Advanced Reciprocating Engine Systems (ARES) Research at Argonne National Laboratory – A Report

Energy Systems Division

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Advanced Reciprocating Engine Systems (ARES) Research at Argonne National Laboratory – A Report

by

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produced for

Dr. Robert Gemmer
Advanced Manufacturing Office, U.S. Department of Energy

August 2014

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Acronyms and Abbreviations

ALIS	Advanced Laser Ignition System
Argonne	Argonne National Laboratory
ARES	Advanced Reciprocating Engine Systems
ASM	air separation membrane
ATDC	after top dead center
BMEP	brake mean effective pressure
BSCO	brake-specific carbon monoxide
BSCRE	Bombardier single-cylinder research engine
BSNO _x	brake-specific NO _x emissions
BTDC	before top dead center
BTE	brake thermal efficiency
C ₂ H ₆	ethane
C ₃ H ₈	propane
CA	crank angle
CAD	crank angle degree
CARB	California Air Resources Board
CCD	charge-coupled device
CDI	capacitance discharge ignition
CEC	California Energy Commission
CFR	compact folded resonator
CHP	combined heat and power
CO	carbon monoxide
CO ₂	carbon dioxide
COV	coefficient of variance
DERC	Distributed Energy Research Center
DG	distributed generation
DOE	U.S. Department of Energy
ECU	engine control unit
EQR	equivalence ratio
FCV	flow control valve
FWHM	full width at half maximum
FTIR	Fourier transform infrared
GBS	gas blending system
GC	gas chromatograph
GHRR	global heat release rate
GSDS	gas storage and delivery system

HGW	hollow glass waveguide
HT	high-temperature
IC	internal combustion
IMEP	indicated mean effective pressure
I/O	input/output
IT	ignition timing
LHS	left hand side
LIBS	laser-induced breakdown spectroscopy
LT	low-temperature
MBT	maximum brake torque
MFB	mass fraction burn
MFC	mass flow controller
MFT	mass flow transmitter
MRE	minimum required laser energy
N ₂	Nitrogen gas
NEA	nitrogen enrichment of intake air
NFPA	National Fire Protection Agency
NO _x	nitrogen oxides
OCS	Operator Control Station
P/A	peak-to-average
PID	proportional-integral-derivative
PM	particulate matter
PO	Princeton Optronics, Inc.
PWM	pulse width modulated
RCM	rapid compression machine
RPEC	rapid prototyping engine control
SCADA	supervisory control and data acquisition
SI	spark ignition
S/N	signal-to-noise
SOC	start of combustion
SS	stainless steel

TEC	thermo electric cooler
THC	total hydrocarbon
TTL	transistor-transistor logic
UEGO	universal exhaust gas oxygen
UHC	unburned hydrocarbon
VCSEL	vertical cavity surface-emitting laser
VDC	volts direct current
VOC	volatile organic compound

Units of Measure

atm	atmosphere	m	meter(s)
		mA	milliampere(s)
bhp	brake horsepower	MHz	megahertz
Btu	British thermal unit(s)	min	minute(s)
		mJ	millijoule(s)
C	Celsius	mm	millimeter(s)
cc	cubic centimeter(s)	ms	millisecond(s)
cm	centimeter(s)	MTBF	mean time between failures
cm ²	square centimeter(s)	MW	megawatt(s)
cu.ft	cubic feet	MWe	megawatt(s) electric
F	Fahrenheit	nm	nanometer(s)
g	gram(s)	ppm	part(s) per million
GW	gigawatt(s)	psig	pounds per square inch gauge
hr(s)	hour(s)		
hp	horsepower	Quad(s)	quadrillion (~10 ¹⁵)
Hz	hertz		
		rev	revolution
kHz	kilohertz	rpm	revolutions per minute
kmol	kilomole(s)		
kPa	kilopascal(s)	slpm	standard liters per minute
kgph	kilogram(s) per hour		
kW	kilowatt(s)	μm	micrometers
kWe	kilowatt(s) electrical		
		V	volt(s)
L	liter(s)		
lb(s)	pound(s)	W	watt(s)

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Executive Summary

1 BACKGROUND

Concerns about the dwindling U.S. energy deposits, uncertainties about the global energy supply chains, human health concerns, greenhouse gas emissions, and other environmental concerns have brought energy efficiency and clean technologies to the forefront. The energy supply matrix for the United States (see Figure 1.1) is a diverse mix — fossil fuels such as coal, natural gas, and petroleum are interspersed with other traditional and nontraditional resources. Among these, because of its availability in abundance, easy transportation through pipelines, and clean-burning nature, natural gas features prominently with total annual consumption of 26.6 Quads, that is, 27.3% of total U.S. energy consumption. Approximately a third of this natural gas is used for electricity generation by peaking power plants and various distributed generation centers spread throughout the country. In addition, because of the fact that high efficiency (as high as ~ 80%) can be achieved via combined heat and power (CHP), the fraction of natural gas used in distributed generation continues to increase.

