DEVELOPMENT AND APPLICATION
OF LASER-BASED SENSORS
FOR HARSH COMBUSTION
ENVIRONMENTS

By

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Abstract

The development of diagnostics based on laser-absorption spectroscopy for combustion applications has been an important and active field of research over the past two decades due to the advantages of this non-intrusive optical sensing technique compared to traditional sensing methods. These optical sensors have shown the ability to provide in situ, time-resolved, line-of-sight measurements of temperature and gas species concentrations. Two propulsion concepts, pulse detonation engines (PDE) and homogeneous-charge compression ignition (HCCI) engines, have received particular interest over the past decade. Sensors based on laser absorption spectroscopy prove useful to the development of these modern propulsion systems to facilitate design advancements, improve efficiency, and reduce pollutant emissions.

Two novel, laser-based sensors employing ultraviolet wavelengths are developed and applied to measure time-resolved temperature and OH concentration in a single-cycle pulse detonation tube. These results, along with pressure data, are employed to evaluate two computational simulations utilizing different chemistry and heat transfer models to predict pulse detonation engine (PDE) flowfields.
A fiber optic-based, wavelength-multiplexed, near-infrared tunable-diode-laser absorption sensor designed to measure temperature is developed and applied to characterize a valveless multi-cycle PDE. The sensor is utilized to measure water vapor temperature profiles for both successful detonations and engine failure modes such as flame-holding. Improvements in both optical engineering and spectroscopic design over previous sensors enable measurements at engine operation rates up to 40Hz. The results provide valuable data for characterizing system performance and investigating component failure thresholds as engine operation rates are increased.

A wavelength-multiplexed, fiber-optic-based, line-of-sight, near-infrared diode-laser absorption sensor is developed for crank-angle-resolved measurements of temperature and water concentration in an HCCI engine. An initial demonstration of its use on two optical HCCI engines at Sandia National Laboratories is reported. The measurements encompassed both motored- and fired-engine operation. Key solutions to select appropriate water linepairs and to suppress crank-angle-dependent noise in the transmitted laser signals are reported. Data obtained through this sensor can provide critical engine characteristics such as combustion efficiency, peak combustion temperature, and autoignition temperature.
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Chapter 1: Introduction

1.1. Motivation and Objectives

The development of diagnostics based on laser-absorption spectroscopy for combustion applications has been an important and active field of research over the past two decades due to the advantages of this non-intrusive optical sensing technique compared to traditional sensing methods. These optical sensors have shown the ability to provide \textit{in situ}, time-resolved, line-of-sight measurements of temperature, gas species concentrations, velocity, density, mass flux, and pressure in a variety of combustion environments (Allen, 1998; Baer \textit{et al.}, 1996; Kohse-Höinghaus and Jeffries, 2002; Philippe and Hanson, 1992, Sanders \textit{et al.}, 2000; Sanders \textit{et al.}, 2002). The information supplied by these sensors has been critical to the development of modern propulsion systems to facilitate design advancements, improve efficiency, and reduce pollutant emissions.

Much of early work in the field of laser-absorption diagnostic development for combustion applications focused on the use of these sensors for laboratory devices such
as flat flame burners and shock tubes (Nagali and Hanson, 1997; Philippe and Hanson, 1993; Schoenung and Hanson, 1981). More recently, researchers have begun to develop and apply these sensors to more practical and industrially applicable combustion systems such as coal-fired power plants, incinerators, gas turbine engines, SCRAMJET combustors, pulse detonation engines, and internal combustion engines (Furlong, Baer, and Hanson, 1998; Griffiths and Houwing, 2005; Kranendonk et al., 2005; Liu et al., 2005; Mattison et al. 2005; Mattison et al., 2006; Owens et al., 2005; Rieker et al., 2006; Sanders et al., 2000; Sanders et al., 2002; Teichert et al., 2003). The resulting data have provided critical information to advance the understanding and to improve the performance of these combustion systems. While these pioneering experiments laid the groundwork for development and application of laser absorption sensors for practical combustion systems, both technical and intellectual challenges remain which limit the widespread use of absorption diagnostics to study these extremely harsh and challenging measurement environments.

Two propulsion concepts, one to be employed for transonic missile applications and the other for ground-based automotive and stationary-power applications, have received particular interest over the past decade. The first concept, a pulse detonation engine (PDE), is a missile propulsion device, similar to the deflagration-based German V-1 ‘buzz bomb,’ which produces thrust from intermittent, repeating detonations in a confined tube. Aeropropulsion researchers have reported advantages of PDEs compared to traditional competing propulsion concepts such as turbojets and ramjets (Tangirala et al. 2005). These theoretical advantages include high specific impulse, high thermal efficiency, and mechanical simplicity (Bussing and Pappas, 1994; Eidelman, 1997;
Eidelman and Yang, 1998; Kailasanath, 2001.) While the final device architecture for practical, flight-operable PDEs has yet to be realized, the underlying physics, components, and mechanisms have received much research attention. Conventional diagnostics for studying PDE performance such as pressure and thrust measurements provide valuable data, but they do not provide sufficient information to investigate all the components and stages of this highly transient cycle. Time-resolved measurements of temperature and species concentration are required to accurately characterize PDE system performance, to validate computational simulations, and to investigate engine component failure thresholds both in highly repeatable single-cycle detonation experiments and in more flight-realistic multi-cycle engine studies. Sensors based on line-of-sight, laser-absorption spectroscopy provide an essential toolset to meet these diagnostic needs.

The second propulsion concept is a homogeneous-charge compression-ignition (HCCI) engine. HCCI engines provide potential advantages compared to standard spark-ignition (SI) or compression-ignition direct-injection (CIDI) internal combustion piston engines and thus have received much attention from both the academic and industrial research communities for automotive and ground-based power generation applications. The major advantages of the HCCI cycle compared to convention piston-engine combustion concepts, including high efficiency and ultra-low particulate matter (PM) and oxides of nitrogen (NOx) emissions, result from the combustion and ignition process (Najt and Foster, 1983). HCCI engines operate on the principle of a homogeneous, dilute, premixed charge of fuel-air that reacts and burns volumetrically as a result of the temperature rise and pressurization from the engine compression stroke. As in premixed SI engines, the homogeneous nature of the fuel-air charge minimizes the occurrence of
fuel-rich zones which could lead to the production of soot. Unlike SI engine combustion, the dilute reaction occurs volumetrically without a defined flame-front thus reducing the peak product gas temperatures which in turn reduces the NO\textsubscript{x} formation. Like CIDI engines, HCCI engines incur no throttling losses and operate at high compression ratios (CR) and thus maintain high efficiency.

While HCCI engines have advantages compared to other piston-engine concepts, technical challenges remain which prevent widespread use of this combustion strategy. One main technical challenge for HCCI engines is control of ignition timing. Unlike SI engine combustion where a spark discharge initiates ignition or CIDI engine combustion where fuel injection initiates ignition, HCCI ignition timing is controlled by chemical-kinetics which is very sensitive to the temperature, pressure, and gas mixture composition. While modern electronic control strategies such as variable-valve timing (VVT), variable compression-ratio (VCR), and exhaust-gas recirculation (EGR) provide a control variable to influence the fuel-air reactant mixture, temperature, and pressure, direct measurements of cylinder temperature and gas composition are critical to the understanding and control of the HCCI ignition process. Sensors based on line-of-sight, laser-absorption spectroscopy offer a tool set needed for near-real-time records of in-cylinder temperature and gas composition. These sensors could prove essential to investigate HCCI engine operation and potentially to provide a feedback signal for electronic engine control strategies.

The objective of the work reported here is threefold:

1. Develop and apply ultraviolet-based (UV) laser-absorption sensors for measurement of temperature and species concentration with
microsecond time resolution in a single-cycle PDE to generate a data set for computational simulation validation.


3. Develop and apply a wavelength-multiplexed, fiber-optic-based, near-infrared, laser-absorption temperature and water concentration sensor to an optical HCCI engine to evaluate the compression stroke and ignition process.

Each objective presents a unique set of challenges which must be overcome both in terms of optical-sensing and facility-specific complexities. Single-cycle PDE experiments were performed on a laboratory-scale PDE at Stanford University. Multi-cycle PDE experiments were performed at the Rocket Propulsion Laboratory at the Naval Postgraduate School in Monterey, CA. HCCI engine tests were performed at the Combustion Research Facility at Sandia National Laboratories in Livermore, CA. The challenges and solutions employed for each objective are outlined below; each item will be discussed in greater detail in the following chapters.

1.2. Measurement Challenges

While some sensing challenges are common to all combustion systems, each combustion device reported here presents a unique set of challenges and specialty solutions for the optical-based sensing methods utilized.
The single-cycle PDE experiments focused on the characterization of detonation propagation and blow-down for an ethylene-oxygen fueled PDE resulting in extreme temperature and pressure conditions and very rapid time-scales. A summary of sensing challenges and specialty solutions for this device are outlined in Table 1.1.

<table>
<thead>
<tr>
<th>Single-Cycle PDE Sensing Challenges</th>
<th>Potential Solutions</th>
</tr>
</thead>
<tbody>
<tr>
<td>• High temperature (up to 4000K)</td>
<td>• UV wavelengths to probe electronic transitions of CO₂(broadband) and OH(individual transition) which have strong absorption coefficients and well-characterized spectroscopy</td>
</tr>
<tr>
<td>• High pressure (up to 35 atm)</td>
<td></td>
</tr>
<tr>
<td>• Short optical path length (3.8cm)</td>
<td></td>
</tr>
</tbody>
</table>
| • Flowfield emission                | • Bandpass filters to reject broadband emission  
• Reduced solid collection angle in detector optics |
| • Highly transient event            | • Fixed-wavelength absorption experiments with high-bandwidth detectors and data acquisition |
| • Beamsteering                      | • Large-area, uniform-response detection  
• Focusing lens/integrating sphere/detector optical train to accommodate laser beam displacement  
• Large diameter windows for flowfield optical access |
| • Window fouling and flowfield sooting | • Off-line beam to track non-resonant changes in laser transmission  
• Lean and stoichiometric operation to minimize soot production |

Table 1.1. Optical sensing challenges and potential solutions for single-cycle PDE measurements at Stanford University.

While the experiments on the single-cycle Stanford PDE presented extreme sensing conditions, engine vibration and motion were managed in this laboratory-scale PDE. Measurement challenges associated with the multi-cycle PDE resulted mostly from engine translation and vibration which required an alternative sensing strategy. As opposed to the single-cycle PDE experiments which focused on detonation propagation
and blow-down, the multi-cycle PDE experiments investigated repetition-rate-limiting flowfield phenomena, such as cycle-to-cycle interference and flame-holding, during the relatively low-pressure portion of the PDE cycle. A summary of sensing challenges and specialty solutions for the multi-cycle PDE experiments are outlined in Table 1.2.

<table>
<thead>
<tr>
<th>Multi-Cycle PDE Sensing Challenges</th>
<th>Potential Solutions</th>
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</thead>
<tbody>
<tr>
<td>• Engine translation (thrust stand motion)</td>
<td>• PDE-mounted, fiber-optic-based sensor</td>
</tr>
<tr>
<td>• Engine vibration</td>
<td></td>
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<tr>
<td>• Large temperature sensing range (300K-2000K)</td>
<td>• Wavelength-multiplexed system to probe multiple spectroscopic absorption features</td>
</tr>
<tr>
<td></td>
<td>• Near-IR, diode-laser sensor to measure rovibrational transitions of water vapor near 1.4μm</td>
</tr>
<tr>
<td>• Beamsteering</td>
<td>• Fast laser scan rate (to ‘freeze’ effects of transmission fluctuation)</td>
</tr>
<tr>
<td></td>
<td>• Optical engineering of collection lens/optical fiber combination to accommodate large beam displacement</td>
</tr>
<tr>
<td>• Flowfield emission</td>
<td>• Band-pass filter (diffraction grating)</td>
</tr>
<tr>
<td>• Fiber-optic related noise</td>
<td>• Reduced pitch- and catch-fiber optic vibration and motion</td>
</tr>
<tr>
<td></td>
<td>• Large area detectors to collect all laser light to minimize effects of mode noise</td>
</tr>
<tr>
<td></td>
<td>• Polarization insensitive diffraction grating</td>
</tr>
<tr>
<td>• Window fouling and flowfield sooting</td>
<td>• Scan-wavelength system with baseline fitting to accommodate laser transmission fluctuation</td>
</tr>
</tbody>
</table>

Table 1.2. Optical sensing challenges and potential solutions for multi-cycle PDE measurements at the Naval Postgraduate School.

Compared to the single- and multi-cycle PDE experiments, the HCCI engine presented a unique combination of optical measurement challenges. In order to maintain crank-angle-resolved time resolution for realistic engine operation speeds, the sensing strategy needed to have fast time response. In order to investigate both low-pressure, low-
temperature portions of the engine cycle where EGR characteristics are important, and the high-pressure, high-temperature portions of the engine cycle where ignition, peak combustion temperatures, and pollutant formation are important, the sensor must maintain sensitivity over a large dynamic range of conditions. A summary of sensing challenges and specialty solutions for the HCCI engine experiments are outlined in Table 1.3.

<table>
<thead>
<tr>
<th>HCCI Engine Sensing Challenges</th>
<th>Potential Solutions</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Engine translation (isolation stand motion)</td>
<td>• Engine-mounted, fiber-optic-based sensor</td>
</tr>
<tr>
<td>• Engine vibration</td>
<td>• Wavelength-multiplexed system to probe multiple spectroscopic absorption features</td>
</tr>
<tr>
<td>• Large temperature sensing range (300K-1700K)</td>
<td>• Near-IR, diode-laser sensor to measure rovibrational transitions of water vapor</td>
</tr>
<tr>
<td>• Large pressure sensing range (1atm-55atm)</td>
<td>• Accurate spectroscopic database</td>
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<tr>
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<td>• Spectroscopic simulation</td>
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<tr>
<td></td>
<td>• Spectroscopic line selection</td>
</tr>
<tr>
<td>• Beamsteering</td>
<td>• Optical engineering of collection lens/optical fiber combination to accommodate</td>
</tr>
<tr>
<td></td>
<td>• Non-resonant beam to track laser transmission fluctuation</td>
</tr>
<tr>
<td>• Window fouling and oiling</td>
<td>• Non-resonant beam to track laser transmission fluctuation</td>
</tr>
<tr>
<td>• Polarization fluctuations due to stress-induced birefringence of</td>
<td>• Polarization insensitive collection and dispersion optics (including diffraction</td>
</tr>
<tr>
<td>engine windows</td>
<td>grating)</td>
</tr>
<tr>
<td>• Line-of-sight non-uniformities (including cold boundary layers)</td>
<td>• Spectroscopic line selection</td>
</tr>
<tr>
<td>• Highly transient event</td>
<td>• Fixed-wavelength absorption experiments with high-bandwidth detectors and data</td>
</tr>
<tr>
<td></td>
<td>acquisition</td>
</tr>
</tbody>
</table>

Table 1.3. Optical sensing challenges and potential solutions for HCCI engine measurements at Sandia National Laboratories.
1.3. Previous Work

Researchers have reported the use of laser-absorption sensors to investigate a wide variety of practical combustion systems which demonstrates the power of this optical technique. Only a small number of studies utilize these sensors to study PDEs and IC engines due to the challenges associated with these harsh measurement environments; many important potential applications exist for further studies in these devices. A summary of previous work and limitations of laser-absorption sensors appears below.

1.3.1. Laser Absorption Sensors for Combustion Systems

Laser absorption sensors have proven valuable for studying practical combustion systems. Furlong et al. utilized a diode-laser temperature sensor for closed-loop control of a 50kW incinerator combustor (Furlong, Baer and Hanson, 1998). Teicher investigated temperature, CO and H₂O species concentration in coal-fired power plants utilizing a wavelength-multiplexed diode-laser system (Teicher et al., 2003) Liu et al., and Griffiths and Houwing, studied the temperature profile and stability in a SCRAMJET combustor with a wavelength-multiplexed diode-laser system (Griffiths and Houwing, 2005; Liu et al., 2005). Zhou achieved active control of a swirl-stabilized combustor with a diode-laser temperature sensor (Zhou, 2005). Liu et al. probed the temperature profile of the combustor of a gas-turbine sector rig (Liu et al., 2003). Wang et al. outlined a method to utilized diode laser sensors to monitor CO emissions of automotive exhaust (Wang et al., 2000). Each of these demonstrations reveal the power of line-of-sight, laser-absorption sensors.
1.3.2. Laser Absorption Sensors for PDEs

Previous research in the area of laser-absorption sensor development for PDE applications can be broken down into two main sensing categories: (1) single-cycle experiments for simulation validation; (2) multi-cycle experiments for engine evaluation.

Sanders et al. developed a temperature and pressure sensor based on the simultaneous monitoring of absorption and emission by flowfield-seeded atomic cesium in a single-cycle PDE (Sanders et al., 2000). This technique successfully tracked the temperature and pressure fluctuations from 2000 to 4000K and 1 to 35atm with microsecond time response in an ethylene-oxygen fueled PDE. Comparisons with computational simulations identified potential errors and shortcomings in computational simulations performed at the Naval Research Laboratories and led to improvement of simulation assumptions. Sanders et al., Mattison et al., and Owens et al., developed and utilized burned-gas velocity sensor based on time-of-flight sensing of discretely seeded atomic cesium in single-cycle PDE flowfields with varying exit boundary conditions (Sanders et al., 2003; Mattison et al., 2002; Owens et al., 2003). Comparisons with computational simulations identified assumptions regarding finite-rate chemistry and heat transfer as the leading cause of error in computed PDE performance.

While single-cycle experiments produce data valuable for computation simulation validation, multi-cycle experiments are necessary for investigation of more realistic engine flowfields. Sanders et al. developed a wavelength-multiplexed, fixed-frequency sensor which employed fiber-optic coupling on the light delivery optics to measure water vapor transitions near 1.4 \( \mu \text{m} \) for temperature and water concentration measurements on a PDE operating at 5 Hz (Sanders et al., 2000). Mattison et al. employed a free-space,
single-laser, water thermometry sensor to probe adjacent water transitions in the $v_1^+v_3$ combination band near 1.4 $\mu$m to characterize successful operation and flame-holding on a PDE operating at 5 and 7 Hz (Mattison et al., 2002). Hinckley et al. developed a fiber-optic coupled sensor to probe water absorption transitions near 1.4 $\mu$m to measure temperature on a PDE operating at 10 Hz (Hinckley, Jeffries and Hanson, 2004). Ma et al. and Klingbeil et al. reported sensors to monitor fuel loading on PDEs operating up to 40 Hz (Ma et al., 2005; Klingbeil et al., 2005).

Both the single-cycle and multi-cycle experiments suffer from several drawbacks which limit their usefulness. The cesium-based thermometry experiments supplied valuable, low-noise, accurate data but required a very cumbersome seeding technique to introduce the tracer into the flowfield in a uniform manner. It also employed a complicated data reduction methodology. The results were scaled from a known temperature point (post-detonation Chapman-Jouguet temperature) thus requiring calibration. The multi-cycle PDE experiments provided valuable data for engine evaluation, but constraints of the sensor limited the ability to simultaneously monitor important engine parameters such as thrust. Due to the free space coupling of the optical techniques, both the Sanders et al. and Mattison et al. techniques required the PDE to be locked to the thrust stand to prevent PDE recoil on the spring-mounted thrust stand. While this limited the motion of the engine (and thus prevented thrust measurements), it increased high frequency engine vibration which appeared as additional noise in the laser signals. Both of these results were limited to low engine repetition rates (<10 Hz). By employing fiber optics for both light delivery and collection, the Hinckley et al.

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technique enabled measurements on a translating vibrating engine. But noise in the laser signal limited engine operation rates to 10 Hz.

