

Application of a Tunable-Diode-Laser Absorption Diagnostic for CO Measurements in an Automotive HCCI Engine

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ABSTRACT

An infrared laser absorption technique has been developed to measure in-cylinder concentrations of CO in an optical, automotive HCCI engine. The diagnostic employs a distributed-feedback, tunable diode laser selected to emit light at the R15 line of the first overtone of CO near 2.3 μm . The collimated laser beam makes multiple passes through the cylinder to increase its path length and its sampling volume. High-frequency modulation of the laser output (wavelength modulation spectroscopy) further enhances the signal-to-noise ratio and detection limits of CO. The diagnostic has been tested in the motored and fired engine, exhibiting better than 200-ppm sensitivity for 50-cycle ensemble-average values of CO concentration with 1-ms time resolution. Fired results demonstrate the ability of the diagnostic to quantify CO production during negative valve overlap (NVO) for a range of fueling conditions.

INTRODUCTION

Because CO is an important indicator of hydrocarbon reaction progress and combustion efficiency, its detection is useful for the study of many combustion phenomena, including engine combustion. In-cylinder measurements of CO can provide insight into the location and timing of CO production and consumption in the engine, as well as contribute to the validation of indispensable chemical kinetic models of engine combustion.

In this work, we describe the development of an in-cylinder CO sensor and its first application in an optical engine. Motivation for development of the diagnostic comes from a current need to characterize combustion in an HCCI engine operating with negative valve overlap (NVO). This strategy often involves the injection of fuel during the NVO period as

a means of controlling main combustion, and it is hoped that the CO diagnostic can help sort out NVO reforming reactions.

BACKGROUND

While CO concentration is commonly and conveniently measured using engine exhaust gas analyzers, the technique typically provides long-time-average values that are of little use for in-cylinder analyses. *In situ* CO sensors have been developed for a wide variety of combustion-sensing applications [1,2,3,4,5,6,7,8,9,10,11,12,13,14,15], but few apply to engines. Researchers [13,15] recently employed a deep-UV, two-photon planar laser-induced fluorescence (PLIF) technique for CO detection in the squish volume of a diesel engine. Their 10-Hz measurements revealed locations of CO formation, and provided semi-quantitative data that correlated well with engine-out emission measurements. Although these results are encouraging, the technique is hampered by temperamental and expensive equipment, relatively slow measurement repetition rates, and difficulties accounting for beam attenuation and signal quenching.

Direct absorption (DA) is a path-averaged approach that also has been used to measure CO in a variety of combustion environments [5,7,9,10]. The approach is based on the Beer-Lambert law and often employs a tunable diode laser (TDL) to make spectrally resolved measurements of transmissivity that are directly convertible into species concentrations. Measurement accuracy generally suffers from the effects of window fouling, difficulties in establishing a non-absorbing baseline, and beam steering. As is the case with several different laser-absorption technologies, DA signal strength improves dramatically as wavelength is increased, *e.g.*, moving from second-overtone (~ 1560 nm), to first-overtone (~ 2300 nm), to fundamental (~ 4600 nm) absorption bands.



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However, inadequate signal-to-noise ratio (SNR) can be a problem for DA in harsh combustion environments like engines. Fortunately, techniques exist that significantly enhance the performance of (non-direct) absorption diagnostics, as discussed below.

The advent of new laser technology and enhanced detection techniques has made in-cylinder measurements of CO more feasible. Ebert, *et al.* [9] demonstrated the use of distributed-feedback TDLs to measure low CO concentrations (6.5 ppm) using first-overtone DA in a harsh combustion environment. More recently, Chao, *et al.* [14] have used similar lasers and wavelength-modulation spectroscopy (WMS) to measure exhaust CO at high temperatures. The WMS technique renders a signal that is immune to intensity variations from particle scattering, window fouling, and beam steering. These studies suggest that CO detection using a similar approach is ripe for application in internal combustion engines.

In this work, we describe the application of TDL, wavelength-modulation spectroscopy to measure ensemble-averaged, crank-angle-resolved CO concentrations in an HCCI engine with negative valve overlap. Following a discussion of diagnostic theory, we present measurements obtained in a motored engine seeded with homogeneous mixtures of CO and air that establish detection limits and evaluate accuracy. Finally, we describe time-resolved measurements (*i.e.*, every 10 crank-angle-degrees) made during fired NVO-HCCI operation and briefly discuss in-cylinder CO concentration trends revealed by the diagnostic.