Figure 1.1. Sankey Diagram Showing the Net U.S. Energy Flow Trends as of 2013.
(Courtesy: Lawrence Livermore National Laboratory)

For centralized power generation, the “prime movers” of choice are large gas turbines as they offer very low maintenance. These turbines tend to be > 20 MW in size and are typically ~ 34%

efficient for simple cycle plants and reach have efficiencies as high as 60% for combined cycle plants. For most of the distributed power generation applications, the prime mover requirements are smaller than 20 MW. Though solar turbines offers intermediate turbines ranging between 1 and 20 MW, their efficiencies are < 30%. As a result, for DG the choices remain reciprocating engines, fuel cells, and micro-turbines (see Figure 1.2). Fuel cells are low polluting and highly efficient (~ 60%) but often require very high capital costs. Micro-turbines, on the other hand, are low polluting but have very low efficiencies (~30%). Reciprocating engines offer very low capital costs and further have very high efficiencies (~42%): however, nitrogen oxide (NO_x) emissions are a concern. Furthermore, the maintenance requirements are higher as compared to the other two prime movers.

Figure 1.2. A Performance Comparison of Prime Movers Used for Distributed Power Generation (Projections Based on 2002 Data).

Per recent estimates from the U.S. Department of Energy (DOE), more than 10,000 stationary reciprocating engines fueled by natural gas are already deployed in various parts of the United States for distributed power generation. These are usually large-bore engines, with bore sizes > 6.5 inches, and usually within the power range of 0.5 to 20 MW. It is estimated that more than 80% of such engines are of the power range 1.5 MW or lower. In order to accommodate the fact that these engines need to have high reliability, ensuring an availability rate of >95% throughout the year, most of these engine are of robust design with large lubrication oil reservoirs and very long-lived components, such as bearings and spark plugs equipped with noble metal electrodes.

2 MAIN OPERATING CONCERNS OF RECIPROCATING ENGINES

The main concerns for natural gas-fueled engines revolve around emissions, efficiency, and maintenance.

2.1 Emissions

Natural gas-fueled engines are very low polluting as compared to other hydrocarbon-fueled engines. However, as these engines are operated round the clock and throughout the year, their per-year emissions total to a very large quantity. Of chief concern are NO_x, carbon monoxide (CO), and unburned hydrocarbon (UHC) emissions. NO_x emissions tend to increase with engine efficiency and have pathways of thermal, prompt, NNH and other such mechanisms. Under low-temperature conditions, NO_x formation is inhibited, whereas CO and volatile organic compound (VOC) emissions increase. The final engine operation is optimized for maximum efficiency, while being compliant with local emission regulations.

In the United States, the stationary engines were exempt from emission regulations until June of 2006. The regulations instituted thereafter are summarized in Table 1.1. As it is evident, the applicable regulations are based on the power of the engine, as well as the intended application.

Table 2.1. U.S. Emission Regulations for Prime Power SI Natural Gas Generator Sets ≥ 100 hp.

Engine type and fuel	Maximum engine power	Manufacture date	Emission standards					
			g/HP-hr			ppmvd at 15% O ₂		
			NO _x	CO	VOC	NO _x	CO	VOC
SI Natural Gas	100 ≤ hp < 500	7/1/2008	2.0	4.0	1.0	160	540	86
		1/1/2011	1.0	2.0	0.7	82	270	60
SI Natural Gas (except lean burn 500 ≤ hp < 1350)	hp ≥ 500	7/1/2007	2.0	4.0	1.0	160	540	86
	hp ≥ 500	7/1/2010	1.0	2.0	0.7	82	270	60
SI Lean Burn Natural Gas	500 ≤ hp < 1350	1/1/2008	2.0	4.0	1.0	160	540	86
		7/1/2010	1.0	2.0	0.7	82	270	60

* For details see 40 CFR Part 60 Table 1 to Subpart JJJJ at <http://www.ecfr.gov>

2.2 Efficiency

The primary operating cost of these stationary engines is the fuel cost, which can total up to six times the initial cost of the engine itself within a year of operation. As a result, the efficiency of the engine is of primary concern to the engine operator.