1.3.3. Laser Absorption Sensors for IC Engines

Two previous sensors based on line-of-sight absorption of water vapor to measure time-resolved, in-cylinder temperature for internal combustion engine applications have been developed. Kranendonk, et al. reported the development of a wavelength-agile (i.e. broadly- and rapidly-scanned) external cavity diode laser sensor to measure temperature and water mole fraction during HCCI engine operation (Kranendonk et al., 2005). While this methodology shows promise as an alternative sensor strategy to traditional wavelength-multiplexed, direct-absorption diode laser approaches, it suffers from several drawbacks which are addressed in Chapter 5, such as problems with the laser source and complexities involved with data reduction. Rieker, et al. have reported an alternative approach to TDL thermometry in IC engines utilizing wavelength-modulation spectroscopy with 2f detection (WMS-2f) to measure in-cylinder water vapor temperature over short path lengths (~1 cm) in a modified spark plug (Rieker et al., 2006). While the latter technique provides increased sensitivity enabling short-path-length measurements, it has limitations compared to traditional direct-absorption techniques which are addressed in Chapter 5, such as complications with control electronics and limitations in laser wavelength multiplexing.
1.4. **Scope and New Contributions**

Recently, the advent and advancement of fiber optic and laser technology, and ultra-violet-based techniques has enabled the improvement and continued development of optical sensors for harsh combustion measurement environments. A summary of key achievements and measurement successes reported in this thesis are summarized below.

1.4.1. **Demonstration of thermometry utilizing UV CO\(_2\) absorption for diagnostics in propulsion systems**

Recent progress in diagnostic development and spectroscopic measurements identified broadband UV absorption by CO\(_2\) as a potential technique to measure temperature in combustion systems (Jeffries *et al.*, 2005). Thermometry based on UV CO\(_2\) absorption proves attractive for the PDE environment. For all hydrocarbon-fueled combustors, CO\(_2\) is a major combustion product thus eliminating the need to seed a tracer gas such as cesium. Also, the absorption coefficient of CO\(_2\) at high temperatures (2000-4000 K) is much stronger than typical absorption coefficients of near-infrared molecular transitions (e.g. H\(_2\)O near 1.4 \(\mu\)m) thus improving the signal-to-noise ratio compared to alternative thermometry strategies. While researchers have demonstrated this technique in a laboratory experiment to measure temperature in well-controlled reacting systems such as shock tubes, application of this technique to propulsion systems has not been thoroughly pursued (Oehlschlaeger *et al.*, 2004; Oehlschlaeger *et al.*, 2005). Chapter 3 summarizes the use of UV CO\(_2\) absorption to measure temperature in the single-cycle PDE environment.
1.4.2. Demonstration of device-mounted, multiplexed, fiber-optic-based, TDL thermometry sensor for PDEs operating at high engine repetition rates (>10 Hz)

Researchers have attempted to utilized device-mounted, wavelength-multiplexed, fiber-optic-coupled, tunable-diode-laser (TDL) absorption sensors to measure temperature in high-repetition-rate PDEs, but successful measurements were limited to repetition rates up to 10 Hz. Through careful spectroscopic design and optical engineering, successful measurements are achieved to measure temperature utilizing water vapor absorption transitions near 1.4μm at PDE repetition rates up to 40 Hz, as summarized in Chapter 4. These results detail successful engine operation and identify and quantify repetition-rate-limiting engine components.

1.4.3. Design, construction, and demonstration of multiplexed, TDL-based water temperature sensor for an HCCI engine

A wavelength-multiplexed, fiber-optic-based, line-of-sight, diode-laser absorption sensor is developed for crank-angle-resolved measurements of temperature and water concentration in an HCCI engine, as reported in Chapter 5. An initial demonstration of its use on two optical HCCI engines at Sandia National Laboratories is reported. The measurements encompassed both motored- and fired-engine operation for temperatures between 300 and 1700 K and pressures between 1 and 55 bar. A spectroscopic line selection process identifies the water transitions at frequencies of 7219.61 cm\(^{-1}\) (\(E''=488.1\) cm\(^{-1}\)) and 7416.05 cm\(^{-1}\) (\(E''=488.1\) cm\(^{-1}\)) as the most appropriate water absorption linepair for thermometry under these conditions. Key solutions to suppress
crank-angle-dependent noise in the transmitted laser signals are reported, including careful spectroscopic design, and optical engineering to accommodate beam-steering, engine vibration and polarization-related interference. Data obtained through this sensor can provide critical engine characteristics such as combustion efficiency, peak combustion temperature, and autoignition temperature.

1.4.4. Identification of and solution to polarization-related effects as noise source in multiplexed, TDL sensors

Polarization-related phenomena have appeared as a significant noise source in wavelength-multiplexed, fiber-optic-coupled, diode-laser sensors through fiber-optic motion and window birefringence. For many wavelength-multiplexed systems, diffraction gratings disperse the multiplexed light so that each wavelength can be monitored independently. Typical diffraction gratings have vastly different reflection efficiencies for s-plane and p-plane polarized light. As such, if the polarization of the light shifts, the transmitted intensity at the optical detector changes. Stress-induced birefringence and motion of optical fiber can shift the polarization of light in laser absorption sensors and thus produce noise. Potential solutions to polarization-related noise are addressed in Chapters 2 and 5.

1.5. Organization of Thesis

Chapter 1 contains the background and motivation for the work reported in this thesis. This chapter describes how the present work fits into the context of previous
efforts and to understand how the new contributions extend sensing capabilities for PDE and HCCI engine researchers.

Chapter 2 presents a brief summary of measurement fundamentals and techniques for laser-absorption sensors. This section covers the governing equation, the Beer-Lambert relation, and outlines how spectroscopic methods can be utilized to extract gas temperature and concentration in combustion environments. Chapter 2 will briefly outline sensor theory; further details for the three applications covered in this thesis will be found in Chapters 3-5.

Chapter 3 outlines the use of a UV-based CO$_2$ temperature sensor and an OH concentration sensor to investigate single-cycle operation of an ethylene-oxygen fueled PDE. The results are compared to computation simulations employing differing models regarding reactive chemistry and heat transfer losses to evaluate the impact of these assumptions on predicted PDE performance.

Chapter 4 outlines the development and application of a wavelength-multiplexed, fiber-optic-coupled diode-laser sensor to measure temperature in a multi-cycle PDE operating and engine repetition rates up to 40 Hz. The sensor characterizes both successful engine operation and engine failure modes to assess the repetition-rate limiting engine components and demonstrates the utility of optical sensors compared to traditional pressure-based measurement techniques.

Chapter 5 details the development and application of a wavelength-multiplexed, fiber-optic-based, diode-laser absorption sensor for crank-angle-resolved measurements of temperature and water concentration in an HCCI engine under both motored- and fired-engine operation. Spectroscopic line selection and optical engineering methods are
presented to ensure accurate, low-noise data. Solutions to polarization-related noise in wavelength-multiplexed laser absorption sensors are discussed.

Chapter 6 summarizes the major contributions of this work and suggests future studies to improve the sensing methods and to utilize these sensors to investigate both PDEs and IC engines. An alphabetical listing of cited references appears at the end of this thesis.
Chapter 2: Measurement Techniques and Fundamentals

The theory of direct absorption spectroscopy has been detailed by numerous researchers and will be briefly discussed in this thesis (Allen, 1998; Arroyo and Hanson, 1993; Baer et al., 1996; Mattison et al., 2003; Zhou, 2005). This chapter outlines the measurement techniques utilized to extract temperature and species concentration from line-of-sight, laser absorption measurements focusing on ultraviolet and wavelength-multiplexed techniques. Chapters 3, 4, and 5 expand on the techniques and equipment utilized for the experiments probing single-cycle PDEs, the multi-cycle PDEs, and HCCI engines respectively.

2.1 Beer-Lambert Relation

The fundamental equation governing line-of-sight, laser absorption spectroscopy is the Beer-Lambert Relation. This equation relates the transmission of a laser beam after it traverses a uniform, absorbing gas, as depicted in Fig. 2.1, as a ratio of incident and transmitted monochromatic laser radiation intensities.
In this equation, $T_\nu$ is transmission, $I(\nu)$ is the transmitted laser intensity, $I_o(\nu)$ is the incident laser intensity, $k_\nu$ [cm$^{-1}$] is the spectral absorption coefficient, and $L$ [cm] is the absorbing path length. The product $k_\nu L$ is absorbance. The spectral absorption coefficient for an absorbing species $i$, is a function of linestrength, $S$ [cm$^{-2}$/atm], lineshape function, $\phi$ [cm], and partial pressure of the absorbing species, $P_i$ [atm], as shown in the following equation.

$$k_\nu = S(T) \cdot \phi(T, P, X_i) \cdot P_i \quad (2.2)$$

If multiple absorption features exist in a given spectral region and are sufficiently broad such that they overlap, a summation of spectral absorption coefficients for each
individual transition produces the overall absorption coefficient at the given frequency. The dependence of the spectral absorption coefficient on temperature, \( T \), pressure, \( P \), and gas composition, \( X_i \), enables quantitative measurements of these parameters in combustion systems.

The temperature dependence of linestrength can be expressed in terms of a known linestrength at a specified reference temperature, \( T_o \).

\[
S(T) = S(T_o) \cdot \frac{T}{T_o} \cdot \frac{Q(T_o)}{Q(T)} \cdot \frac{1 - \exp\left(-\frac{hc\nu_o}{kT}\right)}{1 - \exp\left(-\frac{hc\nu_o}{kT_o}\right)} \cdot \exp\left[-\frac{hcE''}{k} \left(\frac{1}{T} - \frac{1}{T_o}\right)\right]
\] (2.3)

In this relation, \( Q(T) \) is the temperature-dependent partition function for the absorbing molecule (evaluated for either rovibronic or rovibrational energy transitions and determined through empirical correlations to analytical calculations), \( h \) is Planck’s constant, \( c \) is the speed of light, \( \nu_o \) is the transition frequency, \( k \) is Boltzmann’s constant, and \( E'' \) is the lower state energy.

The line shape function, \( \phi(\nu) \), reflects the variation in the spectral absorption coefficient for a single transition as a function of frequency. This variation in the line shape function with frequency is caused by broadening mechanisms in the medium that perturb the transition’s energy levels or the way in which individual atoms and molecules interact with light. It is influenced by the temperature, pressure, and gas composition of the medium. Although numerous physical mechanisms influence the line shape function, two main broadening mechanisms are considered for the combustion research reported here: pressure (or collisional) broadening and Doppler (velocity) broadening (Wehe,
2000). The dependence of the line shape function on these two mechanisms is thoroughly described in the literature and can be evaluated using Gaussian, Lorentzian or Voigt line shape functions depending on the temperature and pressure range of interest (Nagali and Hanson, 1997; Nagali et al., 1997b; Wehe, 2000). These functions are all defined as unity functions, as shown in Eqn. 2.4.

\[
\int_{-\infty}^{\infty} \phi(\nu) \cdot d\nu = 1 \quad (2.4)
\]

Figure 2.2 depicts the effect of line broadening on laser transmission measurements of two individual absorption transitions. For each absorption feature, transmission is minimized at line center, \( \nu_0 \), and symmetrically increases at frequencies near line center. Without the effects of line broadening, each absorption transition would instead appear as a delta function.

![Figure 2.2](image_url)

**Figure 2.2.** Incident (I\(_O\)) and transmitted (I) laser intensity as a function of laser frequency (\( \nu \)) for two individual absorption transitions.
2.1.1 Fixed-Wavelength Absorption Sensors

For the laser absorption measurements reported in this thesis, two categories of experimental methods are utilized to quantitatively monitor absorption transitions: fixed-wavelength and scan-wavelength direct absorption techniques. Each exhibits distinct advantages (and disadvantages), depending on experimental conditions, which must be evaluated in designing experiments.

Fixed-wavelength sensors are the most straightforward to understand and to operate. For this technique, the laser source frequency is tuned such that it lases at the peak of an absorption transition. The laser beam is pitched across a test gas of interest and the transmitted intensity is monitored as a function of time with a photodetector coupled to a computer-based data acquisition system. The transmission is recorded as the temperature, pressure, and gas composition in the system changes. The main advantage of this technique, other than the simplicity of the design, is the time response of the system. The sensor bandwidth is limited only by the time response of the detector and data acquisition system, which can readily achieve megahertz (MHz) rates. For rapidly changing combustion flowfields, such as those contained in IC-engines and PDEs, fast time response is important for monitoring system performance. The major disadvantages of the fixed-wavelength system are the difficulty involved with determining the non-absorbing baseline intensity and the complexity associated with extracting quantitative results from the data. In order to determine an accurate absorption measurement, the intensity of the non-absorbing baseline must be determined. In practical combustion systems, non-resonant transmission fluctuations occur due to sooting, window fouling, vibration, beamsteering, etc. In order to estimate the baseline intensity, a non-resonant
(non-absorbing) laser beam can be used to track the optical transmission. Fixed-wavelength sensors provide only relative transmission data and thus require calibration to a predetermined point in the combustion cycle (such as zero absorption or a known pressure and temperature state). Once absorption data are taken, precise models and simulations of line broadening coupled to an accurate spectroscopic database must be utilized to extract quantitative temperature and species concentration results. Fixed-wavelength sensors often employ wavelength multiplexing to maximize the spectral information achieved during combustion experiments; this technique will be described in the next section.

2.1.2 Scanned-Wavelength Absorption Sensors

Scan-wavelength sensors prove useful in measurement environments where spectrally narrow absorption features exist. For this technique, the laser source frequency is tuned across both an absorption transition and the non-absorbing wings, often in a sawtooth manner as shown in Fig. 2.3. The baseline, $I_0$, is typically extrapolated by fitting a polynomial to the non-absorbing wings of the transmission signal. Then, by utilizing the Beer-Lambert relation, absorbance is determined providing individual absorption line shapes for each laser scan. The laser must be scanned rapidly enough such that fluctuations in transmission due to beamsteering, vibration, sooting, and window fouling are frozen on the timescale of the laser scan.

For tunable-diode-laser sensors, the sawtooth laser scan is typically achieved by modulating the laser injection current, although alternative scanning strategies are currently under development (Kranendonk, Bartula, and Sanders, 2005). The major
advantages of this technique compared to fixed-wavelength systems are twofold. (1) Scan-wavelength measurements provide the entire absorption line shape for each laser scan. This increased spectral information provides opportunities to infer additional flowfield properties. (Sanders et al., 2002). By integrating the absorbance trace with respect to frequency, the line shape function and associated uncertainties can be eliminated resulting in $S'P_iL$. The integrated absorbance is directly proportional to concentration and linestrength. Thus, if temperature is known, species concentration can be determined. Or if temperature is unknown, the ratio of integrated absorbance from two carefully selected transitions can be utilized to infer temperature. This thermometry technique is further described in the next section. (2) The transmission measurements inferred from the non-absorbing wings eliminate the need for a non-resonant beam and provide an absolute absorption measurement. Thus, no calibration point is required.

Figure 2.3. Example diode-laser scans across a water absorption feature in a multi-pulse PDE environment. The detonation passage is marked by a dip in transmission as a result of the Schlieren effect.
The major disadvantages of the scan-wavelength technique concern the sensor bandwidth and the pressure sensing range. Diode-lasers exhibit a limited injection current scanning range, as depicted in Fig. 2.4. For example, if spectroscopic simulations indicate that a laser scan range of $3\text{cm}^{-1}$ is required to fully resolve the absorption transition and the surrounding non-absorbing wings, the laser scan rate is limited to $10\text{kHz}$ for the laser performance illustrated in this figure. When the system pressure increases, the absorption line widths increase due to pressure broadening and may overlap with neighboring absorption features. Thus for high-pressure measurement environments, as in PDEs and IC Engines, the laser may not be able to scan across the entire absorption feature. Then, a non-absorbing baseline cannot be determined.

![Scan range of fiber-optic-coupled diode laser supplied by NEL America. For this laser calibration, the injection current was modulated from laser threshold to 200mA in a sawtooth manner, and an etalon monitored the laser tuning range.](image-url)
2.1.3 Direct Absorption Thermometry

Ratio-based thermometry is a powerful technique utilized to measure temperature in harsh combustion environments. The details and theory of this technique have been thoroughly described in the literature and will be briefly summarized here (Arroyo and Hanson, 1993; Ouyang and Varghese, 1990). Ratio-based thermometry can be employed with both fixed- and scan-wavelength techniques, although the method of data reduction and accuracy vary between the two methods.

As stated in the previous section, the linestrength for a particular absorption transition is temperature dependent. This dependency is demonstrated in Fig. 2.5 which plots absorbance for two hypothetical transitions at three different temperatures. As shown in the figure, the integrated area for each transition changes as the system temperature changes.

![Absorbance for two spectral absorption features with varying temperature conditions. Here, $T_{\text{blue}} < T_{\text{green}} < T_{\text{red}}$.](image)

Figure 2.5. Absorbance for two spectral absorption features with varying temperature conditions. Here, $T_{\text{blue}} < T_{\text{green}} < T_{\text{red}}$. 

Absorbance $= k \nu L$
By taking a ratio of integrated absorbance of two properly selected transitions, temperature can be inferred, as depicted in Figure 2.6.

![Graph showing ratio of peak height yields gas temperature]

Figure 2.6. Ratio of absorption coefficients (or integrated absorbance as the ratio of path length is unity) from Fig. 2.5 for three temperatures.

For scan-wavelength, two-line thermometry, the ratio of integrated absorbance, $R$, reduces to a function of temperature, as shown in the following equations. Note, the line shape function is not included in the expanded absorption coefficient as its integrated area becomes unity.

$$R = \frac{k_{\nu 2} \cdot L}{k_{\nu 1} \cdot L} = \frac{S_2 \cdot P_i \cdot L}{S_1 \cdot P_i \cdot L} = \frac{S_2}{S_1} \quad (2.5)$$

In this equation, $k_{\nu 2}$ and $k_{\nu 1}$ are the absorption coefficients and $S_2$ and $S_1$ are the linestrengths for the transitions located at frequencies $\nu_2$ and $\nu_1$ respectively. The ratio of integrated absorption is independent of the partial pressure and path length. The ratio of linestrengths can be reduced to a function of temperature by combining Eqns. 2.3 and 2.5; the result is listed in Eqn. 2.6.
\[ T = \frac{h \cdot c \cdot (E_2'' - E_1'')}{k \ln(R) + \ln \left( \frac{S_2(T_o)}{S_1(T_o)} \right) + \frac{h \cdot c \cdot (E_2'' - E_1'')}{T_o}} \]  \hspace{1cm} (2.6)

In this equation, \( E_2'' \) and \( E_1'' \) are the lower state energies, and \( S_2(T_o) \) and \( S_1(T_o) \) are the linestrengths (at the reference temperature, \( T_o \)) of the transitions located at frequencies \( \nu_2 \) and \( \nu_1 \) respectively.

For fixed-wavelength, two-line thermometry, the ratio of line-center absorbance, \( R_{\text{fixed}} \), reduces to a function of temperature and line shape function as shown in the following equations.

\[ R_{\text{fixed}} = \frac{k_{\nu_2,\text{linecenter}} \cdot L}{k_{\nu_1,\text{linecenter}} \cdot L} = \frac{S_2 \cdot \phi_{2,\text{linecenter}} \cdot P_i \cdot L}{S_1 \cdot \phi_{1,\text{linecenter}} \cdot P_i \cdot L} = \frac{S_2 \cdot \phi_{2,\text{linecenter}}}{S_1 \cdot \phi_{1,\text{linecenter}}} \]  \hspace{1cm} (2.7)

In this equation, \( k_{\nu_2,\text{linecenter}} \) and \( k_{\nu_1,\text{linecenter}} \) are the line-center absorption coefficients, and \( \phi_{2,\text{linecenter}} \) and \( \phi_{1,\text{linecenter}} \) are the line-center line shape functions for the transitions located at frequencies \( \nu_2 \) and \( \nu_1 \) respectively. The line shape functions are dependent on temperature, pressure, and gas composition. In order to reduce \( R_{\text{fixed}} \) to a function of temperature, the two line shape functions have to be assumed equal, or the values for the two line shape functions are estimated. The line shape function depends largely on pressure which can be easily measured with a pressure transducer. Although these assumptions regarding the line shape function add small measurement error compared to the scan-wavelength method, the fixed-wavelength method proves useful for many
different applications especially in high pressure environments where baseline fitting cannot be achieved.

