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Validation of wavelength modulation spectroscopy techniques for oxygen concentration measurement

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ABSTRACT

Tunable Diode Laser Absorption Spectroscopy (TDLAS) based gas sensing technology, has widespread applications, ranging from use in biomedical industry to aerospace applications. An experimental set-up was established to measure concentration of oxygen gas in the range 0–100% using TDLAS technique. The oxygen absorption at 760.241 nm was scanned with a tunable DFB laser, and wavelength modulation spectroscopy was used to obtain the harmonics (1f, 2f, 3f & 4f) of the oxygen absorption signal. The modulation parameters such as the modulation voltage, modulation frequency, reference phase, time constant of lock in amplifier, the tuning voltage, and the tuning frequency were optimized to obtain the harmonics of high amplitude and narrow half width. Keeping the experimental parameters constant, the oxygen concentration measurements were obtained by the following three methodologies, viz, (i) using only the 2nd harmonic, (ii) using the 2nd and 4th harmonics and, (iii) using the 1st and 2nd harmonics. The results of these measurements were compared and the merits and drawbacks of these methods are discussed.

1. Introduction

Most of the optical absorption based commercial gas sensors [1,2] are based on direct absorption methods, and have relatively simple interpretation of the results. But when the absorption is weak, a technique known as modulation spectroscopy [3] is used for improving the signal to noise ratio through phase sensitive detection. Wavelength Modulation Spectroscopy (WMS) [4] is based on the modulation of the monochromatic light emitted by a laser, so that it is tuned across the optical absorption features of the species to be detected. This technique is also called as Tunable Diode Laser Absorption Spectroscopy (TDLAS). An advantage of this technique is shifting the detection to higher frequencies, where the 1/f noise is reduced. The TDLAS based gas sensing technology, has widespread applications, ranging from use in biomedical industry [5] to aerospace applications [6]. The TDLAS technique, apart from yielding the gas concentration, can also be used to obtain other parameters such as temperature and velocity/flux of the gas [7].

TDLAS based sensors have been found to be extremely useful in aerospace industry for the following applications; (a) for monitoring the oxygen concentration in the breathing gas supplied by oxygen generating system to the pilot [8], (b) for monitoring the performance of aircraft fuel tank inerting systems [9], and (c) in optimization of aero-engines performance in both on-ground and in-flight applications by measuring inlet air mass flux, combustor temperature and product exhaust mass flux and trace pollutant emissions etc [10–12].

The theoretical model of WMS has been investigated by Arndt [13] and experimentally proved by Reid and Labrie [14]. The validity of their model was limited to modulation index <0.1 and absorption coefficient <0.01. Zhang [15] had followed the work of Reid and Labrie, and derived the second harmonic, using Taylor series, which depends directly on actual gas concentration, modulation index, derivative of absorption coefficient, and laser intensity that passes through the absorber gas. A drawback was that, the measured concentration was very much affected by laser intensity and modulation index. To improve this, Guo et al. [16] derived equations for gas concentration using 2nd and 4th harmonics of the absorption signal, which however again was limited by the choice of modulation index. To eliminate the limitations posed by the modulation index and variations in laser intensity, on the gas concentration measurement, Hanson and co-workers [17,18] continued the work of Kluczynski and co-workers [19] who had earlier presented a generalized and analytical theory of WMS based on Fourier decomposition of the detected signal, and derived a methodology which

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uses the 1st and 2nd harmonics of the absorption signal. This methodology (called by them as 1f-normalized WMS-2f technique), had overcome all the limitations and drawbacks of earlier techniques, and had improved the signal to noise ratio, and was used for measurement of gas properties in harsh environment. This methodology was adopted by many other researchers for their work [20,21]. In our previous work [22], we had used single pass gas cell of 30 cm length, and optimized the modulation parameters for measurement of oxygen concentration using the above technique.

In this paper we present the results of oxygen gas concentration measurements in our experimental setup, using the methodologies of Zhang [15], Guo et al. [16] and Hanson and co-workers [17], which uses (i) only the 2nd harmonic, (ii) the 2nd and 4th harmonics, and (iii) the 1st and 2nd harmonics, respectively. The results of these measurements are compared and the merits and drawbacks of the methods are discussed.

2. Theory

When a light beam of intensity $I_0(t)$ travels through an absorbing gas with an absorption coefficient $\alpha(\nu)$, based on Beer–Lambert law, the input $I_0(t)$ and output light intensity $I(t)$ may be written as

$$I(t) = I_0(t)\exp[-\alpha(\nu)CL] \tag{1}$$

where, C represents gas concentration and L is interaction length.

If it is assumed that the line width of the incident light is narrower than the line with of the gas absorption line (in the present case the emission line width of the DFB laser is 0.019 pm, and the chosen gas absorption line width is 2.664 pm) and that the laser driving current is modulated, the frequency and the intensity of the output laser light can be written as

$$\nu = \nu_0 + \nu_m \sin(wt) \tag{2}$$

$$I_0(t) = I_0[1 + \eta \sin(wt)] \tag{3}$$

where, ν_0 represents the central frequency, ν_m is the amplitude of the frequency modulation and η is intensity modulation index and $f = w/2\pi$ is the frequency of modulation.