In order to meet the competing demands of emissions regulation, fuel efficiency, and system reliability, two prominent engine operational modes have evolved.

The first mode, referred to as the “rich-burn” engine, is operated primarily at equivalence ratios ≈ 1 in conjunction with a three-way catalyst to reduce CO, hydrocarbon (HC), and NO_x emissions. Rich-burn engines often use exhaust gas recirculation (EGR) to reduce in-cylinder combustion temperatures and, as a result, the engine-out NO_x emissions. To offset the loss in power density, intake air is boosted using a turbocharger. The efficiency levels of rich-burn engines are $\sim 36\%$ as of 2011. The primary advantage of rich-burn engines is that they easily achieve compliance with emissions regulations.

The second operational mode that has evolved prominently over the last two decades is the “lean-burn” engine. Such engines are often operated at very low equivalence ratios, $\phi < 0.65$ ($\lambda > 1.54$). The inert nitrogen gas in the excess air that is used acts as a diluent and reduces the in-cylinder combustion temperature that, in turn, leads to reduced NO_x formation. In fact, the engine-out emissions are so low that there is no need for an after-treatment system to reach compliance with emission regulations.

The thermal efficiency of Otto-cycle engines is represented by

$$\eta = 1 - \frac{1}{CR^{(\gamma-1)}} \quad (2.1).$$

In lean-burn engines, wherein more air is used than is required for complete combustion of the fuel, the value of the ratio of specific heats (γ), increases. This design, in turn, leads to higher engine efficiencies. Quite often, the lean-burn engines are boosted using a turbocharger to offset the loss in power density. The primary advantage of lean-burn engines is that they can achieve thermal efficiencies as high as 42%, leading to significant fuel savings for a typical operator.

2.3 Maintenance

Maintenance-related concerns that affect the performance of natural gas-fueled engines are as follows.

Ignition. Of primary concern to the operation of stationary natural gas engines is the maintenance associated with spark plugs. Modern engines are optimized to meet the demands of increased efficiency, low emissions, and high specific power, and they are operated under conditions that are difficult to ignite. Problems with ignition can result in significant misfires, leading to increased hydrocarbon emissions and, most importantly, increased fuel consumption.

Friction. Because stationary engines are not produced in large volumes, technologically their designs have lagged behind advancements in the automotive field. Besides leading to energy losses of $\sim 7\%$, friction leads to reduced hardware life.

3 THE ADVANCED RECIPROCATING ENGINE SYSTEMS (ARES) PROGRAM

Addressing the above three concerns, DOE initiated a research program in 2002 called Advanced Reciprocating Engine Systems (ARES), with research activities conducted at various universities, national laboratories, and industry (primarily Caterpillar, Cummins, and GE-Waukesha). The main goals of the ARES program were to improve the performance of the gas engines from 36–38% thermal efficiency and 2–4 g/kW-hr NO_x to >50% efficiency, < 0.1 g/bhp-hr NO_x, increased fuel flexibility, and lowered capital costs by 2013 (see Figure 1.3).

Figure 3.1. ARES Program Time Based Targets.

Summaries of various efforts pursued under the ARES program at Argonne National Laboratory (Argonne) are presented below. References to corresponding appendices are noted throughout for detailed discussion.

3.1 Distributed Energy Research Center

A user facility, the Distributed Energy Research Center (DERC) was built with state-of-the-art instrumentation to conduct research on distributed energy. This facility currently includes a 150-hp (112-kW) engine test cell and a 623-hp (465-kW) engine test cell. In addition, a 65-kW micro-turbine system is readily available. The DERC was established to serve as a user facility for distributed generation (DG) system and component manufacturers, university, and other national laboratories that need to conduct DG-related research.

3.2 Laser Ignition

Initially, studies were conducted in a constant volume vessel and then in a rapid compression machine (RCM) comparing conventional ignition and laser ignition. Shorter ignition delays, faster rates of combustion, and extension of lean ignition limits were observed. Subsequent tests conducted in a single-cylinder engine showed up to a 70% reduction in NO_x, and up to a 3% increase in efficiency (from a base of 32% efficiency). Most of the effort that followed was dedicated to developing a viable laser ignition system. After years of developmental effort,

Argonne successfully demonstrated the operation of a mechanically multiplexed laser ignition system on a Cummins QSK-19G engine. The observed benefits were comparable to those obtained previously in tests on the single-cylinder engine.

