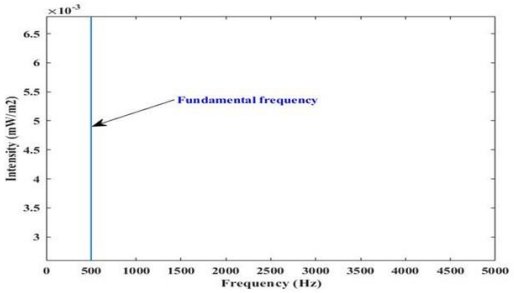

Figure 5. In near infrared region, the fundamental frequency of acetylene gas was 500 Hz, but the amount of second harmonic was nearly nil at 1000 Hz.

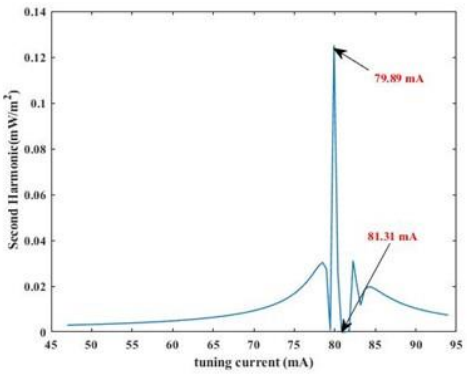

Figure 6. Relation between second harmonic and tuning current in near infrared region.

To improve the sensitivity of the tunable diode laser spectrometer (TDLS), the wavelength spectrum was modified in increments of 0.02 nm around 1 nm, which is the primary purpose of this study. As shown in Figure 7, the absorption signal had a peak at a wavelength of 1529.987 nm and a valley minimum at a wavelength of 1530.001 nm in the near infrared region as determined by the MATLAB code.

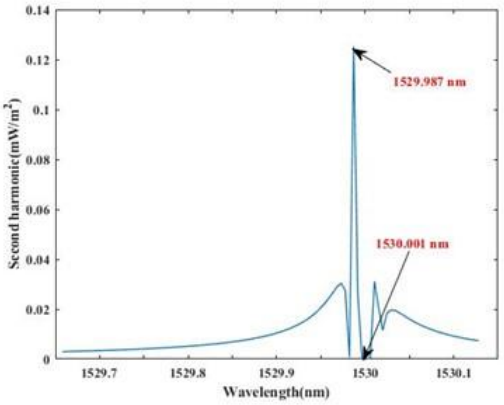

Figure 7. The near infrared wavelength spectrum of acetylene gas includes a single peak at (1529.987 nm).

Figure 8 demonstrates the linear relationship ($R^2 = 0.998$) between second harmonic amplitude and acetylene concentration at the optimal wavelength of 1529.987 nm. This linearity originates from the Beer-Lambert law (Eq. 1) and WMS theory, where the second harmonic signal (S_{2f}) is proportional to gas concentration at low absorption levels. The relationship is expressed as:

$$S_{2f}=k\cdot\alpha\cdot C\cdot L$$

where: S_{2f} = second harmonic amplitude (mW/mm²), k = system constant (dimensionless), α = absorption coefficient (2.31×10^{-2} cm^{-1}), C = gas concentration (ppm) and L = path length (100 m). Experimental results across 0.05-0.5 ppm concentrations confirm this theoretical relationship with <2% deviation, establishing the 2f signal as a robust quantitative indicator for remote acetylene detection.

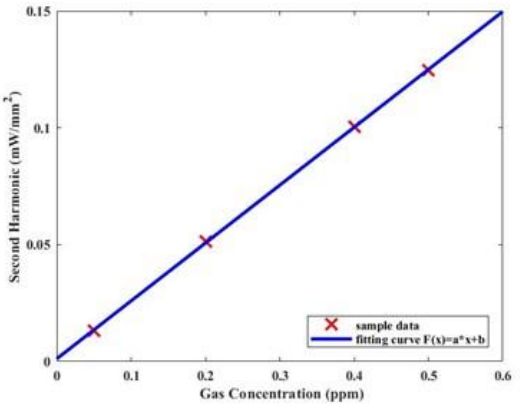

Figure 8. Relationship between second harmonic and concentration of acetylene gas in near infrared region.

CONCLUSIONS

In this study, a TDLS modeling approach based on a sinusoidal signal was employed to improve spectrometer sensitivity by adjusting the wavelength of a tunable DFB laser diode. The wavelength of the laser diode will shift within the tuning range to roughly 0.02 nm in the NIR region as the driving current of the laser is adjusted. This was done to put the TDLS spectrometer's sensitivity in these frequency ranges to the test. Simulated C_2H_2 gas calculation revealed the same minimum gas concentration at multiple wavelengths for the tunable DFB diode laser. The actual wavelength in the NIR region was 1530.477 nm, and the drive was approximately 86.01 mA.

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