While laser absorption thermometry can be achieved by monitoring only two properly selected absorption transitions, incorporating additional absorption transitions can provide benefits. By measuring three or more absorption transitions with varying temperature dependencies (i.e. varying lower state energies, $E''$), the sensing range of the system can be increased and information on non-uniformities along the line-of-sight can potentially be inferred (Liu et al., 2005; Sanders et al., 2001).

### 2.1.4 Direct Absorption Species Concentration

Gas concentration can be inferred from the measurement of a single absorption transitions using either fixed- or scan-wavelength techniques. For scan-wavelength measurements, gas concentration is determined from a measurement of integrated absorbance and pressure, as shown in the following equation.

$$X_i = \frac{A}{S(T) \cdot P \cdot L} \quad (2.8)$$

In this equation, $X_i$ is the species mole fraction, $A$ is the integrated absorbance, $S(T)$ is the temperature-dependent linestrength, and $P$ is the system pressure. If temperature is unknown, it can be measured using a technique such as the two-line thermometry method described in the previous section.
For fixed-wavelength sensors, gas concentration is determined from a measurement of line center absorbance and pressure; the value of the line shape function has to be estimated.

\[
X_{i,\text{fixed}} = \frac{k_{\text{line center}} \cdot L}{S(T) \cdot \phi_{\text{line center}} \cdot P \cdot L} \quad (2.9)
\]

In this equation, \(X_{i,\text{fixed}}\) is the species mole fraction, \(k_{\text{line center}} \cdot L\) is the measured line center absorbance, \(S(T)\) is the temperature-dependent linestrength, \(\phi_{\text{line center}}\) is the estimated line shape function, and \(P\) is the system pressure.

### 2.2 Wavelength-Multiplexed, Near-Infrared TDL Sensors

The previous section outlined how both fixed- and scan-wavelength sensors provide information on single absorption transitions. In order to use laser absorption sensors to measure temperature, multiple transitions need to be monitored, as discussed in the previous section. While TDL thermometry sensors have been developed which utilize a single laser to scan adjacent water absorption features to measure temperature, very few adjacent transitions exist which have proper spectroscopic parameters to enable sensitive measurements of temperature (Arroyo and Hanson, 1993). Eliminating the restriction to utilize adjacent transitions vastly increases the pool of candidate absorption features for spectroscopic line selection, as outlined in Chapter 5.

While two-line techniques show high sensitivity over a narrow temperature range, they do not maintain high sensitivity over the entire temperature range of interest to combustion or propulsion researchers. For example, multi-cycle PDE flowfields may vary from 300-3000K over a single engine cycle; a direct-absorption TDL thermometry
sensor utilizing two absorption transitions cannot maintain high sensitivity and signal over the entire range.

Wavelength-multiplexed systems provide a solution to the limitations of single-laser systems. By adding multiple laser wavelengths to a single measurement path, multiple absorption transitions can be simultaneously monitored thus eliminating the need for adjacent transitions and increasing the temperature sensing range. A simplified schematic of wavelength-multiplexed sensor architecture is shown in Fig. 2.7. For this system, multiple laser beams are optically combined to propagate across the same measurement path such that each laser beam encounters the same gas conditions and flowfield perturbations.

\[ I(v_1) + I(v_2) \]

\[ I_0(v_1) + I_0(v_2) \]

Figure 2.7. A wavelength-multiplexed, line-of-sight, laser absorption schematic depicting incident \( I_0 \) and transmitted \( I \) laser intensity as a function of laser frequency \( v \) for two laser wavelengths. A diffraction grating is utilized to demultiplex the individual wavelengths.

Wavelength multiplexing is achieved utilizing different techniques depending on specific applications. For fiber-optic-coupled systems, individual laser beams are
combined using telecommunications beam combiners which are plug-and-play components. For free space systems, beams can be combined utilizing diffraction gratings or dichroic mirrors. In order to monitor each individual laser wavelength after it traverses the measurement flowfield, many techniques can be utilized to separate the signals. The most common method is to use a dispersive optic such as a diffraction grating (shown in Fig.2.7) or a prism to demultiplex the wavelengths spatially. Other methods include time-division or frequency-division demultiplexing. Each of these techniques will be briefly outlined in the next section.

Wavelength-multiplexed systems offer many advantages compared to single laser systems. For two-line thermometry applications, by monitoring three or more absorption transitions and using different line pairs for specific temperature intervals, the sensing range of the system can be improved. Similarly, multiple species can be monitored by simply adding additional wavelengths. For fixed-wavelength sensors, the wavelength-multiplexed architecture enables the addition of a non-resonant beam to track flowfield transmission thus enabling measurements in harsh combustion environments. With the recent advancement and increased availability of fiber-optic-coupled lasers and telecommunications equipment, wavelength-multiplexed systems are more readily achieved.

### 2.3 Wavelength-Multiplexed, Device-Mounted Sensors

Often for research on propulsion engines, it is necessary to perform optical measurements on devices that move and vibrate throughout the engine cycle. For example, the pulse detonation engine at the Naval Postgraduate School in Monterey, CA (discussed in Chapter 4) is mounted to a thrust stand that allows the engine to translate up
to three inches during the engine cycle. Similarly, the HCCI engine at Sandia National Laboratories in Livermore, CA (discussed in Chapter 5) is mounted to an air-dampened isolation stand to minimize the effects of engine vibration on the surrounding equipment; this allows the engine to move centimeters during engine operation. In order to make possible the use of line-of-sight optical sensors on either of these devices, the sensor must be mounted to the moving, vibrating engines. This is readily achieved using device-mounted, fiber-optic-coupled, wavelength-multiplexed diode-laser sensors. A generalized layout for this type of sensor is shown in Fig. 2.8. This system shows great potential for sensing in industrial applications to enable real-time process monitoring or even combustion control. In order to overcome the effects of beamsteering, optical emission, device vibration, device motion, and other potential noise sources specialized solutions must be employed, as outlined below.

![Figure 2.8. A generalized fiber-optic-coupled, wavelength-multiplexed, diode-laser sensor schematic.](image)

### 2.3.1 Sensor Layout and Optical Components

Figure 2.8 shows a schematic for a typical fiber-optic-coupled, wavelength-multiplexed, TDL sensor utilized for measurements on propulsion systems. The vibration sensitive lasers, laser control electronics, demultiplexing optics, detectors, and data acquisition system are remotely located. The sensor is directly connected to the
combustion device by fiber optics enabling measurements on a translating, vibrating engine.

The fiber-pigtailed diode lasers are multiplexed into a single-mode fiber using a fiber combiner. In this schematic, four laser beams are combined into a single fiber using a 4x1 fused combiner, but additional wavelengths can be added by utilizing alternative combiners. Commercial sensor manufacturers have developed systems capable of multiplexing up to 16 individual laser wavelengths and potentially more.

![Diagram](image)

Figure 2.9. Laser control electronics, diode lasers, and fiber combiner for wavelength multiplexed TDL sensor setup.

Figure 2.9 shows a photograph of laser control electronics, fiber-pigtailed diode lasers, and the fiber combiner. Compared to traditional laser sources such as a solid-state or a dye laser, the small footprint of these components facilitates the development and application of portable systems. The multiplexed laser light is brought from the laser control room to the combustion device through single-mode fiber. This light is then collimated and pitched across the combustor (through fused silica or sapphire windows) using an aspheric collimator which is directly mounted to the combustion device. For the measurements reported in this thesis, the laser light is typically collimated to beam...
diameters ranging from 1 to 3mm depending on the particular application. Smaller beam diameters typically improve the collection efficiency but are more prone to occlusion from window fouling and flowfield particulates. After the light traverses the combustion chamber, it is collected using an aspheric collection lens (mounted to the combustion device) and focused into multi-mode fiber. The collection lens is chosen such that the f-number matches the numerical aperture of the multi-mode fiber and such that the diameter is sufficiently large to accommodate beam steering, as outlined further in Chapter 5.

Multi-mode fiber has a larger core diameter than single mode fiber (thus improving the collection efficiency) but increases sensor noise in the form of fiber mode noise. Mode noise results from fiber motion and laser scanning; the propagation mode of the light in the fiber optic is affected by fiber spatial arrangement and light frequency. For the results reported in this thesis, the single-mode fiber has a 9μm core diameter and the multi-mode fiber has a 400μm core diameter. Both the single-mode pitch fiber and the multi-mode catch fiber are constrained to minimize fiber motion to reduce the effects of fiber optic-based noise (from both mode noise and polarization noise).

The multiplexed light coming from the combustion device is brought to a remote location via the multi-mode fiber optic where the light is then demultiplexed, as shown in Fig. 2.10. For the water-based sensors reported in this thesis, the demultiplexing optics are enclosed in a nitrogen-purged environment to eliminate interference from atmospheric humidity.
In this demultiplexing setup, the light exiting the multimode fiber is collimated using an aspheric lens and then pitched onto a diffraction grating from which the individual wavelengths diffract at different angles. The grating simultaneously acts as a band-pass filter, eliminating interference from flowfield emissions. The demultiplexed beams are then focused onto individual large-area (3mm diameter) amplified InGaAs photodetectors using a spherical focusing mirror. The large-area detectors are necessary to ensure that the entire beam is focused on the active area of the detector to reduce the effects of fiber mode noise.

2.3.2 Demultiplexing Using Diffraction Grating

In order to monitor each of the multiplexed wavelengths individually, they must be separated either spatially, temporally, or spectrally. For the sensors reported in this thesis, a diffraction grating disperses the individual wavelengths spatially; other demultiplexing strategies will be discussed at the end of this section.

In designing a demultiplexing setup utilizing a diffraction grating, numerous factors must be considered to maximize signal intensity, to minimize wavelength cross talk, to maintain polarization insensitivity, and to minimize device footprint. In order to
maximize signal intensity, a high reflection efficiency grating must be utilized with a large fraction of the grooves illuminated. At the near-infrared wavelengths used for the sensors reported in this thesis, gold reflection gratings blazed at wavelengths near the operating wavelength of 1.4μm show the highest efficiencies. In order to ensure that a large fraction of the grating grooves is illuminated, the light exiting the multi-mode fiber must be collimated to a large beam diameter. For the results reported in this thesis, a 2.5cm diameter, f/1 aspheric lens is used. The advantages of using this lens are twofold. The large area, small f-number combination collimates the light to a sufficiently large beam diameter and ensures a low divergence angle collimated beam compared to previously developed demultiplexing systems (Hinckley, Jeffries, and Hanson, 2004). Low divergence angle minimizes cross talk between wavelengths and maximizes signal intensity by ensuring that all of the diffracted light is able to be collected onto the detectors.

A schematic of a three-wavelength demultiplexing setup is shown in Fig. 2.11. For this setup utilized in the HCCI engine measurements reported in Chapter 5, the light exiting the multi-mode fiber (with a emitted included angle of approximately 30 degrees) is collimated to a 10mm beam diameter at the diffraction grating. Because the multi-mode fiber has a finite diameter of 400μm and thus deviates from a perfect point source, the multiplexed light diverges. After traversing the approximately 60cm from the diffraction grating to the spherical focusing mirror, the beam diameter typically increases from 10mm to 20mm.
In order to minimize device footprint and wavelength cross talk, a high dispersion grating must be used. High dispersion gratings diffract the individual wavelengths with larger angles of separation between the wavelengths compared to low dispersion gratings. Thus, the diffracted beams will have to travel shorter distances before they are separated enough spatially to enable collection without cross talk. For the results reported in this thesis, either a 600 or 1200 groove/mm grating is utilized operating in a first-order Littrow configuration. This combination enables the demultiplexing of wavelengths near 1.4 μm separated by greater than 50cm⁻¹ along a diffraction path of less than 60cm.

2.3.3 Impact, Cause, and Solutions to Polarization-Related Noise

Polarization-related effects can lead to potential sensor noise for wavelength-multiplexed TDL systems and must be considered during sensor design. Two
mechanisms can shift the polarization of light in these systems: (1) fiber motion, (2) stress-induced birefringence. The light exiting fiber-coupled diode lasers is typically linearly polarized. As the single-mode fiber that carries the light from the lasers to the combustion device moves during engine operation, the polarization of the light emitted from the fiber changes. Similarly, as the multi-mode fiber that collects the light moves, the polarization shifts. The windows that provide optical access to the combustors can also change the polarization of the transmitted light. During engine operation (both in PDEs and IC engines) the stress state of the window material changes due to varying combustor pressure or thermal expansion of the window and surrounding metal mount. As the stress state changes, the polarization of the transmitted light can rotate as a result of stress-induced birefringence (Musculus and Pickett, 2005).

Diffraction gratings show reflection efficiencies that depend greatly on the polarization of the incident light, as shown in Fig. 2.12. For example, a 1200g/mm grating blazed at 1μm has reflection efficiencies of 90 percent for s-plane polarized light and 20 percent for p-plane polarized light. Thus if the polarization of the incident light onto the diffraction grating (used for demultiplexing) changes, transmission fluctuations result. These effects will be further detailed in Chapter 5.
There are multiple strategies that would help mitigate the effects of polarization-related noise. Polarization-maintaining (PM) single-mode fiber could be used on both the lasers and the single-mode fiber transmitting the light to the combustor (although PM fiber combiners that couple more than two laser wavelengths are currently unavailable). Thus as this fiber moves, rotates, and vibrates, the polarization of the transmitted light would remain constant. In order to overcome stress-induced birefringence effects resulting from the window material, the windows on the combustion device could be manufactured from crystalline material (such as sapphire) and aligned such that the light propagates along the optical axis thus minimizing the effects of stress-induced birefringence. Alternative gratings with better matched polarization-dependent efficiencies, such as a 600g/mm 1.6μm blazed grating shown on the right of Fig. 2.12, would also reduce the effects of polarization fluctuation.
2.3.4 Alternative Demultiplexing Strategies

Alternative demultiplexing strategies such as time-division, and spectral-filtering can be advantageous for certain situations. Time-division multiplexing is achieved by alternating between laser wavelengths rapidly (kHz rates) either by fiber switching or by laser current modulation, thus each laser wavelength is active for a fraction of the total time. This enables relatively simple optical setup compared to spatial demultiplexing as a single detector can be utilized. The main disadvantages relate to sensor bandwidth. As each laser operates for only a fraction of the time, data is collected periodically rather than continuously decreasing the total bandwidth of the sensor. The sensor bandwidth also decreases proportional to the number of wavelengths used. This technique is used rarely, only in situations where the combustion device operates at relatively steady state and sensor bandwidth is not a limitation.

Spectral filter demultiplexing provides another alternative to separate the individual wavelengths. For this technique, the multiplexed light is split into multiple channels and a band-pass filter rejects all but a single wavelength. This can be achieved either through in-line fiber-optic filters or free-space filters. The demultiplexed light is then collected onto individual detectors. While this technique is relatively straightforward to implement, it suffers from several drawbacks. Band-pass filters are available only at specific wavelengths, thus limiting the selection of wavelengths. The system also suffers from signal loss as the laser power degrades proportional to the number of filters utilized. This system does not provide the flexibility of spatial demultiplexing scheme for interchanging laser wavelengths.
2.4 **Ultraviolet Sensors**

The previous sections focused on the use of fiber-optic-coupled, wavelength-multiplexed, diode-laser sensors which are used primarily to probe rovibrational absorption transitions (most commonly water vapor for sensors reported in this thesis) for thermometry or gas concentration measurements. Ultraviolet laser absorption sensors probing rovibronic transitions can prove advantageous for specific sensing situations, especially for high temperatures, low gas concentrations, or short optical path length measurement conditions. For these sensing environments, rovibrational absorption strengths often are too weak for direct absorption measurements. Chapter 3 describes two UV-based sensors to measure CO\textsubscript{2} temperature and OH concentration in a single-cycle PDE.

### 2.4.1 CO\textsubscript{2}-Based Thermometry

Recent progress in shock tube research has provided a detailed characterization of the absorption coefficient of carbon dioxide in the wavelength region from 190-320nm and the temperature range from 1800-4500K (Oehlschlaeger *et al.*, 2004; Schulz *et al.*, 2002). For these conditions, CO\textsubscript{2} exhibits a spectrally broad absorption coefficient with strong temperature dependence as shown in Fig. 2.13. While the initial investigation and shock tube characterization of the CO\textsubscript{2} absorption coefficient at high temperatures was motivated by the need to correct for laser attenuation in high-pressure PLIF measurements in IC engines, researchers have demonstrated the utility of the technique to measure temperature in a variety of combustion environments (Jeffries *et al.*, 2005; Mattison *et al.*, 2005; Oehlschlaeger, Davidson, and Hanson, 2005).
Figure 2.13. Calculated absorbance at 266nm (for a 3.8cm optical path length) for the equilibrium products of a stoichiometric ethylene-oxygen mixture as a function of temperature and pressure.

### 2.4.2 OH Concentration

The hydroxyl radical, OH, is a significant gas species for combustion research due to its importance in the heat release process and as a marker of chemical reaction progress. Numerous researchers have measured OH concentration in flames and shock tubes by probing individual absorption features in the (0, 0) band of the A-X system near 306nm using direct absorption spectroscopy (Herbon, 2004; Rea, 1991). The rovibronic transitions in this system, shown in Fig. 2.14, have strong absorption coefficients enabling measurements at low concentrations and high temperatures. While OH absorption measurements have been widely demonstrated in highly controlled experimental facilities such as shock tubes, fewer studies have been performed which utilize this technique for extremely harsh measurement environments such as PDEs.
Researchers developing computational simulations to predict the performance of pulse detonation engines have employed numerous models of chemistry and heat transfer to account for chemical recombination and energy loss mechanisms in PDE systems. In order to evaluate and validate the accuracy of these simulation subroutines, accurate measurements of chemical composition and temperature are needed. Because predicted OH concentration histories are sensitive to the chemistry model and temperature, they serve as an important metric of simulation performance. Chapter 3 includes a description of techniques and results for time resolved measurements of CO₂ temperature and OH concentration designed to evaluate computational simulation performance.
Chapter 3: UV-based $T_{CO2}$ and $X_{OH}$ for Single-Pulse PDE: Simulation Validation

3.1 Introduction

As outlined in Chapter 1, pulse detonation engines have received much interest in recent years due to their potential advantages compared to conventional aero-propulsion systems, including high thermodynamic efficiency, high specific impulse ($I_{sp}$), and reduced mechanical complexity. (Bussing and Pappas, 1994; Eidelman, 1997; Eidelman and Yang, 1998; Kailasanath, 2001.) Thus, researchers have performed both computational and experimental studies designed to characterize the performance, study feasibility, and investigate limitations of the device. However, detailed experimental measurements of key characteristic parameters (including temperature, pressure, and gas composition) have not been available to allow critical evaluation of the various physical and chemical models imbedded in currently available PDE simulations.

Assumptions regarding reactive chemistry employed in most computational simulations of PDE performance can be broken down into two main strategies: 1) frozen
chemistry, with composition typically fixed at the Chapman-Jouguet (C-J) plane values, and 2) finite-rate chemistry. While comparisons between these two approaches indicate that there are small differences in overall performance for straight tubes (as determined by $I_{sp}$ and head-end pressure calculations), differences in secondary performance characteristics, such as temperature and species concentrations, can arise and become important when thermally dependent loss mechanisms such as energy loss due to heat transfer are included in PDE simulations (Radulescu and Hanson, 2005). Inclusion of heat transfer losses can degrade $I_{sp}$ by 10-15% for typical tube lengths. The secondary differences and heat transfer losses could become more important in overall performance when additional thrust-enhancement devices such as nozzles are included in system calculations.