3.3 NEA Membrane for NO_x Reduction

Current reciprocating engines rely on EGR and after-treatment to meet the regulatory limits for NO_x. However, the EGR control scheme is beset with a wide range of issues that result from the induction of corrosive gases. In this study, the technique of nitrogen enrichment of intake air (NEA) using air separation membranes (ASMs) has been proven to reduce NO_x because of lower combustion temperatures while avoiding the undesired and adverse ramifications of EGR.

This technology relies on using polymeric membranes to separate air into oxygen-rich and nitrogen-rich streams. The nitrogen-rich stream is used as combustion air in the engine. As nitrogen acts as a diluent, the combustion temperatures are reduced thereby mitigating NO_x formation. Tests conducted in a single-cylinder engine have shown NO_x reductions of up to 70%. The associated efficiency penalty (excluding that attributable to work done to separate the air streams) remains modest. This pretreatment technology is an alternative to EGR, and therefore can be applied in almost all engines implementing EGR. It is also suited as an upgrade for older engines installed in the field for NO_x abatement.

This concept was demonstrated in three phases. Phase 1 included conceptual studies performed on a Kohler 4-kW natural gas generator using bottled nitrogen. A 50–70% reduction in NO_x was observed with a modest 2% NEA. Ignition timing was also optimized to account for best engine performance. Subsequently, in Phase 2 and after the DERC was commissioned, a single-cylinder research engine was utilized to evaluate this technology on state-of-the-art, research-grade equipment. Initially, bottled nitrogen was used to introduce NEA. Test results followed similar trends as those found with the conceptual experiments. In Phase 3, experiments were performed using an ASM module to generate the NEA for engine operation. At all conditions of engine testing, NEA had a profound impact on the reduction of NO_x emissions. A new patent was awarded for this concept in 2009. In addition, Argonne has a suite of patents on this technology applied to various engine configurations.

Several industrial partners have expressed interest in this technology. However, the membrane manufacturers currently do not have a business model to tap into the potential engine market. Argonne's role in demonstrating the technology's benefits has been very successful.

3.4 Gas-Blending System

A number of gaseous fuels are readily available that could serve as alternative fuels to natural gas. Most of these fuels fall into two categories: (1) syngas — fuels that primarily consist of H₂ and CO as the primary constituents, and (2) digester gases — a variety of gases that have CO₂ as a primary diluent. Because of the low energy content (< 350 Btu/ft³) of these fuels, large amounts currently are flared without being used effectively. To promote use of these fuels using engines tuned for their use, Argonne developed a system that can mix up to seven different gases to a user-specified composition. Furthermore, this gas-blending system

facilitates research to be conducted to study the effect of variations in natural gas composition on engine performance. Details of this system are provided in Appendix D.

3.5 In-Cylinder Optical Diagnostics Development

The laser ignition system provides a unique opportunity to study in-cylinder combustion and use optical diagnostic techniques, conventionally that are not possible to be employed in real engines because of optically inaccessible system structures. Most of the research in the field of combustion using optically accessible engines is limited to low loads and speeds due to the very nature of optical engines. Optically accessible engines are typically modified to accommodate large quartz windows/mirrors and/or a piston/ring assembly. Further, these engines cannot use lubricants; as a result, they can only be operated for very short intervals. Typically, there is not enough time for engines to warm up properly and run in a stable mode before data are collected. Thus, the information obtained does not represent normal engine operation. The sapphire lens/window used in the laser ignition setup enabled researchers to collect an optical signal originating inside the cylinder while operating the engine at full speeds and loads, and to devise diagnostic methods.

In reciprocating internal combustion (IC) engines, the global heat release rates (GHRRs), combustion temperatures, and equivalence ratios (EQRs) are important metrics as they provide valuable insights into the efficacy of various combustion strategies and their influence on the overall engine efficiency. Two types of spectral signals (chemiluminescence and optical emission due to laser-induced breakdown) were investigated, and correlations were made to engine metrics, which are described in Appendix E.