THEORETICAL DESCRIPTION

The general theory and development of direct absorption and wavelength modulation spectroscopy for concentration measurements are described in Refs. [16,17,18,19,20,21], with relevant details summarized here. Additional details of the optimization of this technique for our particular application will be the focus of a future publication.

The general relationship between absorption and species concentration is based on Beer's law:

$$\tau_v = \frac{I}{I_o} \Big|_v = \exp(-SP\chi\phi_v L) \quad (1)$$

in which τ_v is the spectral transmissivity, I is transmitted intensity, I_o is incident intensity, S is the linestrength of the absorption line of interest [$\text{cm}^{-2}/\text{atm}$], P is pressure [atm], χ is the species mole fraction, ϕ_v is the lineshape function [cm], and L is the absorbing path length [cm]. An example of absorption for a single broadened CO line is plotted in Figure 1. This spectral transmissivity can be measured by ramping the diode laser frequency across the line of interest and detecting the transmitted signal. Once transmissivity is

determined (*i.e.*, by normalizing the transmitted signal with its non-absorbing baseline), Eq. 1 is inverted to find species concentration.

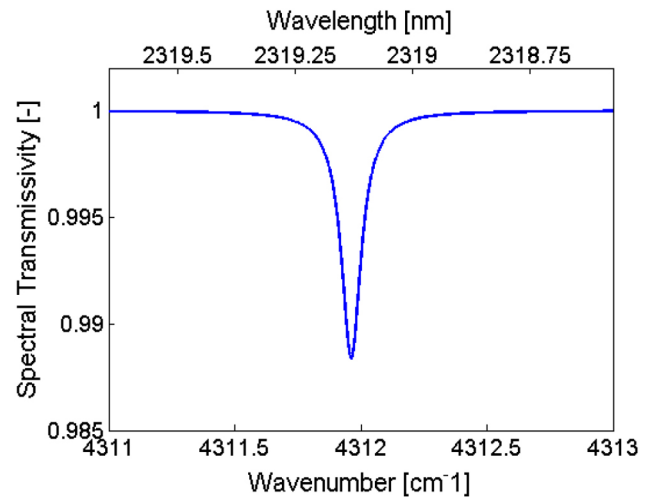


Figure 1. Spectral transmissivity for a single, broadened CO line demonstrating direct absorption.

This simple, DA approach is effective for high-concentration, low-noise conditions. For trace species detection in relatively harsh environments, noise levels can swamp the signal and confound determination of the non-absorbing baseline, resulting in poor detection limits. Many of these problems are alleviated by using wavelength modulation spectroscopy.

WMS reduces susceptibility to interfering effects through the use of phase-sensitive detection (*i.e.*, lock-in amplification) to reject broadband noise. This requires dithering the laser's injection current, which in turn produces the desired laser frequency modulation (FM):

$$\nu(t) = \nu_L + a \cos(\omega t) \quad (2)$$

for which ω is the sinusoidal modulation frequency, ν_L is the laser frequency without modulation, and a is the modulation depth defined as half peak-to-peak FM. Unwanted intensity modulation (IM), with linear and non-linear components, also arises from the dither, and its impact on the signal must be evaluated. The resulting time-varying laser intensity is given by:

$$I_o(t) = I_{oL} \{1 + i_o \cos(\omega t + \psi_1) + i_2 \cos(2\omega t + \psi_2)\} \quad (3)$$

where I_{oL} is the mean laser intensity, i_o and i_2 are the linear and non-linear IM amplitudes normalized by I_{oL} , ψ_1 and ψ_2 are the linear and non-linear IM/FM phase shifts, and higher order harmonics have been truncated. Once the modulated light passes through the absorbing media, the transmitted

signal is detected and demodulated using a lock-in amplifier. The lock-in amplifier electronically demodulates the signal by mixing with a reference signal that is a harmonic of the laser modulation frequency. Typically (as in this work) the second harmonic is used, and the result is termed the $2f$ signal.

For many absorption measurements, a periodic ramp is used to repeatedly scan the laser frequency across the absorbing feature. In WMS, the much higher frequency dither is superimposed on this low-frequency ramp to create a combined waveform as illustrated in Fig. 2. Probing a single absorbing line with this waveform results in a demodulated signal as shown in Fig. 3.