As discussed in Chapter 1, diagnostics based on laser absorption spectroscopy have been successfully demonstrated even in harsh measurement environments, such as the PDE. Hence these diagnostics, capable of measuring several pertinent gas properties, can play an important role in assessing and refining PDE simulations. Most recent studies of single-cycle PDE experiments used for assessing computational simulations have concentrated on characterizing the time integral of head-wall pressure, since this quantity is most closely associated with overall PDE propulsion performance parameters such as thrust and specific impulse. In order to evaluate chemistry and heat transfer assumptions employed in computational simulations, transient measurements of temperature and species concentration are needed. Time-resolved velocity measurements could also play a critical role in simulation validation, especially in the case of multi-tube PDEs and PDEs with nozzles.
In this chapter, two new diagnostics and associated results are introduced for a straight-tube PDE operating on C_2H_4-O_2. The first technique, based on UV absorption of a major combustion product, CO_2, provides a new method of determining temporally resolved gas temperature. The second diagnostic, based on UV absorption of OH, monitors the transient OH concentration behind the detonation wave during product gas blowdown. The two methods, example results, and the evaluation of two PDE computational simulations are described below.

3.2 Experimental Setup

This section will describe the UV absorption experimental techniques employed to measure CO_2 gas temperature and OH concentration in the single-cycle pulse detonation tube at Stanford University shown in Fig. 3.1.

Figure 3.1 Stanford pulse detonation tube facility.
3.2.1 Stanford Pulse Detonation Tube Facility

Experiments were performed on the Stanford pulse detonation tube facility. The detonation tube, shown in Fig 3.2, is 3.8 cm in diameter and 160 cm in length, and is instrumented with pressure ports, ion probes (to track wave front position), and optical access ports to enable laser-based absorption measurements.

![Diagram of Stanford Pulse Detonation Tube Facility](image)

Figure 3.2. Schematic of Stanford PDE facility with CW UV laser diagnostics.

For these experiments, the tube was operated in a single-shot mode on premixed, stoichiometric ethylene-oxygen, as measured by a diode-laser-based ethylene sensor (Ma
et al., 2002). The ethylene and oxygen gas is premixed upstream of the gas injection point ensuring a uniform charge. The tube is instrumented with 16 pressure transducer and ion probe ports to track the wave trajectory and measure both head-end and side-wall pressure using Kistler® piezoelectric pressure transducers (model 603B1) coupled to charge-mode amplifiers (model 5010B). Nine optical access ports permit laser-based measurements along the length of the tube through UV-grade fused silica windows. Results of pressure and wave trajectory studies confirm a deflagration-to-detonation transition distance (DDT) of less than 30 cm and a measured wave velocity within 3% of the predicted C-J value; repeatability of side-wall pressure traces confirm reliable shot-to-shot repeatability. All results reported here are measured at the 144 cm measurement station.

### 3.2.2 CO₂ Thermometry

Recent progress in shock tube research has enabled spectrally resolved characterization of a strong, UV absorption band of CO₂ (Oehlschalaeger et al., 2004; Schulz et al., 2002). This absorption band provides a new and promising tool for measuring temperature via line-of-sight absorption measurements in hot combustion gases, as discussed in Chapter 2. The temperature sensor reported here utilizes 266 nm and 306 nm CW UV laser radiation to measure CO₂ absorption, enabling accurate, time-resolved temperature measurements from 2000K to 4000K (conditions pertinent to the PDE operating range).

The theoretical groundwork for extracting temperature or species concentration in high temperature combustion environments from laser absorption measurements of
spectroscopic features is described in Chapter 2. In brief, a laser beam tuned to resonant
CO₂ absorption is pitched through a test gas of interest and its transmitted intensity is
monitored using a photo-detector. For harsh environments, such as the PDE, in which
non-resonant effects such as extinction due to soot and intensity modulation due to
window effects cause changes in the transmitted beam intensity, the laser is also tuned off
the absorption band for some experiments to provide an accurate baseline transmission
measurement.

\[ k_{\nu, \text{CO}_2} = k_{\nu, \text{CO}_2}(T) \]  (3.1)

The CO₂ absorption coefficient (Eqn. 3.1) has strong dependence on temperature
over UV wavelengths from about 190 nm to 320 nm. The functional dependence has
been well-characterized at high temperature (900K - 3050K) and recently extended to
4500K at 266 nm.

Figure 3.3 shows the calculated product of the absorption coefficient and the
partial pressure of equilibrium CO₂ at 266 nm and 306 nm as a function of temperature
for 6 pressures typical of a PDE operation cycle. The equilibrium mole fraction of CO₂ is
calculated at each temperature and pressure assuming an initial gas composition of
stoichiometric ethylene-oxygen using the STANJAN equilibrium gas solver. The results
of the OH diagnostic (reported in the next section) and calculations using CHEMKIN
indicate that the chemical kinetics in this system are fast enough to ensure a quasi-
equilibrium gas composition on the time-scales of interest in this study. For each
wavelength as pressure is held constant, the absorbance by CO₂ per unit path length
changes with temperature. This functional dependence enables CO₂-based thermometry.
Figure 3.3. Product of absorption coefficient and CO\textsubscript{2} partial pressure at 306 nm (top) and 266 nm (bottom) as a function of pressure for equilibrium products of stoichiometric C\textsubscript{2}H\textsubscript{4}-O\textsubscript{2}.

Typical temperature sensors utilizing spectroscopic absorption require measurements of two separate absorption features or measurements of a single absorption feature and pressure at known gas composition. For this sensor, two independent measurements are made: transmission at 306 nm and 266 nm, and pressure. At each time step during the PDE cycle, the measured pressure is used to calculate the temperature-dependent absorbance quantity, as shown in Fig. 3.3. By taking the intersection point of the measured and temperature-dependent, calculated absorbance at each time step, temperature is inferred. Two resonant wavelengths are utilized here to ensure appropriate sensitivity and accuracy of the measurement throughout the cycle.
A 632 nm (HeNe laser) off-line beam is used to track extinction due to soot, beam steering, and window transmission variation and thereby correct the $I_0$ signal used in equation 1 for each of the two UV wavelengths used to measure CO$_2$ absorption. A cw, frequency-doubled, Nd:YAG-pumped tunable dye laser produces 4 mW of light near 306nm. A second 532 nm Nd:YAG laser is doubled with a beta-BaB$_2$O$_4$ (BBO) crystal producing 0.5 mW of 266 nm light. Each beam is simultaneously pitched through the 144 cm measurement station, shown in Fig. 3.2. The intensities of the transmitted beams are individually monitored using silicon photo-detectors (Thorlabs® model PDA555). A National Instruments® analog-to-digital converter card coupled to a personal computer monitors the output of each detector with a sampling rate of 1 MHz.

![Figure 3.4](image)

Figure 3.4. Normalized detector signals for 4 wavelengths used to measure temperature and OH concentration in the PDE tube filled with stoichiometric C$_2$H$_4$-O$_2$ at 1 atm, 296 K.
Sample laser transmission data as a function of time after detonation ignition are shown in Fig. 3.4. The detonation arrives at the measurement station at 0.6 ms; a significant decrease in transmission of the resonant beams occurs due to CO₂ absorption. The transmission continues to change as the pressure and temperature decrease until the blow-down is complete at 8 ms. The simultaneously measured pressure data at the measurement station are shown in Fig 3.5.

![Figure 3.5](image)

Figure 3.5. Measured and simulated pressure at the 144 cm measurement location.

The temperature is inferred from the measured pressure and transmission data, as shown in Figs. 3.6 and 3.7. The measurement error for the temperature results is estimated to be ±4 percent. The 266 nm and 306 nm wavelengths are used for different periods of the cycle to maximize sensitivity and accuracy of the temperature
measurement. A small gap in the reported temperature appears from 5 to 6 ms; future iterations of this sensing technique could include additional UV wavelengths to enable accurate temperature measurements over the entire blowdown cycle. This time-resolved temperature measurement enables sensitive evaluation of computational simulations as discussed in later sections of this paper.

![Figure 3.6](image)

Figure 3.6. Inferred temperature from CO₂ absorption and measured pressure compared to simulation results. Both simulations assume frozen composition and fixed γ.
Figure 3.7. Inferred temperature from measured CO₂ absorption and pressure compared to two finite-rate chemistry simulation results.

The results obtained with this sensor demonstrate the potential for using UV absorption by CO₂ to determine temperature in harsh measurement environments using native combustion product species. This sensing technique also provides the advantage of being an absolute temperature sensor. Previously developed temperature sensors for PDEs provided relative temperature results, but required a calibration point (usually the well-established C-J condition) to infer absolute temperature (Sanders et al., 2000; Sanders et al., 2002.)

3.2.3 OH Concentration

The second diagnostic introduced in this study, based on an in situ UV laser absorption measurement of OH, provides transient OH concentration behind the
detonation wave during the product gas blowdown. These OH concentration data provide another sensitive tool needed to evaluate computational simulation results, specifically differences caused by the inclusion of finite-rate chemistry and heat transfer losses.

Previous, laser-based measurements of species concentration in PDE flows have utilized near-infrared diode lasers to probe rovibrational spectroscopic transitions such as those of water vapor (Sanders et al., 2000). The present OH concentration measurement uses UV laser light from a cw Nd:YAG-pumped dye laser to probe electronic transitions of OH. These transitions provide the advantage of increased absorption strength compared to rovibrational transitions in the electronic ground state, but require use of a more complicated laser source.

As shown in Fig. 3.8, the absorption spectra of the OH A-X(0,0) system contains a number of features near 306 nm that have previously been well-characterized and could potentially be used to determine the species concentration (Herbon, 2004; Rea, 1991). For this set of measurements, the relatively weak S_{21}(1) transition was chosen for measuring the OH concentration behind the detonation wave during the blowdown process for two reasons. Firstly, the transition is well-isolated from surrounding absorption features, which minimizes the effects of interference caused by line-broadening during high pressure portion of the cycle. Secondly, the S_{21}(1) transition also has an appropriate absorption strength for the test conditions of interest. The absorption is strong enough to provide a high signal-to-noise ratio, yet is not so strong as to cause the gas to become optically thick.
A measurement cycle consists of two consecutive detonation experiments for which the dye laser, shown in Fig. 3.2, is tuned to two different wavelengths. The raw laser transmission data is shown in Fig. 3.4. The gas mixture is ignited at time 0; the detonation wave reaches the measurement station at 0.6 ms. The first wavelength (off-line OH, 306 nm) is used to track non-resonant extinction caused by soot and window effects and resonant absorption by CO₂, providing the I₀ signal for the OH concentration measurement. At this wavelength, hot CO₂ in the combustion products absorbs the laser light, as discussed in the thermometry section, reducing its transmitted value. For the second wavelength (306.3413 nm, the line center of S₂₁(1)), absorption by OH further reduces the transmitted laser intensity values compared to the 306 nm signal. Because the absorption by CO₂ in this region is a spectrally broad feature, it can be considered constant in the 306 nm and the 306.3413 nm signals. Therefore, transmission and thus
absorbance by the $S_{21}(1)$ OH feature is calculated from the ratio of the 306 nm and the 306.3413 nm signals using the Beer-Lambert relation.

In order to determine OH concentration from the absorption measurements, the temperature and pressure of the gas need to be known to determine the appropriate linestrength ($S$) and lineshape function ($\phi$) values for the spectral absorption coefficient, as shown in Eqn. 3.2 and further described in Chapter 2. The temperature and pressure dependence of these parameters have been well-characterized for the OH $A-X(0,0)$ system.

$$k_v = S(T) \ast \phi(T, P, X_i) \quad (3.2)$$

Using the temporally resolved temperature and pressure results from the previous section, the absorption coefficient can be calculated at each time step. Using this calculated trace in conjunction with the measured OH absorption, OH mole fraction is inferred. As shown in Fig. 3.9, the measured OH mole fraction decreases by a factor of four during the first 4 ms of the burnt gas blowdown. The measurement error for the OH concentration results is estimated to be $\pm 7$ percent.
Figure 3.9. OH mole fraction (from measured absorption, temperature, and pressure) compared to two simulation results. Both frozen chemistry simulations yield a constant value of $X_{OH} = 0.126$.

### 3.3 Description of Simulation

Numerous researchers have developed both simplified and complex simulations designed to predict and evaluate PDE performance and to optimize designs for both single- and multi-cycle engines (Kailasanath and Patnaik, 2000; Morris, 2003; Povinelli and Yungster, 2002; Owens et al., 2005; Radulescu and Hanson, 2005; Wu, Ma, and Yang, 2003). Two of the sub-mechanism included in simulations that impact predicted PDE parameters and performance are chemistry and heat transfer. By including additional heat release due to chemical recombination of the highly dissociated C-J state during blowdown through a finite-rate chemistry routine or by including energy loss due to heat transfer, the temperature and gas composition predicted by PDE simulations can
be altered, leading to differences in predicted performance. The following section evaluates the impact of chemistry and heat transfer by applying varying postulations of these two sub-mechanisms and comparing the predicted parameters with the measured experimental data.

The results from two simulations employing different models for chemistry and heat transfer are evaluated. Although the details of the simulations can be found in the references; brief descriptions are reported here. The first simulation, developed by Owens and Hanson, assumes frozen chemical composition at the C-J condition and neglects the influence of heat transfer losses (Owens et al., 2005). The simulation solves the quasi-one-dimensional Euler equations using the Roe, flux-splitting algorithm. It utilizes a constant $\gamma$ with a choked-flow or fixed-pressure exit boundary condition with no relaxation length (depending on whether the exit pressure differential is sufficient to maintain sonic flow). Results are reported for two values of $\gamma$ (which arise from two potential definitions of sound speed: equilibrium and frozen), as defined in Eqns. 3.3 and 3.4.

$$\gamma_s = \frac{d \ln(P)}{d \ln(\rho)} \frac{a_e^2}{R \cdot T} \quad (3.3)$$

$$\gamma_f = \frac{c_p}{c_v} \frac{a_f^2}{R \cdot T} \quad (3.4)$$

In these definitions, $P$ is pressure, $\rho$ is density, $a_e$ is the equilibrium sound speed, $a_f$ is the frozen sound speed, $R$ is the universal gas constant, $c_p$ is the constant pressure specific heat, $c_v$ is the constant volume specific heat, and $T$ is temperature. For the stoichiometric ethylene-oxygen C-J state, $\gamma_s = 1.14$ and $\gamma_f = 1.24$. 
The second simulation, developed by Morris, includes finite-rate chemistry and investigates the influence of heat transfer losses (Morris, 2003). The code implements a slightly modified version of the ethylene-oxygen reduced chemistry mechanism developed by Varatharajan and Williams, utilizing the 21 species and 33 forward reactions of that mechanism, but with all 33 reverse reaction rates computed using the equilibrium constants (Varatharajan and F.A. Williams, 2002). The simulation accurately calculates the C-J detonation velocity and state. The solution method to the quasi-one-dimensional Euler equations can be found in the Morris reference. Results here are reported for cases neglecting and including energy loss due to heat transfer. The heat loss term utilized in this simulation is similar to that reported by Radulescu and Hanson, as shown in Eqn 3.5 (Radulescu and Hanson, 2005).

\[
Q_{\text{loss}} = \frac{2 \cdot C_f}{Pr^{2/3} \cdot D_h} \cdot \rho_e \cdot |u_e| \cdot (h_{w,eq} - h_{aw})
\]  

(3.5)

In this equation, \(C_f\) is the skin friction coefficient (for this analysis, \(C_f = 0.0062\)), \(Pr\) is the Prandtl number, \(D_h\) is the hydraulic diameter, \(\rho_e\) is the freestream density, \(u_e\) is the freestream velocity, \(h_{w,eq}\) is the wall enthalpy (equilibrium composition), and \(h_{aw}\) is the adiabatic wall enthalpy. The heat loss simulation also includes losses due to frictional effects, but these cause only minor effects on temperature, pressure and gas composition.

Results from 4 simulation runs (frozen chemistry \(\gamma = 1.24 = \gamma_f\), frozen chemistry \(\gamma = 1.14 = \gamma_s\), finite-rate chemistry, and finite rate chemistry with heat transfer) compared to current measurements are shown in Figs. 3.5-3.7 and 3.9.
3.4 Results

The differing assumptions and sub-mechanisms employed in the computational simulations have varying effects on the pressure, temperature and gas composition characteristics of PDEs. As shown in Fig. 3.5, each of the four simulation runs accurately predicts the measured side-wall pressure during the Taylor expansion region from 0 to 1.5 ms. During the lower pressure portion of the blowdown from 1.5 to 5 ms, the simulations over-predict the measured pressure with the frozen chemistry simulations providing the best agreement to the measured results. This result is consistent with specific impulse ($I_{sp}$) comparisons between measurements and simulations for which the simulations overpredict $I_{sp}$ by 6 percent. The relative agreement between the simulated pressure traces demonstrates that side-wall pressure is relatively insensitive to changes in the chemistry and heat transfer models.

Temperature provides a more sensitive metric to evaluate these simulations. As shown in Fig. 3.6, the predicted temperatures for the frozen chemistry, constant $\gamma$ simulations differ by 20-30% between the two definitions of $\gamma$. The results from the simulation utilizing $\gamma_s$ agree well with the measured temperature throughout the PDE cycle, although this agreement is somewhat artificial owing to the neglect of heat transfer and chemical recombination. The results from the simulation utilizing $\gamma_f$ consistently underpredict the measured temperature. The rapid decrease in measured temperature at 7.7 ms is consistent with previous measurements; this decrease is thought to be due to interaction of the detonation wave with the walls of the dump-tank vessel used to capture product combustion gases.
The C-J state for an ethylene-oxygen detonation consists of thermally dissociated product gases. As the temperature and pressure decrease during the blowdown cycle of PDE operation, the temperature should increase compared to a chemically frozen system due to chemical recombination of the dissociated gases. As shown in Fig. 3.7, the predicted temperature from the simulation utilizing finite-rate chemistry is higher than the measured temperature and is therefore greater than both frozen chemistry simulation results shown in Fig. 3.6. When energy loss due to heat transfer is included in the simulation, however, the temperature decreases and agrees very well with the measured data.

OH mole fraction data provide another metric to evaluate the accuracy of the finite-rate chemistry and heat transfer simulations, and validate the equilibrium product composition assumption employed for the thermometry measurement. During the first 4.5 ms of the product gas blowdown, the OH mole fraction decreases by a factor of four, as shown in Fig. 3.9, due to its high sensitivity to changes in temperature for these test conditions. This demonstrates that chemical recombination rapidly occurs as the temperature decreases from the C-J state. The simulation utilizing finite-rate chemistry (without heat transfer) consistently overpredicts the measured OH mole fraction; the simulation employing both finite-rate chemistry and heat transfer matches the measured data well, with slight disagreement only for the first 1 ms of blowdown. For both frozen chemistry models, OH mole fraction remains constant at the initial C-J value, hence differing substantially from the measured OH time history.
Figure 3.10. Measured OH mole fraction compared to two calculated results. The trace labeled equilibrium is determined for stoichiometric C$_2$H$_4$-O$_2$ from measured T and P using an equilibrium gas solver. The second calculated trace is based on the finite-rate chemistry solution with losses due to heat transfer and wall friction.