4 ARES COORDINATION ACTIVITIES

Argonne has taken a leading role in the ARES Program since its inception in 2002. In addition to building appropriate research facilities and conducting several related supporting technology projects in-house, Argonne has coordinated the work of development contractors at many levels and arranged three national conferences on distributed generation and CHP. These conferences were well attended and resulted in generated productive directions for the ARES program to take as a whole. In addition, Argonne took an active role in organizing conferences in association with ASME and the California Energy Commission. In addition, Argonne staff coordinated the visits of DOE managers at the three development contractors (Waukesha Engines, Cummins, and Caterpillar).

Apart from consortium activities, Argonne organized or led the following roundtable meetings, peer reviews, and conferences:

1. Initial meeting of the ARES Program, Argonne National Laboratory, March 2001.
2. Ignition Roundtable, Argonne National Laboratory, November 2002.
3. ARES Peer Review, Argonne National Laboratory, Dec. 2, 2003.
4. Emissions Roundtable, Argonne National Laboratory, Feb. 10–11, 2003.
5. Large bore engine and ignition track at the *ASME Fall Technical Conference*, Long Beach, California, 2004.
6. 1st Advanced Stationary Reciprocating Engine Systems (ASRE), organized by DOE and the California Energy Commission (CEC), Sacramento, California, April 14–15, 2004.
7. Advanced Laser Ignition System (ALIS) components meeting, Argonne National Laboratory, January 18–19, 2005.
8. 2nd Advanced Stationary Reciprocating Engine Systems (ASRE), organized by DOE and CEC, SCAQMD headquarters, Diamond Bar, California, March 15–16, 2005.
9. *ASME Spring Technical Conference*, Chicago, Illinois, 2005.
10. *ASME-ICE 2005 Fall Technical Conference*, Ottawa, Canada, 2005.
11. 3rd Advanced Stationary Reciprocating Engine Systems (ASRE), organized by DOE and CEC, Argonne National Laboratory, June 28–30, 2006.
12. Ignition Roundtable, Argonne National Laboratory, Nov. 17–18, 2009.
13. *2010 ASME Fall Technical Conference*, San Antonio, Texas, 2010.

Meetings after 2010 were organized mainly by DOE's Advanced Manufacturing Office and were held in Washington, D.C.

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APPENDICES

A APPENDIX A: DISTRIBUTED ENERGY RESEARCH CENTER

A.1 DERC FACILITY

At the beginning of the Advanced Reciprocating Engine Systems (ARES) Program, most of the distributed generation (DG)-related research was conducted by the three major engine manufacturers — Caterpillar, Cummins, and GE-Waukesha. The need for a common platform for testing newer technologies soon became apparent. To meet this impending necessity, the Distributed Energy Research Center (DERC) was established at Argonne National Laboratory (Argonne) to serve as a user facility for use by national laboratories, component manufacturers, and academia.

A floor plan of the DERC facility is shown in Figure A1. It consists mainly of three test cells and ancillary equipment that support engine testing within each of the test cells. Test Cell #1 (TC #1) houses a single-cylinder research engine. Test Cell #2 (TC #2) houses a micro-turbine engine and emissions measurement equipment. Test Cell #3 (TC #3) houses a 6-cylinder Cummins QSK-19G engine.

Figure A1. Floor Plan of DERC.

A.1.1 Fuel Supply

At the heart of the DERC facility is a 4-inch natural gas supply system that was established early in the program. This system is capable of supplying natural gas at 4,500 cu. ft/hr. at a pressure of 10 psig (15 psig max.) without affecting natural gas supply to buildings across the Argonne campus. Furthermore, from the natural gas supply system south of the 362-Hibay, a 3-inch pipeline was extended to each of the engine test cells for uninterrupted natural gas supply. Combustible gas sensors placed at several strategic locations monitor the DERC facility to ensure safety.

A.1.2 Cooling Water System

A cooling water system circulates a glycol/water mixture across the three engine test cells. The circulating fluid transfers the waste heat from each of the engine test cells to an external radiator bank to vent it into the environment.

A.1.3 Exhaust System

TC #1 and TC #2 are connected to a common exhaust system equipped with a high-temperature fan. The exhaust from the micro-turbine and single-cylinder engine are diluted with room air prior to venting outside of the DERC facility. TC #3 vents the exhaust directly outside of the facility after passing through an appropriate muffler.