Eq. (1) can be rewritten as

$$I(t) = I_0[1 + \eta \sin(wt)]\exp[-\alpha(\nu_0 + \nu_m \sin(wt))CL] \tag{4}$$

When, gas absorption and the intensity modulation are very small $a((\nu) \ll 1$ and $\eta \ll 1)$, $I(t)$ may be approximated as

$$I(t) = I_0[1 + \eta \sin(wt) - \alpha(\nu_0 + \nu_m \sin(wt))CL] \tag{5}$$

where the higher order terms have been neglected.

Under atmospheric pressure and temperature, the line shape is given by Lorentzian distribution $\alpha(\nu) = \frac{\alpha_0}{\left(\frac{\nu-\nu_g}{\Delta\nu}\right)^2+1}$ where, α_0 is the absorption coefficient for pure gas at the center of the absorption line, ν_g and $\Delta\nu$ are the central frequency and the half width of the absorption line.

Zhang et al**.:** Eq. (4) has been expanded using Taylor series, and the higher harmonics have been neglected when the modulation amplitude is sufficiently small and absorbance is very low. The concentration measurement using the 2nd Fourier components of absorption signal at center of the absorption line is expressed as.

$$C = 2H_2\Delta\nu^2/(I_0 L \nu_m^2 \alpha_0) \tag{6}$$

where, H_2 represents the amplitude of the 2nd harmonic of the absorption signal and C is the gas concentration.

Guo et al**.:** to improve the result, and ensure better accuracy, Eq. (4) has been expanded using Taylor series, and then considering the 2nd and 4th harmonics of the center of the absorption line and neglecting other higher harmonics. Using 2nd and 4th harmonics of absorption line, a formula for concentration measurement was derived.

$$C = -\frac{I_{4\max}}{2\alpha_0 L I_0}\left[\left(\frac{I_{2\max}}{I_{4\max}}\right)^2 + 8\left(\frac{I_{2\max}}{I_{4\max}}\right) + 16\right] \tag{7}$$

where, $I_{4\max}$ and $I_{2\max}$ are the amplitudes of the 4th and 2nd harmonics of the absorption signal.

Hanson et al**.:** had derived the 1st and 2nd harmonics at the center wavelength of the absorption line using Eq. (4). Using the 1st and 2nd harmonics they derived an equation for the concentration of the gas as,

$$C = -\frac{2F}{1F}\frac{\eta}{\alpha_0 Lk} \tag{8}$$

where k is represented by $k = (-2)\frac{\left[2+x^2-2(x^2+1)^{\frac{1}{2}}\right]}{x^2(x^2+1)^{\frac{1}{2}}}$ and $x = \nu_m/\Delta\nu$

3. Experimental details

The schematic of the TDLAS based oxygen sensor and the actual experimental setup are shown in Figs. 1 and 2.

The laser source was a DFB diode laser with a power of 10 mW (Sacher Laser Technik GmbH, Germany) emitting single mode at 760 nm (25 °C, 70 mA). The fiber pigtailed laser diode was connected to a collimator (Thorlab, USA), and the collimated beam passes through a variable path length multi pass optical gas cell (Analytical Corporation, USA). The beam exiting out of the gas cell was refocused by another collimator (Thorlab, USA) onto an optical fiber, which sends the collected light to an optical power meter (Newport, USA). A modular laser diode controller (Newport Inc., Model 6000) provides the working current to the laser diode with ripple noise smaller than 1 μA, so that the frequency fluctuations of the laser, that are due to current noise can be neglected (<1 MHz). The laser wavelength is driven by a 200 Hz triangular wave generated by waveform generator (Tektronix, Model AFG3022B), and summed by an adder with a 10 kHz sine wave, to provide the required wavelength modulation. This sine wave signal was generated by a dual channel lock-in amplifier (Signal Recovery Inc., model 7270), and it is also its internal reference signal. The laser diode driver (Newport, Model 6000), also provides the temperature control for the DFB laser diode (with Peltier cooler) within ±0.01 °C, near 32 °C. The electrical signal from the optical power meter was then demodulated by dual channel lock-in amplifier (Signal Recovery, Model 7270), to recover the harmonic (1st, 2nd, etc) signals with a time constant of 200 μs and filter slope of 12 dB/octave, which leads a noise equivalent bandwidth of the low pass filter to be 880 Hz. The demodulated signals, the harmonics of the absorption signal viz. 1f, 2f, 3f, 4f, etc from the lock-in amplifier were sent to a PC, via data acquisition card, to display the waveforms and for further calculations.

The sample gas for concentration measurements were supplied from a combination of two mass flow controllers supplying nitrogen and oxygen gases. For the measurements a total flow of 500 ccm was used. The data reported in this paper are for an optical path length 56 cm of the multipass gas cell. The laser temperature was set at 32 °C and the laser operating current was set at 72 mA to operate the laser wavelength near 760.241 nm which corresponds to oxygen absorption line termed as RQ(11). A tuning voltage of 130 mV/200 Hz was used to scan laser wavelength across oxygen absorption line (760.241 nm ± 10 pm) and modulation voltage of 77 mV/10 kHz (modulation index of 2.2) to modulate the signal, for achieving a high signal to noise ratio. (In our experimental set up, laser driver controller transfer function is 50 mA/V. A 130 mV tuning signal corresponds 6.5 mA current and 77 mV modulation