A close examination of the finite-rate simulations reveals that the combustion gases for this PDE case remain close to chemical equilibrium. Hence, it is of interest to compare OH measurements with a simple solution assuming chemical equilibrium. Figure 3.10 shows two calculated traces and one measured trace of OH mole fraction. The first calculation is the finite-rate chemistry simulation, including heat transfer. The second calculation utilizes the measured temperature and pressure and a simple chemical equilibrium assumption to determine a temporally resolved, equilibrium OH
concentration using the STANJAN equilibrium code. The measured values determined using the OH sensor agree well with both calculations, confirming that the reactive chemistry is well-approximated by a quasi-equilibrium process in this PDE environment. This observation is substantiated by chemical modeling using CHEMKIN that indicates the gases quickly equilibrate (<1 μs) at these conditions. The OH concentration quickly drops below its initial C-J value (X_{OH}=0.12) as the temperature and pressure decrease, clearly showing the error inherent in the frozen chemistry models. Finally, these results confirm the assumption of equilibrium product gases employed for the CO₂-based thermometry measurement.

3.5 Summary

In this chapter, we introduced two new diagnostics based on UV laser absorption to measure time-resolved T and X_{OH} in high-temperature, harsh measurement environments characteristic of PDE flowfields. These results prove useful for evaluating PDE models to reveal the differences resulting from finite-rate and frozen-chemistry assumptions and to evaluate loss mechanisms such as heat transfer which may be significant in PDE flows.

The first simulation, utilizing frozen gas composition, can accurately predict the measured pressure and temperature profiles if an appropriate γ is utilized, γ=γ_s. While such simulations neglect additional heat release due to chemical recombination and energy loss due to heat transfer, the two missing effects appear to negate each other. Of course, the frozen chemistry model (constant X_{OH}) fails badly with regard to properly simulating the decay of OH mole fraction. The second and more correct simulation...
incorporates finite-rate chemistry and includes losses due to heat transfer and friction. With the proper inclusion of losses due to heat-transfer, the finite-rate chemistry code accurately predicts temperature, pressure, and OH concentration. Agreement between the measured and predicted metrics inspires confidence in the accuracy of the simulations to be utilized to predict the performance of more complicated PDE systems such as multi-pulse tubes or tubes with nozzles.
Chapter 4:

\( T_{\text{H}_2\text{O}} \) Measurements using a Fiber-Optic TDL Water Vapor Absorption Sensor in a Multi-Pulse PDE: Engine Evaluation

4.1 Introduction

Multi-pulse PDEs utilize a number of varying designs. The most widely studied PDE design relies on a closed wall tube. For this design, a fuel-air mixture is injected into the closed end of a detonation tube through a robust valve. After the mixture injected, an ignition system at the closed end of the tube ignites the mixture and a detonation wave rapidly forms and traverses the tube. The resulting pressure increase and momentum flux across the open end of the tube produces thrust. A valveless PDE architecture, which relies on a constant air-flow stream, eliminates the need for a robust valve to meter the air flow (Brophy et al., 2002; Brophy and Hanson, 2005; Wittmers, 2004). While the valveless design simplifies the mechanical requirements of the PDE, it increases the complexity of the engine flowfield and the ignition system, especially as engine operation
rates increase. While conventional methods of studying multi-cycle device performance such as pressure and thrust measurements provide valuable data, measurements of temperature and species concentration are needed to accurately characterize system performance and to investigate engine component failure thresholds as engine operation rates are increased. Diagnostics based on tunable-diode-laser absorption spectroscopy (TDLAS) provide a unique tool to meet these requirements.

In this Chapter, an advanced, fiber-optic-based, multiplexed-wavelength tunable diode-laser sensor is described which is used to measure temperature during multi-pulse operation of a valveless PDE at the Naval Postgraduate School in Monterey, CA. The fiber-optic sensor demonstrates improvements in both optical engineering and spectroscopic design over previous sensors to enable remote measurements at engine operation rates up to 40Hz on a translating, vibrating PDE (Hinckley, Jeffries, and Hanson, 2004; Mattison et al., 2003). Three engine operation modes were studied: (1) 40 Hz cold-flow operation during which the engine flows with the fuel charge but the igniter is turned off; (2) 40 Hz hot-flow operation; (3) 40 Hz operation during which the purge air flow in the initiator is reduced until the onset of flame-holding.

### 4.2 Experimental Setup

Multi-cycle PDEs present vastly different sensing challenges and thus specialty solutions compared to the single-cycle PDE operation described in Chapter 3. In this section, the operation of the valveless PDE and the sensor design and layout are discussed.
4.2.1 Naval Postgraduate School PDE Facility

The tunable diode laser sensor described in this chapter was utilized to characterize and evaluate the valveless pulse detonation engine at the Naval Postgraduate School in Monterey, CA shown in Fig. 4.1. A detailed description of this engine can be found in the references. In brief, the PDE which is mounted to a six degree-of-freedom thrust stand can be fueled by either liquid or gaseous fuels and utilizes a valveless air delivery system to supply the main combustor. The PDE employs an initiator/main tube configuration for which a detonation is formed in a small-volume, oxygen-enriched initiator and then diffracted into a large volume, fuel-air charged main combustor tube which produces a majority of the thrust. For the set of experiments reported in this paper, the ethylene/air configured PDE was evaluated at repetition rates up to 40 Hz in both successful detonation modes and artificially created engine failure modes designed to investigate sensor performance and engine component failure thresholds.

Figure 4.1. Schematic of NPS PDE facility with optical access provided at the exit of the initiator.

This engine consists of a 10 cm diameter main combustor tube and a 4.4 cm diameter initiator tube. The main combustor tube is fed by a constant flow of vitiated air and intermittently injected ethylene which are mixed upstream of the main combustor in
four inlet arms which discharge into a common manifold. A vitiator (hydrogen fueled) in the compressed air stream generates the heated air used to supply the main tube. The initiator is fed by a constant flow air stream and an intermittently injected oxygen/ethylene charge; the oxygen supplement ensures charge detonability in the short initiator section. A fuel sensor based on ethylene absorption at 3.39\,\text{um} monitors the equivalence ratio of both the main combustor and the initiator (Klingbeil et al., 2005).

1.) Main combustor fuel injection:

2.) Initiator fuel/O\textsubscript{2} injection:

3.) Ignition/ Detonation propagation

4.) Thrust, exhaust blow-down, purge:

Figure 4.2. Schematic of the four stages of a single operation cycle of the NPS PDE.

During normal operation, the main combustor and initiator are charged simultaneously as shown in stages 1 and 2 of Fig 4.2. When the fuel mixtures in both
sections reach their respective exit planes, a spark system ignites the initiator. After a short deflagration-to-detonation (DDT) length in the initiator, a detonation forms and then transmits to the main combustor as shown in stage 3 of Fig. 4.2. After a short blow-down period during which the high pressure gases in the combustor exhaust producing thrust as shown in stage 4 of Fig. 4.2, the constant-flow air purges the remaining combustion products. Then, a fresh fuel charge is injected into both sections and the cycle repeats. This entire process is controlled by a PC-based LABVIEW system coupled to a BNC pulse generator (Wittmers, 2004).

Figure 4.3. Timing diagram of a single operation cycle of the NPS PDE.

Optical access for the line-of-sight laser sensors is provided 5 cm downstream of the initiator exit through 1.2 cm diameter wedged sapphire windows. High-speed piezoelectric pressure transducers are utilized to monitor the pressure and wave position at
both the optical measurement plane and along the main combustor. A generalized time sequence of a single PDE cycle is shown in Fig. 4.3. As depicted, the pressure and temperature relaxation times are quite different demonstrating the need for a near-real-time temperature sensor to fully characterize the engine operation.

In this chapter, temperature histories measured using the TDL-based thermometry sensor for three engine operation modes are reported. The first mode consists of cold-flow operation during which the engine runs with the fuel charge at 40 Hz but the igniter is turned off. The second mode consists of 40 Hz operation hot flows for which the igniter is turned on and successful detonations are formed. The third mode consists of 40 Hz operation during which the purge air flow in the initiator is reduced until the onset of flame-holding during which the residual combustion products prematurely ignite the fresh fuel charge injected for the next engine cycle. These types of measurements will become more important to help understand engine failure modes as engine operation rates are increased and the effects such as pulse-to-pulse interference and flame-holding begin to appear. The results from the TDL-based sensor provide a unique tool (in addition to pressure and thrust data) to evaluate and characterize both successful operation and PDE failure modes.

4.2.2 Multiplexed TDL Sensor

Sensors based on tunable diode-laser absorption spectroscopy provide unique diagnostic capabilities for investigating and characterizing the performance of PDEs, as outlined in Chapter 1. These sensors, capable of measuring several pertinent parameters such as temperature, fuel concentration, burned-gas concentration, burned-gas velocity,
and pressure are used to characterize idealized single-cycle laboratory engines for computation simulation validation and high-repetition-rate engines for performance evaluation.

Thermometry based on line-of-sight TDLAS has been detailed and described in Chapter 2. In brief, when spectrally narrow absorption features exist, distributed-feedback lasers (DFB) can be scanned across the feature by modulating the injection current to the laser in a sawtooth manner, as shown in Fig. 4.4. As the intensity of the laser increases, the wavelength also changes. By fitting a polynomial to the non-absorbing wings surrounding the absorption feature, a zero absorbance baseline can be determined. Then, by utilizing the Beer-Lambert relation, the spectral absorption coefficient is determined. The temperature-dependent variation of two water absorption features utilized for thermometry in this paper is shown in Fig. 4.5. As shown, the peak centerline absorbance changes as a function of temperature. By measuring two absorption features and taking the ratio of the absorption coefficients, temperature can be inferred.

![Example laser scans across the 7185.59 cm⁻¹ absorption feature during the detonation arrival at the optical measurement location.](image)

Figure 4.4. Example laser scans across the 7185.59 cm⁻¹ absorption feature during the detonation arrival at the optical measurement location.
A previous sensor based on TDLAS for studying high-repetition-rate PDE operation utilized a single free-space laser to measure two adjacent near infrared (NIR) water transitions to measure temperature and water mole-fraction (Mattison et al., 2003). While this sensor provided valuable information for characterizing normal PDE operation and engine failure modes caused by multi-pulse operation such as flame-holding, it possessed a few limitations. First, the laser had to be fixed to the thrust stand (rather than the engine itself) as the free-space laser could not withstand the fast axial movements caused by engine firing. Second, the sensor had a limited temperature range, as only two water transitions were measured. A wavelength-multiplexed sensor in which the lasers are fiber-coupled can overcome these limitations, as demonstrated in this chapter. By employing a fiber-coupled system, several laser wavelengths are multiplexed into a single fiber enabling the measurement of individual absorption transitions. By utilizing multiple absorption features both the sensitivity and measurement range of the sensor can be improved. Also, by remotely locating the vibration sensitive optics and electronics by employing fiber optics, the sensor can be directly connected to the PDE enabling measurements on a translating, vibrating engine. A first generation sensor of this type has been reported previously (Hinckley, Jeffries, and Hanson, 2004); this paper reports several advances over the previous system including improved accuracy and the ability to perform low noise measurements at engine repetition rates up to 40Hz.
Figure 4.5. Temperature-dependent absorbance for two water absorption features used in TDL-based sensor.

Figure 4.6 shows the temperature-dependent centerline absorption by four water transitions which are utilized for this sensor at the resulting ratio of three line pairs. The spectroscopic parameters ($\nu$, centerline frequency; $S_{296K}$, linestrength at 296 K; $E^\prime$, lower state energy) for each of the transitions utilized are shown in Table 4.1. By utilizing multiple line pairs, the temperature sensitivity and sensing range of the diagnostic is improved. A validation of the sensor using a heated cell containing a water vapor and air in a temperature controlled furnace is shown in Fig. 4.7.
Figure 4.6. Centerline absorbance (top) for four water absorption transitions and three ratios of centerline absorbance (bottom) used for thermometry in TDL-based sensor.

Table 4.1. Spectroscopic parameters of water transitions used in TDLAS sensor (HITRAN 2000; Liu et al., 2005).

<table>
<thead>
<tr>
<th>$\nu$ [cm$^{-1}$]</th>
<th>$S_{296K}$ [cm$^{-1}$/atm]</th>
<th>$E^\prime$ [cm$^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>7390.13</td>
<td>8.53*10$^{-2}$</td>
<td>446.5</td>
</tr>
<tr>
<td>7185.59</td>
<td>1.97*10$^{-2}$</td>
<td>1045.1</td>
</tr>
<tr>
<td>7444.36</td>
<td>5.40*10$^{-4}$</td>
<td>1774.8</td>
</tr>
<tr>
<td>7444.37</td>
<td>5.76*10$^{-4}$</td>
<td>1806.7</td>
</tr>
<tr>
<td>6708.83</td>
<td>1.02*10$^{-6}$</td>
<td>3319.4</td>
</tr>
</tbody>
</table>
Figure 4.7. Heated furnace validation of TDL-based temperature sensor.

4.2.3 Optical Hardware

Figure 4.8. Schematic of Stanford TDL-based temperature sensor applied to the NPS PDE facility.
Figure 4.9. Photograph of Naval Postgraduate School PDE facility (left) with the fiber-optic coupled sensor attached to the engine. The optical test section (right) contains two axial measurement locations. The $T_{H2O}$ sensor is mounted at the upstream measurement location.

Figure 4.10. Schematic of optical arrangement for TDL sensor mounted to PDE.

The experimental setup for this multiplexed, fiber-based TDLAS sensor is shown in Fig. 4.8. Four fiber-coupled DFB lasers (NEL America, Inc.) are multiplexed using a
single-mode 1x4 combiner. Each laser produces approximately 10 mW of peak power.

Each laser is scanned across its targeted absorption feature at 5 kHz using a sawtooth function generated by a National Instruments PCI-6115 DAQ card coupled to a PC. The multiplexed laser light is then brought to the PDE through single-mode fiber (9 μm core) which is attached the PDE. This light is then collimated and pitched across the PDE combustor using a Thorlabs aspheric collimator (F230FC-C). After the light (2 mm beam diameter) traverses the combustion chamber, it is collected using an aspheric lens from Oz Optics (HPUCO-25-1300-M-10BQ) and focused into a 400 um core multi-mode fiber with a numerical aperture (NA) of 0.39. Wedged sapphire windows provide optical access to the PDE approximately 5 cm downstream of the initiator exit. The total transmission loss from the laser source to the optical detector is approximately 30 percent of the laser power which arises largely from reflection losses at the sapphire windows. A photograph of the optical test section and fiber optics appear is Fig. 4.9. The schematic of the PDE-mounted optics are detailed in Fig. 4.10. The T H2O sensor is mounted in the upstream optical measurement location. In the highlighted photograph shown in Fig. 4.9, the single-mode fiber appears in the lower portion of the photograph in yellow, and the multi-mode fiber appears in the upper portion of the photograph in orange. The path length across the combustor at this position is 7.2 cm.

As discussed in Chapter 2, each optical component utilized in these tests was chosen to optimize the signal quality. Single-mode fiber carries the light from the laser sources to the PDE to eliminate the effects of mode noise, compared to previously developed systems which employed multi-mode fiber on the delivery optics (Sanders et al., 2000). The light is then collimated to a 2 mm beam diameter and pitched across the
combustion chamber. A wide variety of commercial pitch lenses are available to collimate the multiplexed light to various beam diameters. The Thorlabs collimators were chosen due to their compact and rugged design which easily attaches to the 30mm diameter optical bosses supplied by the PDE optical test section. Within the Thorlabs suite of collimators, multiple collimated beam diameters are available. Compared to smaller beam diameter collimators, the 2mm version showed smaller susceptibility to window fouling especially from soot deposition on the sapphire windows. Wedged sapphire windows were chosen to provide optical access due to their toughness, optical transmission properties, and availability in custom shapes. The windows were both tapered and wedged. The taper enabled press mounting in the optical boss receptacle eliminating the need for chemical bonding. The wedge eliminated etalon formation in the optical train. The major improvement over previously developed systems included the use of a large diameter, small f/no aspheric collection lens which proved insensitive to beam translation of approximately 4mm in both the x and y directions.

The light collected by the collection lens traverses a 5m long section multi-mode fiber to the dispersion optical setup. The multiplexed light from the fiber is collimating using an aspheric lens (Optosigma 023-2392) and then pitched onto a diffraction grating (30mm x 30mm, 1200g/mm, 1st order) where it is demultiplexed. The demultiplexed beams are then focused onto individual 4 MHz large-area (3 mm diameter) amplified InGaAs photodetectors from Electro-Optical Systems Inc. (IGA-030-E5 / 4MHz) using concave mirrors. The resulting intensity is recorded by the same National Instruments card used to generate the sawtooth modulation function. The entire dispersion setup is enclosed in a N2 purge to eliminate interference absorption caused by atmospheric water.
The details of the dispersion setup of shown in Fig. 2.11 of Chapter 2. Both the single-mode pitch fiber and the multi-mode catch fiber are constrained to minimize the effects of fiber optic-based noise.

This optical setup is tolerant to both beamsteering and to engine vibration and translation. A set of benchtop experiments were conducted to evaluate the robustness of the fiber-based pitch and catch to beamsteering. The system was able to maintain full signal power while the pitch fiber was translated 4mm in both the x and y directions. Thus in performing optical alignment on the NPS PDE, after the pitch beam was centered in both window, a 5-axis optical stage was adjusted such that the beam was centered in the collection lens and such that the lens was rotated to be perpendicular to the incoming light.

![Figure 4.11. Schematic of Stanford TDL-based temperature sensor applied to the NPS PDE facility.](image)

As shown in Fig. 4.11, less than a single scan is lost due to detonation arrival at the measurement station during 40Hz operation of the PDE. This shows nearly an order
of magnitude improvement compared to a previously developed system which showed 4 to 5 lost scans at 5kHz repetition rate for 10Hz PDE operation (Hinckley, Jeffries, and Hanson, 2004). The major improvements compared to the previously developed system included the use of a large-area, small f/ collection lens to improve the robustness to beamsteering and the use of large-area detectors to minimize the effects of fiber mode noise resulting from engine motion.

4.3 Results

In this section, three engine operation modes are reported: (1) 40 Hz cold-flow operation during which the engine runs with the fuel charge but the igniter is turned off; (2) 40 Hz hot-flow operation; and (3) 40 Hz operation during which the purge air flow in the initiator is reduced until the onset of flame-holding. For each of these cases, temperature (from TDL-based sensor) and side-wall pressure (from PZT pressure transducer) are recorded at the optical measurement station 5cm downstream of the initiator exit.

4.3.1 Cold-Flow Operation Temperature Results

As shown in Fig. 4.12, the flowfield temperature varies during 40 Hz cold-flow operation of the PDE. As the heated, vitiated air mixes with the cooler fuel (which has been expanded through a choked orifice from high pressure, room temperature gas cylinders) the flowfield temperature decreases. The change in temperature, ~10-15 K, agrees with mixing calculation based on adding a stoichiometric amount of ethylene (6.5 percent by volume) to the vitiated air. The low noise (~5K) apparent in the data showing
40Hz modulation of temperature demonstrates the fidelity of the TDL-based sensor. The temperature information provided by the sensor during fuel charge loading enables accurate characterization of the fuel concentration using simultaneous 3.39um laser absorption (the ethylene absorption coefficient is temperature-dependent).

![Temperature Sensor Results](image)

**Figure 4.12.** Temperature sensor results for 40 Hz cold flow tests during which fuel is injected into the vitiated air without igniting the mixture.

### 4.3.2 Hot-Fire Operation Temperature Results

Standard operation of the PDE at 40 Hz results in repeatable temperature and pressure traces as demonstrated in Fig. 4.13 which shows eight consecutive cycles of the PDE. The fifth and sixth cycle from this experiment are detailed in the expanded display shown in Fig. 4.14. Prior to the detonation arrival, the TDL-based sensor accurately captures the vitiated air temperature, as both the cold-flow and hot-flow provide the same
pre-detonation temperature. After the detonation arrival at the measurement station, both the temperature and pressure spike and then rapidly decrease to a plateau value (within 200μs, or 1 laser scan), which is typically referred to as $T_3$ and $P_3$ in closed-end-wall PDEs.