A.1.4 Emissions Measurement System

The DERC facility is equipped with state-of-the-art emissions measurement systems (see Figure A2). A Horiba 7100 D emissions bench is used for measuring regulated emissions — carbon monoxide (CO), carbon dioxide (CO₂), hydrogen (H₂), oxygen (O₂), unburned hydrocarbon (UHC), and oxides of nitrogen (NO_x). The Horiba 6000 FTIR system facilitates measurement of unregulated emissions. A set of heated lines and solenoid valves facilitates sharing of these two pieces of equipment among the three engine test cells. In addition, an Agilent Micro GC equipped with the G2801A and 3000A modules allows speciation of the natural gas used in any of the engine test cells.

Figure A2. DERC Emissions Measurement System: (a) Horiba 7100 D Emissions Bench, (b) Horiba 6000 FTIR, and (c) Agilent 3000 Micro GC.

A.1.5 Compressed Air System

An Atlas Copco air compressor (model ZT75-150, with a maximum air flow capacity of 390 cfm) equipped with a 1,550-gallon air receiver tank supplies an uninterrupted compressed air supply at ~ 100 psig to the DERC facility.

Details of other major elements that constitute DERC are given below.

A.2 TEST CELL #1

TC #1 consists of a single-cylinder engine coupled to an alternating current (AC) dynamometer (see Figure A3). An intake surge tank and an exhaust surge tank equipped with appropriate valves facilitate engine operation under turbocharged conditions.

Figure A3. Schematic of the EngineTech Single-Cylinder Engine Setup.

A.2.1 Single-Cylinder Engine

An EngineTech single-cylinder, spark-ignited research engine (RSi 130Q), as shown in Figure A4, is used in Test Cell #2. The engine is anchored to a base plate weighing about 18,000 lbs. Spring isolators dampen the engine vibration being transmitted elsewhere in the facility. The engine specifications are given in Figure A4.

The engine is of 1.87-liter displacement. The engine cylinder head is equipped with two valves and a centrally located 18-mm spark plug. In addition, a pressure port carrying a Kistler pressure transducer facilitates combustion pressure data acquisition. An AVL indicom system along with a Kistler encoder facilitate high-speed data acquisition and analysis.

A.2.2 The 150-hp AC Dynamometer

A trunnion-mounted, dual-ended, four-pole, blower-cooled Dyne Systems Dymond Series AC dynamometer (dyno) is used. This dyno is rated at a maximum power of 150 hp (between 1,800 and 3,600 rev/min) for both continuous motoring and absorption with decreasing power to the maximum speed of 5,000 rev/min. Correspondingly, the dyno has a maximum continuous motoring or absorbing torque rating of 437 lb-ft from 0–1,800 rev/min with 150% overload available for 60 seconds.

A dyno interlock system monitors various elements, such as dyno cooling, dyno winding temperature, over speed, and over torque conditions, and shuts down the dyno when a fault is detected.

Engine Specifications	Single-Cylinder, 4-Stroke, SI
Bore (mm)	130
Stroke (mm)	140
Comp. Ratio	11:1
Displacement (L)	1.857
Power (kW/hp)	33/45
Speed (rpm)	1,800

Figure A4. Specifications and a Photograph of the EngineTech Single-Cylinder Engine.

A.2.3 Inter-Loc V Digital Dynamometer Controller

An Inter-Loc V digital dynamometer controller supplied by DyneSystems LLC is used for controlling engine speed and torque (through the dyno). The Inter-Loc V is a software-based, multi-loop controller capable of providing closed-loop control (with a microprocessor-controlled, pulse width modulated [PWM] control method). The Inter-Loc V obtains feedback signals for speed and torque from an encoder and the load cell, respectively, and performs closed-loop control by supplying the required power to the vector motor drive that powers the dynamometer. Operator Control Station (OCS) is used to control the Inter-Loc V dyno controller.

A Companion Data Acquisition System was used to acquire slow-speed data from transducers placed at various points on the engine. A GE-Fanuc Horner programmable logic controller (PLC) mounted in the Companion enclosure monitors various relays and other such hardware to help ensure safety.

A.2.4 Natural Gas Fuel

Facility-supplied natural gas at 15 psig is compressed to 160 psig using a compressor and stored in a 20-gallon tank. This gas is introduced into the engine intake manifold using an injector block consisting of two electronically controlled gas injectors manufactured by Clean Air Power, Inc. These stainless steel injectors (model SP-010) can operate up to the rated pressure of 125 psig. Gas delivery is adjusted by a pulse-width, modulation-controlled solenoid.