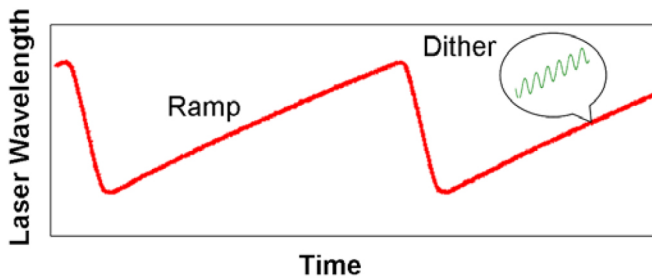


Figure 2. Superimposed ramp and dither characterizing laser wavelength and intensity variations for measurements using WMS.

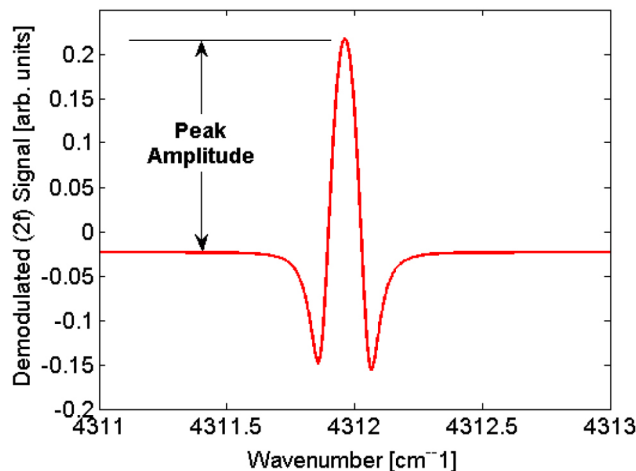


Figure 3. A theoretical demodulated $2f$ signal for a single absorbing CO line. Denoted peak amplitude plays a crucial role in determining species concentration.

The peak amplitude of the $2f$ signal denoted in Fig. 3 is an important parameter for quantifying species concentration. For a specific set of simplifying conditions, this amplitude (hereafter referred to as D_{2f}) can be expressed as:

$$D_{2f} = -\frac{GI_{oL}P\chi_{CO}L}{2\pi} \int_{-\pi}^{\pi} S(T)\phi(T, P, \nu_{peak} + a \cos \theta) \cos 2\theta d\theta \quad (4)$$

for which G is the optical gain of the system. This expression is valid for optically thin conditions with negligible contributions from nonlinear laser IM terms. In this work, relatively low modulation depths (a) were selected to minimize the nonlinear terms. A more general equation [21] containing non-linear terms i_2 and ψ_2 confirmed the negligible impact of these terms on our results. One consequence of selecting low modulation depths is a reduced-pressure operating range. However, this is of little consequence in this work since measurements are made during low-pressure (1 to 5 atm) portions of the engine cycle. Alternatively, by increasing the TDL modulation depth and accounting for laser non-linearities, accurate measurements at higher in-cylinder pressures can also be obtained.

Equation 4 indicates that D_{2f} varies linearly with species concentration. To extract concentration values, we require a calibration measurement at known concentration, pressure, and temperature:

$$D_{2f,cal} = -\frac{GI_{oL,cal}P_{cal}\chi_{CO,cal}L}{2\pi} \int_{-\pi}^{\pi} S(T_{cal})\phi(T_{cal}, P_{cal}, \nu_{peak} + a \cos \theta) \cos 2\theta d\theta \quad (5)$$

Dividing Eq. 4 by Eq. 5 and canceling terms provides an expression for CO concentration in terms of measured parameters:

$$\chi_{CO} = \chi_{CO,cal} \frac{D_{2f,norm}}{D_{2f,norm,cal}} \frac{P_{cal}}{P} \frac{S(T_{cal})}{S(T)} \left(\frac{\int_{-\pi}^{\pi} \phi(T_{cal}, P_{cal}, \nu_{peak} + a \cos \theta) \cos 2\theta d\theta}{\int_{-\pi}^{\pi} \phi(T, P, \nu_{peak} + a \cos \theta) \cos 2\theta d\theta} \right) \quad (6)$$

in which peak amplitudes of the demodulated $2f$ signals (D_{2f}) have been normalized by their corresponding mean laser intensities (I_{oL}). Summarizing Eq. 6, we see that CO concentration is determined by scaling the calibration concentration with measured ratios of peak signal amplitudes, pressures, line strengths, and line-shape parameters. Line-

shape parameters are computed using known line-broadening relationships and measured reference data [7] that depend on measured pressure, temperature, and estimated composition. For motored engine operation, in-cylinder composition is determined directly from measured intake flow rates. For fired engine operation, composition is estimated from measured combustion efficiency and residual gas fraction (RGF). Analysis of uncertainty in our estimates of composition indicates a minor impact (<5% error) on our CO measurements.