![Temperature and pressure results for 40 Hz PDE operation.](image)

Figure 4.13. Temperature and pressure results for 40 Hz PDE operation.

The plateau temperatures highlighted in Fig. 4.14 are lower than the expected value (both lower than simulated temperatures and the adiabatic combustion temperature). The measured plateau temperature is approximately 1350K. This temperature is much less than the Chapman-Jouguet temperature of 2926 K, as expected, but it also lower than the predicted plateau temperature as discussed in the following section. This discrepancy is hypothesized to result from both physical mechanisms and experimental setup and data reduction techniques.
Figure 4.14. Expanded display of the temperature and pressure results for 40 Hz PDE operation from Fig. 7 detailing two detonation cycles.

The valveless design in the air-flow system utilized in this PDE cause the $T_3$ and $P_3$ values to be lower than the corresponding values in a closed-wall PDE due to gas expansion upstream. There are three distinct temperature regions during the blowdown and purge portion of an open-end-wall PDE cycle, as outlined in appendix A and depicted in Fig. 4.15. After the detonation exits the initiator and transmits to the main combustor, the temperature rapidly decreases from the Chapman-Jouguet condition to the plateau condition. This relaxation takes approximately 0.03ms, as estimated in appendix A. The plateau region lasts approximately 2.3 ms. After the plateau region, the gas relaxes to ambient pressure and cools further. After the product gases reach ambient pressure, the air flow in the PDE purges the high temperature gases before a fresh charge of fuel is injected into the system. This purge time lasts approximately 5ms, and thus accounts for two-thirds of the total blow-down and purge time at the optical measurement.
station. The temperature during this purge period is estimated to be between 1650K and 1950K, which is greater than the measured temperature of 1350K.

Figure 4.15. Predicted temperature history at the exit of the initiator tube for a single cycle of the NPS PDE with $L=1\text{m}$ operating on stoichiometric ethylene-air.

Figure 4.15 includes two calculated temperatures, each utilizing either a frozen or an equilibrium value for $\gamma$ as discussed in chapter 3, for both the plateau and purge portions of the PDE cycle. For high temperature and pressure flowfields (such as those reported for ethylene-oxygen detonations in chapter 3), the equilibrium value more accurately predicts the system temperature. As the flowfield temperature decreases (for the ethylene-air detonation case reported in Fig. 4.15), the effects of finite-rate chemistry can begin to appear. Thus, the actual temperature in the system should fall between the frozen and equilibrium values reported in Fig. 4.15. These predictions provide a simple estimate of the expected temperatures during operation of the open-head-wall PDE tube for comparison with measured data. In order to accurately predict the actual system
temperatures and performance, a more sophisticated simulation that utilizes finite-rate chemistry (and thus eliminates the constant specific heat assumption) should be utilized.

There are numerous experimental details and physical mechanisms that could lead to a falsely low temperature for each region of the PDE cycle. The first region consists of the detonation arrival at the measurement location and the rapid relaxation to the plateau temperature and pressure. As stated previously, the relaxation from the Chapman-Jouguet to the plateau condition takes approximately 0.03ms. As the sensor bandwidth is 0.2ms due to the finite scan rate of the laser, this relaxation cannot be captured by this sensor.

The second temperature region consists of the 2.3ms long plateau region. During this period, the system pressure at the measurement station is approximately 4 atm. While the laser sensor maintains sensitivity up to the ~2200K temperature that occurs during this region for atmospheric pressure conditions, the higher system pressure during this period leads to increased error. A poor polynomial fit to the non-absorbing baseline could lead to temperature errors. For higher system pressures, the spectroscopic features broaden. Thus, the polynomial may actually fit part of the absorbing wings. Also, higher transmission noise due to beamsteering slightly shifts the measured laser scan profile leading to varying polynomial fits. In the high temperature portion of the cycle where the sensitivity of the TDL diagnostic is lowest, even small errors in baseline fitting can lead to large errors in temperature. Methods to improve the accuracy of the sensor are discussed in chapter 6.

The third temperature region consists of a 5ms purge region during which the near atmospheric pressure gases are purged out of the tube by the air flow feed. Two physical mechanisms are hypothesized to lead to a lower measured than predicted temperature:
temperature non-uniformity and mixing with purge gas. First, the measurement location is less than one tube diameter downstream of the initiator. Thus, there could be significant temperature non-uniformity across the line-of-sight. The initiator tube blow down and purge period lasts approximately 1.6ms; after that time, purge air flowing through the initiator enters the main combustor. Thus after 1.6ms, the line-of-sight temperature distribution at the measurement station consists of a cool inner core from the initiator purge and a hot surrounded by hot purge gases from the upstream combustion products. This non-uniformity would skew the temperature measurement. Second, the combustion products upstream of the measurement station are mixing with the air purge. The calculation results shown in Fig. 4.15 assume plug flow during the purge portion of the PDE cycle. Mixing between the combustion products and the purge air would decrease the measured temperature and could account for the relatively low measured temperature during this period.

For the first and second periods of the PDE cycle, the accuracy of the temperature measurement could be improved by employing alternative measurement strategies such as wavelength-modulation spectroscopy with 2-f detection or a wavelength-agile strategy. Both of these techniques do not rely on accurate baseline fits and are thus better suited to high-pressure measurement environments. The accuracy of the measured temperature during the purge portion of the PDE cycle could be improved by performing the measurement at an axial position farther downstream of the initiator where the occurrence of temperature non-uniformities would be reduced. The true utility of the sensor is shown in the next section where the effects of cycle-to-cycle interference are investigated. The
sensor location at the exit of the initiator tube optimizes the sensor utility for these studies.

### 4.3.3 Component Failure Temperature Results

When engine operation parameters are modified to the threshold of flame-holding, vastly different temperature and pressure profiles result, as shown in Fig. 4.16. This figure shows four engine cycles after the purge air flow in the initiator has been reduced to the threshold of flame-holding; three distinct temperature and pressure profiles are apparent.

![Graph showing temperature and pressure results](image)

**Figure 4.16.** Temperature and pressure results for 40 Hz PDE operation with flame-holding showing cycles containing a successful detonation, partial flame-holding, and full flame-holding.

The first engine cycle shows a successful detonation, and the resulting temperature and pressure profiles are similar to those shown in Figs. 4.13 and 4.14. But,
the temperature near the exit of the initiator does not decay to the vitiated air value before the next main-combustor fuel charge reaches that axial location. This results in premature ignition of the main-combustor fuel charge as shown by the increase in temperature at 20ms, during which the pressure remains near atmospheric. The spike in temperature and pressure at 28ms is due to ignition of the initiator fuel charge and the resulting blast-wave reaching the measurement station. While a detonation was formed in the initiator, the thrust produced from this cycle is substantially decreased because the main-combustor fuel charge was ignited before the detonation could be transitioned to the main combustor. The same engine failure mode appears in the 3rd engine cycle which shows a rapid increase in temperature at 45ms and 53ms and only one rapid pressure increase at 53ms. The fourth engine cycle reveals full flame-holding. Both the main-combustor and initiator fuel charges are ignited from the residual combustion products before the spark ignition as indicated by the two temperature plateaus and constant near-atmospheric pressure.

4.4 Summary

A TDL-based temperature sensor was developed and applied to characterize a valveless pulse detonation engine. The fiber optic-based sensor was shown to withstand a vibrating, translating measurement environment at engine operating rates up to 40Hz. Results from cold-flow operation enables accurate characterization of the fuel concentration during fuel charge loading. Results from hot-flow operation show repeatable temperature and pressure profiles. The sensor also shows utility for investigating and diagnosing engine failure modes, especially as engine operation rates
are increased and the effects pulse-to-pulse interference becomes more important. Future work could seek to further improve the data quality through advanced optical engineering and to apply the sensor to high-repetition-rate PDE operation to investigate and optimize specific engine component performance.
Chapter 5: In-Cylinder T and $X_{\text{H}_2\text{O}}$ Measurements in HCCI Engines Using a Multiplexed-Wavelength Diode-Laser System

5.1 Introduction

Modern combustion strategies for internal combustion engines, such as Homogeneous Charge Compression Ignition (HCCI), rely on accurate knowledge and control of the in-cylinder temperature and gas composition to realize successful operation (Epping, et al., 2002; Najt and Foster, 1983). Many optical diagnostics currently used for in-cylinder measurements in internal combustion (IC) engine research, such as planar laser-induced fluorescence (PLIF), laser-induced incandescence (LII), and Rayleigh scattering, can provide instantaneous 2-dimensional images of in-cylinder properties but do not provide a continuous, crank-angle-resolved record of these quantities and thus can be susceptible to cycle-to-cycle variation. Other diagnostic techniques such as exhaust gas analysis can provide continuous, time-resolved gas composition and temperature of the combustion products but are decoupled from the instantaneous in-cylinder dynamics.
By contrast, sensors based on wavelength-multiplexed TDL spectroscopy show potential for highly accurate, non-intrusive measurements of time-resolved in-cylinder temperature and gas composition. Coupled with a spatially-resolved technique such as PLIF, the time-resolved, line-of-sight TDL sensors could provide a critical diagnostic toolset needed to advance modern IC engine design and development, e.g. through validation of engine simulations and development of engine control strategies.

Two previous sensors based on line-of-sight absorption of water vapor to measure time-resolved, in-cylinder temperature for internal combustion engine applications have been developed, but these systems have utilized different approaches compared to the sensor reported in this chapter (Kranendonk, et al., 2004; Mattison et al., 2006; Rieker et al., 2006). Kranendonk reported the development of a wavelength-agile (i.e. broadly and rapidly scanned) external cavity diode-laser sensor to measure temperature and water mole fraction during HCCI engine operation. While this methodology shows promise as an alternative sensor strategy to traditional wavelength-multiplexed, direct-absorption diode-laser approaches, it suffers from several drawbacks. First, the wavelength-agile system requires the development and maintenance of a somewhat complex laser source that exhibits high intensity noise and multi-spectral- and multi-spatial-mode output. These characteristics limit the sensor’s ability to probe individual water absorption transitions, thus reducing the accuracy of the sensor during low-pressure portions of the engine cycle where parameters such as exhaust gas recirculation (EGR) and combustion residuals become important. Second, it requires the use of more complicated data acquisition and reduction techniques.
Rieker, *et al.* have reported an alternative approach to TDL thermometry in IC engines which utilizes wavelength-modulation spectroscopy with 2f detection (WMS-2f) to measure in-cylinder water vapor temperature over short path lengths (~6mm) in a modified spark plug. While this technique provides increased sensitivity enabling short-path-length measurements, it has limitations compared to traditional direct-absorption techniques. First, this system requires more expensive and complex electronic components to generate the laser modulation and to ‘lock-in’ to the correct output signal. Second, due to the frequency multiplexing of the individual laser sources, this approach is restricted to the simultaneous use of a limited number of laser wavelengths, thus reducing the potential temperature-sensing range. Lastly, this technique relies on the use of an intrusive optical probe which may perturb normal engine operation.

The current study reports the development and initial demonstration of a fiber-optic-coupled, wavelength-multiplexed, direct-absorption diode-laser sensor to measure temperature and water concentration during motored and fired operation of optical HCCI engines. This technique exhibits advantages enabling high-quality, low-noise data throughout the entire engine cycle. The wavelength-multiplexed architecture will allow expansion of the current system to include many individual laser wavelengths (if used in conjunction with a demultiplexing strategy able to accommodate many wavelengths such as high-order grating demultiplexing units being developed by Zolo Technologies, Inc.). By probing multiple water absorption features, the temperature-sensing range of the sensor can be maximized and the influence of temperature and species non-uniformity can be investigated. Other important combustion species could be monitored simultaneously by adding additional lasers and wavelengths. This architecture utilizes
well-developed diode-laser sources that have high-power, single-mode, narrow-linewidth, low-noise characteristics, and fiber-optic coupling that enables remote location of the laser control and data acquisition electronics and demultiplexing optics. The relatively simple data reduction and interpretation for these wavelength-multiplexed, direct-absorption sensors shows the potential for rapid automation and thus real-time sensing for active engine-control strategies.

5.2 Sensing Theory

The sensor reported in this chapter utilizes multiplexed-wavelength, fiber-optic-coupled laser absorption to probe rovibrational water transitions for temperature and water concentration measurements in HCCI engines. Because of the high pressures achieved during both motored- and fired-engine operation which cause severe pressure broadening of the spectroscopic absorption features, the sensor utilizes fixed-wavelength absorption with the laser wavelengths fixed at the linecenter of water absorption features and one wavelength offline to quantify non-resonant transmission fluctuations. The theory utilized to extract temperature and water concentration is fully described in Chapter 2. Careful spectroscopic design and accurate simulations of interference from surrounding absorption features enable the utilization of this technique throughout the compression and combustion portions of the engine cycle where temperatures and pressures can reach 1700K and 55bar respectively in the demonstration reported here.
5.3 Spectroscopic Line Selection

Water vapor serves as a convenient ‘tracer’ gas for laser-based thermometry in combustion systems due to its natural presence as nascent humidity in the inlet air, its ease of seeding, and of course its presence in the product gases of hydrocarbon combustion. Water vapor also exhibits many thousands of rovibrational transitions in the 1μm to 2μm wavelength region where telecommunications lasers and fiber technology are readily available. For example, the absorption band of water near 1.4μm contains over 6000 absorption features, providing numerous options for water-based thermometry. To ensure accurate temperature and gas concentration measurements, careful and quantitative selection of appropriate spectroscopic absorption features must be performed. The spectroscopic selection process is outlined below.

To begin the spectroscopic selection, the temperature, pressure, and water concentration state space are specified. Figure 5.1 plots the measured pressure history for a motored optical HCCI engine at Sandia National Laboratories (described fully below) along with the temperature history computed using the WAVE cycle-simulation model, tuned to match experimental pressure data, for a typical operating condition (Sjöberg and Dec, 2004). The remaining constraints governing the selection process are water concentration, optical path length, and laser wavelength region. For the selection reported here, the nominal water mole-fraction is 0.02 (relative humidity of 64% at 25°C), the path length is 92mm (the bore of one of the optical engines studied here), and the laser frequency range is 6000 to 8000cm⁻¹ (where telecommunications lasers and fiber optic components are readily available).
A selection process for near-infrared water vapor transitions to be used for in-cylinder measurement of temperature in an IC-engine was outlined previously and provides a starting point for this sensor design (Zhou et al., 2005b). The first three selection criteria address sufficient absorbance over the engine cycle, influence from potentially cold boundary layers, and interference from nearby transitions. Utilizing the temperature, pressure, and water mole fraction state-space described above in conjunction with spectroscopic parameters prescribed by HITRAN 2004 for individual rovibrational water transitions, the minimum absorbance values for each transition over the entire engine cycle can be calculated from Eq. 5.1.

\[
k_v = S(T) \cdot P \cdot X_{H_2O} \cdot \phi_{peak}
\]  

(1)

In this equation, \( S \) is the linestrength, \( P \) is the pressure, \( X_{H_2O} \), is the water mole-fraction, and \( \phi_{peak} \) is the line shape parameter at line center. To meet the first criterion, the minimum acceptable absorbance, \( k_v \cdot L \), is set at 0.03 which provides a signal-to-noise ratio of 10, assuming that the minimum detectable absorbance is 0.003 as estimated from initial experiments. The second selection criterion rejects molecular transitions with lower state energies, \( E'' \), less than 350cm\(^{-1}\) to minimize the influence of cold boundary layers along the line-of-sight measurement path and interference from air humidity in the purged demultiplexing setup (Ouyang and Varghese, 1990). The third criterion eliminates absorption features with strong surrounding neighbors, unless those neighbors have similar lower state energies and are close enough to be considered a single transition. By applying these three selection criteria, the 6000 potential water lines are reduced to 22 candidate absorption features, as listed in Table 5.1.
Table 5.1. Most promising water absorption features (from HITRAN 2004).

The transitions were further down-selected by the requirements that they must maintain high temperature sensitivity over the range of conditions to be investigated, maximize sensing accuracy, and show the ability to be separated (or demultiplexed) utilizing a diffraction grating. These three additional selection criteria are addressed as follows. The thermometry performance of line pairs formed from every combination of transitions listed in Table 5.1 is evaluated. First, the temperature sensitivity of a potential line pair is optimized when the difference in lower state energy, $\Delta E' = E'_\text{high} - E'_\text{low}$, is maximized. For this evaluation, line pairs with $\Delta E' < 300\text{cm}^{-1}$ are rejected for
temperatures ranging from ~300K to 900K. Second, each line pair must contain a minimum wavelength separation such that it can be demultiplexed using a diffraction grating. Here, we reject line pairs with centerline frequency separation, $\nu_1 - \nu_2$ less than 50cm$^{-1}$. This criteria can be relaxed if other demultiplexing techniques (such as time division) or alternate high-dispersion, high-order gratings are utilized. Lastly, the line pair must exhibit good measurement accuracy.

$$\sigma_T = \frac{\sigma_M}{dR/dT} \cdot \frac{1}{L} \cdot \sqrt{1 + R^2} \quad (4)$$

The measurement uncertainty, $\sigma_T$[K], is a function of the line pair ratio, $R=H/L$, where $H$ and $L$ are the centerline absorbance ($k_\nu * L$) of the high E” and low E” lines, respectively, the measured noise floor, $\sigma_M$, and the derivative of the ratio with respect to $T$, $dR/dT$. These criteria lead to the selection of line 6 at 7219.61cm$^{-1}$, and line 22 at 7416.05cm$^{-1}$. Figure 5.1 shows the simulated centerline absorbance and measurement uncertainty for this line pair. For these line pairs and the estimated noise floor, the measurement uncertainty ranges from 14K at BDC and 26K at 26° BTDC. With this low level of measurement uncertainty, the sensor could prove useful for quantifying the effects of residual gases and the effects of EGR as well as potentially characterizing the cool-flame heat release commonly observed in HCCI engines. For example, an engine utilizing approximately 20 percent residuals operating on a stoichiometric mixture of iso-octane and air can experience an increase in BDC mixture temperature of approximately 250K compared to a mixture consisting of consisting of 0 percent residuals. Thus, a measurement uncertainty of 14K would be sufficiently low to quantify the effects of residuals in the reactant gases.
If the selection process described previously does not result in a line pair with acceptable measurement accuracy, the cycle state space can be broken down into multiple temperature and pressure regions and separate line pairs can be utilized for each region, or more than two lasers (and hence more than two water lines) can be used. This is one of the major advantages of utilizing wavelength-multiplexed techniques.

5.4 Experimental Setup

This section describes the optical HCCI engine facilities at Sandia National Laboratories and the optical equipment utilized for the laser absorption sensor. Measurements were performed on two separate engines: a gasoline-like HCCI engine and a diesel-like HCCI engine.
5.4.1 Sandia National Laboratory Optical HCCI Engine Facility

The sensor performance is demonstrated in two optical HCCI engine facilities at Sandia National Laboratories which have been previously described in detail (Dec, Hwang, and Sjöberg, 2006; De Zilwa and Steeper, 2005). In-cylinder optical access to both engines is enabled by fused-silica rings and windows in the top of the cylinder liner which provide a line-of-sight path across the cylinder. The gasoline-engine-based HCCI engine shown in Fig. 5.2, with compression ratio (CR) of 11.8 and bore of 92mm, utilizes a fused-silica ring mounted to the top of the cylinder liner. However, optical access into the clearance volume is limited because the pent-roof design places the clearance volume above the fused-silica ring. Thus, for the motored engine measurements, data are reported until 30° before-top-dead-center (BTDC) where the piston begins to occlude the laser beam. The diesel-engine-based HCCI engine, with CR of 18 and bore of 102mm, has a flat cylinder-head surface and piston top, creating a pancake combustion chamber. With this configuration, the fused-silica windows mounted at the top the cylinder liner permit optical access into the clearance volume through top-dead-center (TDC). This allowed measurements over the full engine cycle for fired-engine operation.
Figure 5.2. Optical gasoline-engine-based HCCI engine at Sandia National Laboratories.