A.2.5 Lube Oil and Coolant Conditioning Unit

Engine lubrication is achieved through an external “lube/coolant unit.” Engine oil at 85°C is pressurized to 30 psig and transferred to the engine. The same unit supplies coolant to the engine at 80°C and 15 psig.

A.3 TEST CELL #3

TC #3 houses a Cummins QSK-19G engine coupled to an AC dynamometer. This test cell was established to test various technologies on a production “ARES class” engine. The engine and dynamometer are fixed to a 25,000-lb bed plate.

A.3.1 The Cummins QSK-19G Research Engine

A Cummins spark-ignited natural gas QSK-19G engine (as shown in Figure A5) is used for performing all baseline and research components of testing. The engine is anchored to the base plate and is coupled to the AC dynamometer via a drive line. All rotating components are very well guarded.

Engine Specifications	Cummins QSK-19G
6-Cylinder, 4-Stroke, SI	
Bore (mm)	159
Stroke (mm)	159
Comp. Ratio	11:1
Displacement (L)	19
Power (kW)	350
Speed (rpm)	1800
Lube oil	133 Liter

Figure A5. Specifications and a Photograph of the 6-Cylinder Cummins QSK-19G Engine.

A.3.2 Engine Control Unit

The engine control unit (ECU) used for this project was provided by Cummins to allow the ECU to function with the engine operating on an engine dynamometer. The engine control unit controls engine operation parameters based on sensor inputs as well as load demand which is commanded by the operator.

The engine is equipped with several sensors to allow for determination of operating conditions. These sensors deliver input signals for the ECU and influence the operational behavior. The sensors available on this particular engine setup are as follows:

- Crank angle position sensor
- Cam shaft position sensor
- Fuel pressure sensor
- Engine coolant temperature sensor

- Knock sensor
- Throttle position feedback
- Exhaust oxygen sensor

Based on these sensor inputs and the load demand, the ECU calculates the engine's operational settings using equations and look-up tables. The main output functions of the ECU are:

- Throttle Position
- Ignition Timing
- Equivalence Ratio
- Boost Pressure

In TC #3, the ECU controlled the ignition timing and equivalence ratio. The throttle position was controlled separately using a ProACT-II controller supplied with an analog signal. The engine boost pressure was the result of the turbocharger operation. In addition, the system was equipped with a mechanically actuated waste gate. Monitoring, recording, and changing of operational parameters in the ECU was made possible by Calterm-II software supplied by Cummins.

A.3.3 Dyne Systems AC Dynamometer

A trunnion-mounted, dual-ended, four-pole, liquid-cooled Dyne Systems AC dynamometer (dyno) is anchored on the base plate for engine testing. The power/torque vs. speed curves for this dynamometer are shown in Figure A6. The maximum rated power of the dyno is 623 hp (between 1,530 and 3,650 rev/min) for both continuous motoring and absorption with decreasing power (200 hp) at 4,800 rev/min. Correspondingly, the dyno has a maximum continuous motoring or absorbing torque rating of 2,138 lb-ft from 0–1,530 rev/min with 140% overload available for 60 seconds. The dyno is powered by a 480–VAC, 3-phase power line with the maximum current drawn for full load motoring at approximately 800 amps. A precision strain-gage load cell (rated at 5,000 lbs.) connected between a welded calibration arm and the dynamometer base through a mechanical linkage provides the torque measurement. The drive shaft is protected with heavy-gauge steel guards to avoid unintentional personnel mishaps in the unlikely event of a shaft breakdown. A dyno interlock system monitors various elements such as dyno cooling, dyno winding temperature, over speed, and over torque conditions and shuts down the dyno when a fault is detected.

Figure A6. Power/Torque versus Speed Curves for a 623-hp (465-kW) AC Dynamometer.

A.3.4 Inter-Loc V Digital Dynamometer Controller

An Inter-Loc V digital dynamometer controller supplied by DyneSystems LLC is used for controlling engine speed (through the dyno). The Inter-Loc V is a software-based, multi-loop controller capable of providing closed-loop control (with a microprocessor-controlled, pulse width modulated (PWM) control method) for up to three dynos. The Inter-Loc V obtains feedback signals for speed and torque from an encoder and the load cell, respectively, and performs closed-loop control by supplying the required power to the vector motor drive that powers the dynamometer. Operator Control Station (OCS) is used to control the Inter-Loc V dyno controller.