EXPERIMENTAL APPROACH

DIAGNOSTIC SETUP

Selecting the first CO overtone near 2300 nm enables low detection limits and a spectral range compatible with the engine's quartz windows. The TDL required for these measurements is housed in a laser diode mount (Thorlabs - LDM21) coupled with a fast aspheric IR lens (NA = 0.68) that collimates the laser output. The 3-mm beam is pitched through the engine's quartz cylinder and reflected between opposing mirrors to obtain multiple passes before being collected and focused on an extended-range IR detector (Thorlabs - PDA10DT) as shown in Figure 4. Because the quartz engine cylinder acts as a negative lens, one of the opposing mirrors is concave ($d = 75.0$ mm, $f = 200$ mm) to minimize divergence. Zemax® ray-tracing software was instrumental in selecting and positioning optics to obtain a satisfactory multi-pass arrangement.

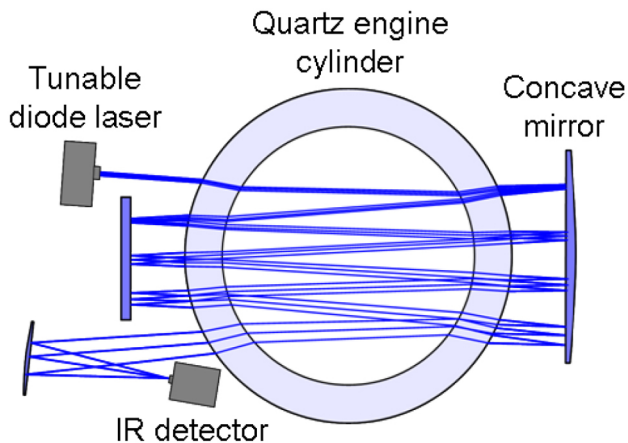


Figure 4. Diagram of the diagnostic setup for in-cylinder measurements of CO; 8-pass arrangement, $L = 65$ cm.

The multi-pass arrangement serves a dual purpose of increasing cylinder coverage to obtain a more representative measurement of average CO concentration in the measurement plane, as well as increasing total path length to boost signal (*cf.* Eq. 4). The process of optimizing the beam path is largely concerned with minimizing etalon fringes that appear as noise in the $2f$ signal. These fringes arise from reflections off of parallel surfaces in the optical path. They

can be reduced by avoiding beam paths near cylinder centerlines, but this becomes more difficult with increasing number of passes. For this work, we employ 6- and 8-pass arrangements with total path lengths from 50 to 65 cm that yield good signal-to-noise ratios (SNR) and low detection limits.

On the input side of the diagnostic is the tunable diode laser cooled by embedded thermo-electric coolers (TEC). The TEC controller (ILX Lightwave) regulates the diode temperature to maintain a mean output wavelength near the R15 transition of the first vibrational overtone of CO near 2319 nm. This absorption line was selected to avoid interference from an overlapping H₂O absorption band [7].

A TDL driver creates both the low-frequency ramp and the high-frequency WMS dither by modulating laser current. Ramp frequency is set at 1 kHz, causing the TDL to scan across the R15 absorption feature in 7.2 CAD at an engine speed of 1200 RPM. (For simplicity, a short delay is included in the current measurements so that data are collected every 10 CAD.) The dither frequency is set high enough (300 kHz) relative to the ramp to ensure that mean laser frequency is nearly constant during each dither cycle. The modulation depth is adjusted to maximize the $2f$ signal for near-atmospheric CO measurements, resulting in a value of $a \approx 0.11$ cm⁻¹. This value is near the theoretical optimum [19] of 2.2 times the half-width at half-maximum (HWHM) of the absorption feature.

On the output side, the transmitted signal is captured with a 1-MHz-bandwidth IR detector, satisfying the Nyquist collection criterion for the 300-kHz modulation frequency. A lock-in amplifier mixes the detected signal with a 600 kHz (second harmonic) reference signal and low-pass filters the result at 20 kHz to generate the $2f$ signal. This signal is then digitized with a 12-bit A/D board at $\frac{1}{4}$ -CAD resolution (28.8 kHz at 1200 rpm). The resulting temporal output is one CO concentration measurement every 10 CAD.

ENGINE SETUP AND MEASUREMENTS

Experiments are carried out in our single-cylinder automotive HCCI research engine [22] with specifications listed in Table 1. The engine is configured with a 25-mm-tall quartz cylinder incorporated in the cylinder liner for optical access. Beam passes are constrained to a single horizontal plane through the quartz cylinder about 5 mm below the firedeck.