Each optical engine is equipped with intake air temperature, pressure, and mass flow-rate controls enabling the simulation of realistic inlet air conditions. Water vapor is injected far upstream of the intake valve ($\chi_{H2O} \approx 0.02$) utilizing a metering pump and an electrically heated vaporizer to ensure uniform mixing. The engines are operated at engine speeds up to 1200rpm for the data reported here. Cylinder pressure is monitored utilizing a transducer mounted in the cylinder head. The engine temperature is controlled by flowing heated oil and coolant water, thereby eliminating potential water vapor condensation. For fired engine operation, the iso-octane fuel is supplied by a gasoline-type direct fuel injector early in the intake stroke to provide a well-mixed charge.
5.4.2 Sensor Hardware

The optical arrangement for the multiplexed-wavelength diode-laser sensor is shown in Fig. 5.3; photos of the sensor applied to the diesel-like HCCI engine appear in Figs. 5.4-5.6. The vibration-sensitive laser, detector optics, and electronics are remotely located. The laser light is coupled by fiber optics to the pitch and catch lenses of the sensor, which are directly mounted on the vibrating engine. The multiplexed laser light, consisting of the two resonant beams and a non-resonant beam, is brought to the device through single-mode fiber. This light is then collimated to a 0.5mm beam diameter and pitched across the combustor using an aspheric collimator (CFS-T-2-1400nm, Optics for Research). This collimator was chosen due to the small diameter of the housing which enabled flush mounting to the engine head to minimize the effects of beam occlusion by the piston (discussed in next section). After the light traverses the combustion chamber, it is collected using an aspheric lens and focused into a 400μm-core-diameter, multi-mode fiber. The collection lens is chosen such that the f-number matches the numerical aperture of the multi-mode fiber (NA=0.39) and so that the diameter is sufficiently large to accommodate beam steering (10mm-diameter, f/1 lens in this case). The collimator/fiber combination permits beam translation of 4mm without signal degradation ensuring robustness to density-gradient-induced beam-steering.
Figure 5.3. Generalized schematic of sensor applied to HCCI engine.

The multiplexed light leaving the multi-mode fiber is collimated using an aspheric lens and then pitched onto a diffraction grating where it is demultiplexed, as detailed in Fig. 5.4 and further discussed in Chapter 2. The grating simultaneously acts as a band-pass filter, eliminating interference from flowfield emissions. The demultiplexed beams are then focused onto individual large-area (3mm diameter) amplified photodetectors (4MHz bandwidth). The large-area detectors are necessary to ensure that the entire beam is focused on the active area of the detector thus minimizing the effects of fiber mode noise on the signal. The entire dispersion setup is housed in a nitrogen-filled enclosure to eliminate interference absorption caused by atmospheric water.
As shown in Fig. 5.5, the entire engine is surrounded by an optical table on one side and a dynamometer and an intake-air heater on the other side. While the optical table provides a convenient location to place the sensor dispersion setup, the fiber pitch and
catch had to be mounted on the engine. The engine is attached to an air-suspended isolation stand to minimize the effect of engine vibration on the surrounding optics. The isolation stand resulted in engine movement of up to 1 inch this necessitating the engine mounted pitch and catch setup.

Figure 5.6. Diesel-like HCCI engine cylinder and optical access windows.

As shown in Fig. 5.6, small optical windows provided access to the combustion chamber of the diesel-like HCCI engine. The single cylinder and head are mounted far above the original engine block to enable optical measurements. The relatively small window access limited the potential laser paths available for line-of-sight measurements; thus only near-cylinder-center paths were available.
Figure 5.7. Diesel-like HCCI engine cylinder and optical access windows with collection lens mounted.

Figure 5.7 shows a close-up picture of Fig. 5.6 with the collection lens of the fiber-based sensor mounted. The optical access windows showed large transmission fluctuations during engine operation necessitating frequent cleaning (cleaned approximately every minute of engine operation). The small space confinement near the optical access locations limited the potential optical paths for the line-of-sight measurements, as shown in the schematic of Fig. 5.8. The optical pitch is mounted flush to the engine head such that the laser beam is as high in the engine cylinder as possible. This enables tracking of temperature to the top-dead-center crank angle position where the pancake-style combustion chamber allows optical access across the cylinder.
5.5 Results

This section contains results for both motored- and fired-engine operation and data detailing the effects of polarization-related noise on wavelength-multiplexed systems. The polarization-related noise section expands on the discussing included in Chapter 2.

5.5.1 Polarization-Related Noise

For the first set of tests, the sensor was applied to the automotive HCCI engine operating at 1200RPM motored conditions. In order to isolate and characterize the vibration and beam-steering noise for the multiplexed diode-laser sensor, the water
injection scheme was disabled such that dry air was fed to the engine intake. Under such conditions where the effects of water absorption are eliminated from the two resonant wavelengths, the transmitted signal of the three laser wavelengths should be self-similar.

![Graph showing measured pressure and laser transmission for motored engine operation]

Figure 5.9. Measured pressure and laser transmission for motored engine operation showing polarization related problem and solution.

Shown in Fig. 5.9 are the measured pressure signal and the transmitted beam intensity for two cases. The first case, labeled ‘polarization problem’ shows variation in the transmitted signal as the engine cylinder pressure increases during the compression stroke of the engine. Because the non-resonant signal fails to track the resonant signals, accurate absorption measurements cannot be performed. For this case, the demultiplexing grating consists of a 1200 grooves/mm gold grating blazed at 1μm. The second case,
labeled ‘polarization solution’, shows the transmitted signal for the same sensor utilizing a demultiplexing grating of 600 grooves/mm blazed at 1.6 μm. These two gratings exhibit vastly different polarization efficiencies, as discussed in Chapter 2.

Typical reflective diffraction gratings are very sensitive to the polarization state of the incoming light. For example, a 1200 groove/mm ruled grating blazed at 1 μm chosen for its high dispersion may have reflection efficiencies of 90% for s-plane polarized light and 20% for p-plane polarized light. Thus, if the polarization of the light changes anywhere along the optical path before the grating, fluctuations in the transmitted signal will result. Many different effects can change the polarization state of the transmitted light. For example, if the birefringence of the cylinder windows change with varying stress, it can shift the polarization of the transmitted light (Musculus and Pickett, 2005). For these engine experiments, the non-crystalline fused silica is stressed by time-varying cylinder pressure producing a changing birefringent behavior. Because the grating efficiency is sensitive to polarization, it results in fluctuation of the transmitted signal, as shown in Fig. 5.9. The single-mode fiber used to carry the laser light to the engine can also induce changes in the polarization since it is sensitive to movement. As the fiber moves, bends, and vibrates during engine operation, the polarization of the light emitted from the fiber changes, resulting in noise in the transmitted signal.

These effects of polarization can be overcome by redesign of the optical system. Use of a diffraction grating with matched s- and p-plane efficiencies at the sensing wavelength, such as our current 600 grooves/mm grating blazed at 1.6 μm, eliminates polarization-related noise as shown in the ‘polarization solution’ graph in Fig. 5.9.
While the 600 grooves/mm grating blazed at 1.6 \( \mu \text{m} \) solves the polarization-related noise problem, it imparts limitations to the wavelength-multiplexed system. The lower dispersion of this grating compared to other gratings employed in past measurement (such as the 1200 g/mm grating) limits the number of and the spacing of wavelengths that can be utilized. For example, the sensor reported in Chapter 4 for measurements on multi-cycle PDEs employed four lasers to track water temperature over a large temperature range. The 600g/mm grating reported provides only enough dispersion to separate three laser wavelengths (two resonant and one non-resonant) from the water band near 1.4 \( \mu \text{m} \) thus limiting the temperature sensitivity of the sensor. This limitation could be overcome by employing alternative dispersion strategies. For example, high-order gratings typically exhibit better-matched polarization efficiencies while providing the necessary dispersion to separate a larger number of wavelengths. Holographic gratings also provide the potential for high optic dispersion and matched polarization efficiency. The availability of holographic gratings with high dispersion for wavelengths near 1.4 microns is currently increasing. Also, hybrid demultiplexing schemes could increase the wavelength-multiplexing of these sensors. For example, utilizing time-division multiplexing in conjunction with a grating dispersion system could increase the total number of wavelengths used in a sensor. These alternatives will be discussed further in Chapter 6.

5.5.2 Motored Engine Demonstration

The ability of the sensor to provide accurate temperature results is demonstrated during motored operation of the automotive HCCI engine. Figure 5.10 shows the low-
noise transmission signals of motored engine operation at 1200RPM with water injection into the feedstock gases. The resulting centerline absorbance is measured by taking a ratio of the resonant and non-resonant beams and utilizing the Beer-Lambert relation. The BDC absorbance at each wavelength is fixed at the value determined by utilizing the sensor in scanned-wavelength mode. By evaluating the ratio of peak absorbance at each crank angle position, the temperature can be inferred as discussed in the sensing theory section.

Figure 5.10. Measured transmission and resulting absorbance during motored gasoline-engine-based HCCI engine operation.
As shown in Fig. 5.11, the measured temperature agrees well with the mass-averaged temperature derived from the measured pressure (as discussed with respect to Fig. 5.1) giving confidence in the measurement technique. The estimated uncertainty in temperature throughout the entire compression stroke is less than 3%. At 30°BTDC, the piston occludes the transmitted beam preventing further measurements. The noise appearing near 30°BTDC is believed to result from beam steering caused by the thermal boundary layer formed just above the piston.

![Graph showing temperature and pressure results](image)

Figure 5.11. Measured (single cycle) and pressure-derived temperatures and measured pressure during compression stroke of the gasoline-engine-based HCCI engine.

Results showing the repeatability of the multiplexed-wavelength diode-laser sensor for motored operation of an HCCI engine are shown below (a full set of data appears in Appendix B). Figure 5.12. plots measured temperature results for 5
consecutive cycles of the motored gasoline-engine-based HCCI engine compared to simulated temperature. This Figure reveals small cycle-to-cycle variation until approximately 45° BTDC. The noise appearing after this crank angle position is hypothesized to result from thermal boundary layer growth and from possible condensation of water in the feedstock gases.

Figure 5.12. Measured temperature (top) for 5 consecutive cycles gasoline-engine-based HCCI engine motoring at 1200 RPM compared to pressure-derived temperature, and pressure (bottom).

The average measured temperature from 5 consecutive cycles compared to the simulated value, and the residual fraction are shown in Fig. 5.13 confirming variation between the measured and simulated temperature of less than 3 percent. The measured standard deviation of temperature for 5 consecutive cycles compared to the simulated measurement accuracy is shown in Fig. 5.14. This comparison reveals that the sensor performance exceeds simulated performance providing confidence in the spectroscopic line selection procedure and optical engineering.
Figure 5.13. Measured average temperature (top) for 5 consecutive cycles gasoline-engine-based HCCI engine motoring at 1200RPM compared to pressure-derived temperature, residual fraction (middle), and pressure (bottom).

Figure 5.14. Measured standard deviation of temperature (top) for 5 consecutive cycles gasoline-engine-based HCCI engine motoring at 1200RPM compared to simulated standard deviation of temperature (measurement uncertainty), and pressure (bottom).
5.5.3 Fired Engine Demonstration

For fired HCCI engine operation, the intake temperature was adjusted so that compression-induced autoignition of the premixed gases occurred a few degrees after TDC. In order to evaluate the sensor performance under fired HCCI engine operation, the sensor was applied to the diesel-based HCCI engine, which has optical access to the clearance volume.

Figure 5.15 shows the resulting measured temperature compared to the pressure-derived temperature for fired operation at 900 RPM. This mass-averaged temperature is computed from the measured cylinder pressure and the known volume change due to piston motion using the ideal gas law. Also, the average molecular weight and the system mass are assumed to be constant. During the compression stroke, the measured temperature tracks the pressure-derived temperature within the measurement accuracy of the sensor. A little after TDC, the mixture of iso-octane and air (equivalence ratio 0.38) begins to ignite resulting in a rapid increase in temperature. The sensor accurately tracks the temperature increase, and the sensor accuracy in temperature is estimated to be better than 8%. At crank angle positions after 45°ATDC, some disagreement appears between the measured and pressure-derived temperature. This is hypothesized to result from temperature non-uniformities along the line-of-sight, possibly induced by heat transfer from the gas to the engine wall.
Figure 5.15. Measured and pressure-derived temperatures, water mole-fraction, and pressure during fired diesel-engine-based HCCI engine operation.

The water mole-fraction during the entire engine cycle is inferred from a single-wavelength measured absorbance, measured pressure, and measured temperature as described in the sensor theory section. This result is plotted in panel 2 of Fig. 5.12. Near TDC, the water mole-fraction rapidly increases from the seeded tracer gas concentration as water is produced during the combustion process. The uncertainty in water mole-fraction after ignition is estimated to be less than 15%. The large noise near 5°ATDC results from the ignition process during which large beam steering effects are hypothesized to be present, thus the dip in mole-fraction during the ignition process is unrealistic. From the plateau in water concentration, the overall conversion efficiency (as estimated by comparing the measured water mole-fraction to the theoretical value
assuming complete combustion) is 70%-85% which is consistent with previous estimates of HCCI engine operation under similar conditions. The relatively low values of conversion efficiency results from the mechanical design of the optical engine. A large clearance area between the piston and cylinder windows designed to minimize window damage results in large a large crevice volume at TDC. This crevice volume suffers from extremely high heat transfer losses; thus fuel reaching the crevice volume remains unburned due to the low-temperature quenching. Current production engines do not include large crevice volumes and are thus able to achieve conversion efficiencies approaching 100%.

Results showing the repeatability of the multiplexed-wavelength diode-laser temperature sensor for fired operation of an HCCI engine are shown below (full data set appears in Appendix B). Figure 5.16. plots measured temperature results for 3 consecutive cycles of the fired diesel-engine-based HCCI engine compared to simulated temperature. Each of the single cycle results agree well with the simulated temperature until the ignition process begins at approximately 5° BTDC when the ignition process begins.

The average measured temperature from 3 consecutive cycles compared to the simulated value, and the calculated residual difference are shown in Fig. 5.17. The residual difference between measured and simulate temperature rapidly increases after ignition where large line-of-sight non-uniformities are hypothesized to exist.
Figure 5.16. Measured temperature (top) for 3 consecutive cycles diesel-engine-based HCCI engine firing at 900RPM compared to pressure-derived temperature, and pressure (bottom).

Figure 5.17. Measured average temperature (top) for 3 consecutive cycles diesel-engine-based HCCI engine firing at 900RPM compared to pressure-derived temperature, residual difference (middle), and pressure (bottom).
5.6 Summary

A new non-intrusive optical diagnostic has been demonstrated for measuring crank-angle-resolved, in-cylinder, line-of-sight temperature in HCCI engines. The technique utilizes a wavelength-multiplexed diode-laser-absorption technique to measure temperature and water concentration along the line-of-sight. An initial demonstration of the sensor provides microsecond time-resolved data for both motored- and fired-engine operation under conditions ranging from 300K to 1700K and 1bar to 55bar from two optical HCCI engines at Sandia National Laboratories. The fiber-optic coupling employed for this sensor enables measurements on vibrating engines and simplifies the implementation of the sensor in this harsh environment.

The current wavelength-multiplexed technique utilizes two resonant wavelengths and one non-resonant wavelength to track water absorption throughout the engine cycle. The non-resonant beam successfully tracks fluctuations in the transmitted beam intensities resulting from particulate attenuation (if present), window fouling, and beam steering. Figure 5.17 shows transmission of the non-resonant beam during fired-engine operation. As shown, the non resonant beam transmission remains at 1 until the ignition process. During the ignition event, the transmission decreases sharply to a minimum of 0.2 within 5° of the beginning of combustion. These fluctuations result from both beam steering and engine vibration. After ignition, transmission rapidly recovers to nearly 1 and then fluctuates by approximately 10 percent during the expansion stroke. These fluctuations result largely from fouling of the windows by engine oil.
Figure 5.18. Transmission of non-resonant beam and measured pressure for fired operation of diesel-like HCCI engine.

Key solutions required to suppress crank-angle-dependent noise in the transmitted laser signals are reported. These solutions include careful spectroscopic design, and optical engineering to accommodate beam-steering, engine vibration and polarization-related interference. A spectroscopic line selection process is reported to identify the most appropriate water absorption line pair for thermometry under these conditions. The straightforward data reduction allows for rapid reduction of the raw data to temperature.

The temperature data reported from this sensor accurately track the pressure-derived temperature for both motored- and fired-engine operation with 3% and 5% accuracy, respectively. The sensor also provides autoignition and peak-combustion temperatures during fired-engine operation which can prove critical for understanding the ignition and pollutant formation processes. The sensor also demonstrated the ability to track water concentration changes during the combustion process.
While this initial demonstration focused on the development and application of a two-line water temperature and concentration sensor, the flexibility of the wavelength-multiplexed architecture allows straightforward addition of other wavelengths. This could allow characterization of non-uniformities along the line-of-sight as well as enabling the sensing of multiple engine parameters. Other diode-laser based sensors have been developed to measure hydrocarbon fuel concentration and other combustion species such as CO and CO₂ (Webber et al., 2000). By simply adding additional diode-laser wavelengths, which are continually being developed, to the fiber optic-based wavelength-multiplexed system, these important parameters can potentially be measured.
Chapter 6:
Summary and Future Work

6.1 Summary

Sensors based on laser-absorption spectroscopy could supply important information for the development and advancement of both PDE and HCCI engine technology. In order to succeed making measurements in these harsh environments, numerous technical challenges must be overcome as detailed in the previous four chapters. As stated in Chapter 1, the objective of the work reported here is threefold:

1. Develop and apply ultraviolet-based (UV) laser-absorption sensors for measurement of temperature and species concentration with microsecond time resolution in a single-cycle PDE to generate a data set for computational simulation validation.

3. Develop and apply a wavelength-multiplexed, fiber-optic-based, near-infrared, laser-absorption temperature and water concentration sensor to an optical HCCI engine to evaluate the compression stroke and ignition process.

The following sections outline the milestones accomplished to achieve these goals.

### 6.1.1 Single-Cycle PDE Measurements

Two new diagnostics based on UV laser absorption to measure time-resolved $T$ and $X_{OH}$ for temperatures up to 3800K and pressures up to 33atm were developed and applied to a single-cycle PDE at Stanford University. These results prove useful for evaluating PDE models to reveal the differences resulting from finite-rate and frozen-chemistry assumptions and to evaluate loss mechanisms such as heat transfer which may be significant in PDE flows. Proper inclusion of heat transfer losses in computational simulations can change the predicted $I_{sp}$ by 10-15% for typical tube lengths.

Comparison between computation simulation results (utilizing varying models for chemistry and heat transfer) and experimental measurements confirmed the following conclusions which aid the development of detailed PDE models. The simulation utilizing frozen gas composition can accurately predict the measured pressure and temperature profiles if an appropriate $\gamma$ is utilized, $\gamma = \gamma_s$. While such simulations neglect additional heat release due to chemical recombination and energy loss due to heat transfer, the two missing effects appear to negate each other. Of course, the frozen chemistry model (constant $X_{OH}$) fails badly with regard to properly simulating the decay of OH mole fraction. The second and more correct simulation incorporates finite-rate chemistry and includes losses due to heat transfer and friction. With the proper inclusion of losses due to
heat-transfer, the finite-rate chemistry code accurately predicts temperature, pressure, and OH concentration. Agreement between the measured and predicted metrics inspires confidence in the accuracy of the simulations to be utilized to predict the performance of more complicated PDE systems such as multi-pulse tubes or tubes with nozzles. Accurate models of both heat transfer and chemistry are critical to the accurate simulation of PDE flowfields.

6.1.2 Multi-Cycle PDE Measurements

A TDL-based temperature sensor was developed and applied to characterize a valveless pulse detonation engine at the Naval Postgraduate School in Monterey, CA. The fiber optic-based sensor was shown to withstand a vibrating, translating measurement environment at engine operating rates up to 40Hz. Results from cold-flow operation enables accurate characterization of the fuel concentration during fuel charge loading. Results from hot-flow operation show repeatable temperature and pressure profiles. The sensor also shows utility for investigating and diagnosing engine failure modes, especially as engine operation rates are increased and the effects pulse-to-pulse interference becomes more important. While the magnitude of the temperature during the plateau region is lower than predicted values, the sensor shows high utility for characterizing device failure modes and thus proves useful for advancing PDE designs. Future modifications to the sensor, discussed below, could improve the accuracy of the measured plateau temperatures and thus improve the value of the sensor results for validating computation simulations of more practical PDE flowfields.
6.1.3 HCCI Engine Measurements

A new non-intrusive optical diagnostic has been demonstrated for measuring crank-angle-resolved, in-cylinder temperature and water concentration in HCCI engines at Sandia National Laboratories in Livermore, CA. An initial demonstration of the sensor provides microsecond time-resolved data for both motored- and fired-engine operation under conditions ranging from 300K to 1700K and 1bar to 55bar from two optical HCCI engines. The fiber-optic coupling employed for this sensor enables measurements on vibrating engines and simplifies the implementation of the sensor in this harsh environment.

Key solutions required to suppress crank-angle-dependent noise in the transmitted laser signals were reported. These solutions include careful spectroscopic design, and optical engineering to accommodate beam-steering, engine vibration and polarization-related interference. A spectroscopic line selection process is reported to identify the most appropriate water absorption linepair for thermometry under these conditions. The straightforward data reduction allows for rapid reduction of the raw data to temperature.

The temperature data reported from this sensor accurately track the pressure-derived temperature for both motored- and fired-engine operation with 3% and 5% accuracy, respectively. The sensor also provides autoignition and peak-combustion temperatures during fired-engine operation which can prove critical for understanding the ignition and pollutant formation processes. The sensor also demonstrated the ability to track water concentration changes during the combustion process.
6.2 Future Work

Future modification to the sensing techniques reported in this thesis could improve the accuracy and utility of these laser absorption sensors for characterizing and improving modern propulsion concepts. A brief summary of suggestions for future work are included in the following section.

6.2.1 UV Diagnostics for PDEs

While the UV-based temperature diagnostic reported in this thesis extends the sensing capabilities for PDEs to higher temperatures compared to previously developed systems, there are potential areas to improve the diagnostic. The data reported in Chapter 3 includes measured temperature up to 3800K but contains measurement gaps at temperatures near 2800K resulting from condition-specific sensitivity issues. Under portions of the blowdown temperatures and pressures of the single-cycle PDE, the two wavelengths, 266 and 306 nm, do not maintain high enough sensitivity to provide a temperature result. This problem could be overcome by incorporating additional UV wavelengths (between 266 and 306 nm) that would enable coverage of the entire temperature and pressure state space. Additionally, by including higher frequency wavelengths, the temperature sensing range of the system could be extended to temperatures much lower than the 2000K reported here, as the CO₂ absorption coefficient increases drastically at high frequencies. For example, researchers have demonstrated CO₂ temperature sensing in shock tubes utilizing 244nm and 216nm laser radiation. The addition of these wavelengths could increase the temperature sensing range of this system
to 1000K. These temperatures could become more important if thrust enhancement devices such as nozzles are incorporated into the PDE flowfield.

### 6.2.2 Multiplexed TDL Sensors for PDEs

The results reported in this thesis for measurements on multi-cycle PDEs using TDL diagnostics show significant improvement in data quality and an increase in PDE operation rates compared to previous free-space and fiber-coupled systems, but modifications to the sensor could lead to additional improvements in data results. Improvements to the optical engineering and changes in sensing techniques could extend sensing capabilities to higher engine operation rates and to improve the accuracy of the temperature results during the plateau region.

Improvements to data quality could be achieved by adapting the optical engineering to reduce the effects of polarization noise. During engine operation both the single-mode pitch and multi-mode catch fibers move and vibrate. This leads to rapidly changing polarization of the light entering the demultiplexing setup. As outlined in Chapter 2, shifting polarization leads to fluctuations in the measured transmission. Fluctuations in transmission affect the baseline fitting of the data reduction process which can lead to increased error in the temperature results and to lower maximum engine operation rates. Polarization noise could be reduced by utilizing diffraction gratings with matched polarization efficiencies or by employing alternative demultiplexing strategies. For example, high-order gratings or holographic gratings show potential for high dispersion with well-matched polarization efficiencies. Also, hybrid schemes employing time-division demultiplexing with diffraction gratings could greatly increase the number
of wavelengths utilized and thus improve the temperature sensing range of these systems. Polarization maintaining fiber on the pitch would also decrease polarization related noise.

In order to improve the accuracy of laser-absorption sensors during the high-pressure blowdown period, alternate sensing strategies could be employed. Recent advances in sensing technology reveal wavelength-modulation spectroscopy with 2f detection as a viable technique for thermometry under high pressure conditions. This methodology eliminates the need for a baseline fit of the non-absorbing wings thus potentially improving sensing accuracy of the line-of-sight measurement. This technique also could increase the sensor bandwidth enabling measurements on higher operation rate PDEs.

### 6.2.3 Multiplexed TDL sensors for IC engines

While this initial demonstration focused on the development and application of a two-line water temperature and concentration sensor, the flexibility of the wavelength-multiplexed architecture allows straightforward addition of other wavelengths. Recent advancements in sensing technologies which utilize high order (echelle) gratings enable the simultaneous use of many laser wavelengths (potentially up to 40 wavelengths in systems under development). This could allow characterization of non-uniformities along the line-of-sight as well as enabling the sensing of multiple engine parameters. Other diode-laser based sensors have been developed to measure hydrocarbon fuel concentration and other combustion species such as CO and CO$_2$. By simply adding additional diode-laser wavelengths, which are continually being developed, to the fiber optic-based wavelength-multiplexed system, these important parameters can potentially be measured.
Appendix A: PDE Analysis

Model

This appendix outlines the use of an analytical model originally developed by Wintenberger and Shepherd to predict the impulse of a single-cycle PDE (Wintenberger et al., 2003). In the current study, the model is extended to calculate the temperatures, pressures, and characteristic times important to the blowdown period of a closed-end-wall PDE cycle. These results are then utilized in conjunction with simple isentropic expansion relationships to predict the temperatures and pressures that occur during the blowdown period of an open-end-wall PDE cycle for the purpose of comparison with data taken at the Naval Postgraduate School PDE.

Figure A.1 contains a generalized x-t diagram for a closed-end-wall PDE of length L. Three different regions in the diagram, labeled ‘1’, ‘2’, and ‘3’, correspond to the unburned reactants, the Chapman-Jouguet detonation state, and the plateau state, respectively. While the full details of the diagram are contained in the reference, a brief description is included here.
After ignition, a detonation wave instantaneously forms and propagates down the tube at velocity $U_D$. The detonation wave is followed by Taylor region through which the moving gases in region ‘2’ are isentropically stagnated to condition ‘3’, which results from the zero velocity head wall boundary condition (Taylor, 1950). As the detonation wave reaches the end of the tube, expansion waves reflect off of the contact surface (created by the air interface at the exterior of the tube) and move toward the head wall exhausting and cooling the high-pressure, high-temperature gas contained in the tube. Three characteristic times are labeled on the diagram: $t_1$, $t_1 + t_2$, and $t_{23}$ which correspond to the time it takes for the detonation wave to reach the tube exit, the total time required for the first reflected expansion wave to reach the head wall, and the duration of the Taylor wave at location $x_{\text{meas}}$ near the head wall respectively.

Figure A.1. Generalized x-t diagram of a closed-end-wall PDE cycle.
Figures A.2 and A.3 depict the resulting temperature and pressure of the flowfield as a function of time for an axial position at the head wall (x=0). After the detonation wave forms, the pressure and temperature decay nearly instantaneously to the plateau conditions $P_3$ and $T_3$ respectively. This decay time can be evaluated at a position close to the head wall, labeled $t_{23}$ in Fig. A.1. After the first reflected characteristic reaches the head wall, labeled time $t_1+t_2$ in Figs A.1-A.3, the pressure and temperature decrease until the pressure reaches ambient conditions.

![Diagram](image)

Figure A.2. Head wall pressure trace for closed-end-wall PDE cycle.
Figure A.3. Head wall temperature trace for closed-end-wall PDE cycle.

Nomenclature and Equations

This section outlines the equations utilized to estimate the plateau temperature and pressure and the characteristic blow-down times for a closed-end-wall PDE of length $L = 1\text{m}$ operating on stoichiometric ethylene-air. A full description of the model utilized can be found in the references (Taylor, 1950; Wintenberger et al., 2003.)

$c_{\text{CJ}} = c_2$ sound speed of burned gas just behind detonation wave  
$c_3$ sound speed of burned gases behind the Taylor wave  
$L$ length of detonation tube  
$P_2$ Chapman-Jouguet pressure  
$P_3$ pressure of burned gases behind the Taylor wave  
$t_1$ time taken by detonation wave to reach the open end of the tube  
$t_2$ time taken by the first reflected characteristic to reach the thrust wall after reflection off of contact surface  
$t_3$ time associated with pressure decay period  
$T_2$ Chapman-Jouguet temperature
$T_3$ temperature of burned gases behind the Taylor wave
$u_2$ gas velocity of burned gas just behind the detonation wave relative to fixed reference frame on detonation tube wall
$U_{CJ}$ Chapman-Jouguet detonation wave velocity
$\alpha$ nondimensional parameter corresponding to time $t_2$
$\beta$ nondimensional parameter corresponding to pressure decay period, $t_3$
$\gamma$ ratio of specific heats (either frozen or equilibrium)

\[ c_3 = \frac{\gamma + 1}{2} c_{CJ} - \frac{\gamma - 1}{2} U_{CJ} \]  
(1)

\[ \frac{c_3}{c_2} = \frac{\gamma + 1}{2} - \frac{\gamma - 1}{2} \frac{U_{CJ}}{c_{CJ}} \]  
(2)

\[ P_3 = P_2 \left( \frac{c_3}{c_2} \right)^{2\gamma} \]  
(3)

\[ T_3 = T_2 \left( \frac{c_3}{c_2} \right)^2 \]  
(4)

\[ t_1 = \frac{L}{U_{CJ}} \]  
(5)

\[ t_2 = \alpha \cdot \frac{L}{c_3} \]  
(6)

\[ t_3 = \beta \cdot \frac{L}{c_3} \]  
(7)

\[ \alpha = \frac{c_3}{U_{CJ}} \left[ 2 \left( \frac{\gamma - 1}{\gamma + 1} \left[ \frac{c_3 - u_2}{c_2} + \frac{2}{\gamma - 1} \right] \right)^{-\frac{\gamma + 1}{2(\gamma - 1)}} - 1 \right] \]  
(9)

\[ t_{\text{blowdown}} = t_1 + t_2 + t_3 \]  
(10)
Table A.1. Calculated Chapman-Jouguet conditions for stoichiometric mixture of ethylene-air utilizing STANJAN.

<table>
<thead>
<tr>
<th>property</th>
<th>$\gamma=\gamma_f=1.25$</th>
<th>$\gamma=\gamma_e=1.16$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_3$</td>
<td>2361</td>
<td>2554</td>
</tr>
<tr>
<td>$P_3$</td>
<td>6.3</td>
<td>6.9</td>
</tr>
</tbody>
</table>

Table A.2. Estimated plateau conditions for a closed-end-wall PDE operating on a stoichiometric mixture of ethylene-air.

<table>
<thead>
<tr>
<th>property</th>
<th>$\gamma=\gamma_f=1.25$</th>
<th>$\gamma=\gamma_e=1.16$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t_1$</td>
<td>0.55</td>
<td>0.55</td>
</tr>
<tr>
<td>$t_2$</td>
<td>1.23</td>
<td>1.18</td>
</tr>
<tr>
<td>$t_3$</td>
<td>0.59</td>
<td>0.56</td>
</tr>
<tr>
<td>$t_1+t_2$</td>
<td>1.78</td>
<td>1.73</td>
</tr>
<tr>
<td>$t_{\text{blowdown}}$</td>
<td>2.37</td>
<td>2.29</td>
</tr>
<tr>
<td>$t_{23}$</td>
<td>0.03</td>
<td>0.03</td>
</tr>
</tbody>
</table>

Table A.3. Estimated blowdown times and Taylor wave duration for a 1m closed-end-wall PDE operating on stoichiometric ethylene-air.

**Extension to Open-End-Wall PDE**

The previous section contained calculated results of plateau conditions and blowdown times for a closed-end-wall PDE. The PDE at the Naval Postgraduate School
discussed in chapter 4 utilizes a constant air flow system and thus incorporates an open-end-wall configuration. The gases are allowed to expand upstream of the initiator section as the detonation wave transmits to the main combustor. As a result, the plateau conditions reported in the previous section do not apply. In order to estimate the appropriate plateau conditions the gases are allowed to expand isentropically from the plateau pressure, $P_3$, to a lower pressure estimated from the measured pressure traces for the NPS PDE operating at 40 Hz on ethylene-air, as discussed in chapter 4. These results are included in table A.4

<table>
<thead>
<tr>
<th>property</th>
<th>$\gamma = \gamma_f = 1.25$</th>
<th>$\gamma = \gamma_e = 1.16$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{3, \text{open}}$</td>
<td>2157</td>
<td>2368</td>
</tr>
<tr>
<td>$P_{3, \text{open}}$ (estimate from data)</td>
<td>4</td>
<td>4</td>
</tr>
</tbody>
</table>

Table A.4. Estimated plateau conditions for the NPS PDE cycle.

While table A.4 includes estimates of the plateau conditions for an open-end-wall PDE, other temperatures could be important during the operation cycle of the engine. For example after the gasdynamic blowdown period of the PDE cycle, the remaining product gases are purged out of the engine before a fresh fuel charge is introduced into the system. The constant flow of air in the system purges the product gases. The temperature of these purged gases can be estimated by isentropically expanding the gases from the plateau pressure to ambient pressure. The resulting temperatures are shown in Table A.5.

<table>
<thead>
<tr>
<th>property</th>
<th>$\gamma = \gamma_f = 1.25$</th>
<th>$\gamma = \gamma_e = 1.16$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{\text{purge}}$</td>
<td>1635</td>
<td>1953</td>
</tr>
<tr>
<td>$P_{\text{purge}}$</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

Table A.5. Estimated temperature of the product gases during the purge portion of the NPS PDE cycle.
For the NPS PDE operating at 40Hz, the purge time for the gases located between the fuel injector and the optical measurement station is estimated to take approximately 5ms (Klingbeil et al., 2005). This purge time is approximately twice as long as $t_{\text{blowdown}}$ as shown in Table A.3.

**Summary**

The results from the previous sections can be utilized to construct a predicted temperature-time history for a single cycle of the NPS PDE including Chapman-Jouguet, plateau, and purge temperatures as shown in Fig. A.4.

![Graph showing temperature history](Graph.png)

**Figure A.4.** Predicted temperature history at the exit of the initiator tube for a single cycle of the NPS PDE with $L=1\text{m}$ operating on stoichiometric ethylene-air.
Appendix B: HCCI Engine Data

Motored-Engine Data

Results showing the repeatability of the multiplexed-wavelength diode-laser sensor for motored operation of an HCCI engine are shown below. Figure B.1. plots measured temperature results for 5 consecutive cycles of the motored gasoline-engine-based HCCI engine compared to simulated temperature. The average measured temperature from 5 consecutive cycles compared to the simulated value, and the calculated residual difference and residual fraction are shown in Figs. B.2 and B.3. The measured standard deviation of temperature for 5 consecutive cycles compared to the simulated measurement accuracy is shown in Fig. B.4. This comparison reveals that the sensor performance exceeds simulated performance providing confidence in the spectroscopic line selection procedure and optical engineering. Individual temperature results for each of the 5 consecutive cycles are shown in Figs. B.5-B.9.
Figure B.1. Measured temperature (top) for 5 consecutive cycles gasoline-engine-based HCCI engine motoring at 1200RPM compared to pressure-derived temperature, and pressure (bottom).

Figure B.2. Measured average temperature (top) for 5 consecutive cycles gasoline-engine-based HCCI engine motoring at 1200RPM compared to pressure-derived temperature, residual difference (middle), and pressure (bottom).
Figure B.3. Measured average temperature (top) for 5 consecutive cycles gasoline-engine-based HCCI engine motoring at 1200RPM compared to pressure-derived temperature, residual fraction (middle), and pressure (bottom).

Figure B.4. Measured standard deviation of temperature (top) for 5 consecutive cycles gasoline-engine-based HCCI engine motoring at 1200RPM compared to simulated standard deviation of temperature (measurement uncertainty), and pressure (bottom).
Figure B.5. Measured temperature (top) for first of 5 consecutive cycles gasoline-engine-based HCCI engine motoring at 1200RPM compared to pressure-derived temperature, and pressure (bottom).

Figure B.6. Measured temperature (top) for second of 5 consecutive cycles gasoline-engine-based HCCI engine motoring at 1200RPM compared to pressure-derived temperature, and pressure (bottom).
Figure B.7. Measured temperature (top) for third of 5 consecutive cycles gasoline-engine-based HCCI engine motoring at 1200RPM compared to pressure-derived temperature, and pressure (bottom).

Figure B.8. Measured temperature (top) for fourth of 5 consecutive cycles gasoline-engine-based HCCI engine motoring at 1200RPM compared to pressure-derived temperature, and pressure (bottom).
Figure B.9. Measured temperature (top) for fifth of 5 consecutive cycles gasoline-engine-based HCCI engine motoring at 1200RPM compared to pressure-derived temperature, and pressure (bottom).

**Fired-Engine Data**

Results showing the repeatability of the multiplexed-wavelength diode-laser sensor for fired operation of an HCCI engine are shown below. Figure B.10. plots measured temperature results for 3 consecutive cycles of the fired diesel-engine-based HCCI engine compared to simulated temperature. The average measured temperature from 3 consecutive cycles compared to the simulated value, and the calculated residual difference are shown in Fig. B.11. The measured standard deviation of temperature for 3 consecutive cycles is shown in Fig. B.12. The standard deviation rapidly increases during the ignition portion of the cycle. Individual temperature results for each of the 3 consecutive cycles are shown in Figs. B.13-B.15.
Figure B.10. Measured temperature (top) for 3 consecutive cycles diesel-engine-based HCCI engine firing at 900RPM compared to pressure-derived temperature, and pressure (bottom).

Figure B.11. Measured average temperature (top) for 3 consecutive cycles diesel-engine-based HCCI engine firing at 900RPM compared to pressure-derived temperature, residual difference (middle), and pressure (bottom).
Figure B.12. Measured standard deviation of temperature (top) for 3 consecutive cycles diesel-engine-based HCCI engine firing at 900RPM, and pressure (bottom).

Figure B.13. Measured temperature (top) for first of 3 consecutive cycles diesel-engine-based HCCI engine firing at 900RPM compared to pressure-derived temperature, and pressure (bottom).
Figure B.14. Measured temperature (top) for second of 3 consecutive cycles diesel-engine-based HCCI engine firing at 900RPM compared to pressure-derived temperature, and pressure (bottom).

Figure B.15. Measured temperature (top) for third of 3 consecutive cycles diesel-engine-based HCCI engine firing at 900RPM compared to pressure-derived temperature, and pressure (bottom).
References