Various National Instruments (NI) CompactRIO modules are used to acquire transducer data at 10 Hz. An “in-house” control software written in LabVIEW that works in tandem with various NI PXI based hardware is used for engine control.

A.3.5 Air System

In lieu of using the engine’s stock intake air filter, a custom intake air system was designed; this system includes an air filter for filtering air and a Flowmaxx subsonic Venturi flow meter to measure the air mass flow rate. This custom component is attached to the stock air intake system.

A.3.6 Exhaust System

The stock exhaust manifold was modified to accept thermocouples for cylinder-to-cylinder exhaust temperature measurement and emissions measurement. In lieu of the stock exhaust system, the engine exhaust is expelled out of the building through an 8-inch stainless steel exhaust system.

A.3.7 Fuel System

The fuel system broadly consists of the following:

- A Micro Motion Coriolis-type (ELITE) flow meter coupled to a single-variable flow transmitter to measure fuel flow rate.
- Two solenoid valves to enable fuel flow remotely which are programmed to shut off during the E-stop condition.
- The Cummins Venturi fuel flow controller, which modulates the fuel flow based upon user demand for specific load, equivalence ratio, etc.

A.3.8 Cooling Water Systems

The engine is equipped with two coolant circuits — high-temperature (HT) circuit for cooling the engine block and areas in proximity to the combustion chamber and a low-temperature (LT) circuit to supply cooling to the after-cooler. Engine coolant in the HT circuit flows through a liquid-to-liquid heat exchanger, typically used for steady-state testing. The engine's stock internal coolant pump, in combination with an external liquid-to-liquid heat exchanger, is used to cool the engine. A 50/50 mixture of long-life engine coolant (ethylene-glycol) and distilled water are used as the coolant medium. Temperature-controlled flow valves on the process water outlet of the liquid-to-liquid heat exchangers are used to control the engine coolant to a preset temperature (85°C for the HT circuit and 40°C for the LT circuit).

A.3.9 Lubricating Oil Systems

The stock lubricating oil system of this engine was used in the tests. The overall volume of the engine-lubricating oil used is about 33 gallons (125 liters). The engine oil system is equipped with an internal engine oil pump, as well as two oil filters. An engine oil temperature sensor and a pressure sensor were added to monitor engine operation.

A.3.10 Cylinder Pressure Data Acquisition

With help from Cummins, pressure ports were machined in each of the six cylinder heads. Signals from Kistler pressure transducers installed in each of these ports, conditioned using appropriate charge amplifiers, and were routed to an AVL indicom unit for high-speed data acquisition and processing. The AVL indicom system also used signals from a Kistler rotary encoder mounted on the engine crank shaft.

B APPENDIX B: LASER IGNITION

B.1 BACKGROUND

As mentioned earlier in this report, the main objective of the ARES Program is to achieve **high thermal efficiency** (>50%) and **low NO_x emissions** (< 0.1 g/kw-hr) for stationary natural gas engines. An additional and important requirement, usually mandated by customer preference is **high specific power**. As shown in Figure B1, commercial engines in 2002 were of 18 bar brake mean effective pressure (BMEP), and market forces subsequently pushed engine manufacturers to trend toward 27 bar BMEP by 2010. Quite often, an engine design is achieved as a trade-off among these three conflicting requirements.

Figure B1. Engine BMEP Trend at GE-Jenbacher [1].

Primarily, there are two technical approaches to meet such targets:

- (A) Rich-burn ($\phi \sim 1.0$) operation with Exhaust Gas Recirculation (EGR) and use of a three-way catalyst, and
- (B) Lean-burn operation ($\phi \sim 0.6$ -0.7).

Rich-burn engine operation ($\phi \sim 1.0$), usually entails the use of an exhaust gas oxygen (UEGO) sensor, along with an advanced engine controller. The controller varies the combustion

equivalence ratio between 0.95 and 1.05, thereby enabling the oxidation and reduction processes in a three-way catalyst. EGR helps keep the combustion temperatures low, thereby mitigating engine knocking. This facilitates ignition advance, which results in overall high efficiency. Although such a strategy can provide very low emission levels for easy compliance with emission regulations, engine efficiencies are limited to values below 38%.

Lean-burn operation ($\phi \sim 0.6\text{--}0.7$), has remained the favorite approach of the gas engine industry. In this strategy, combustion air, far in excess of that required for complete combustion of the fuel, is inducted into the cylinder during each combustion cycle. Following a simple thermodynamic model, one can represent the efficiency of an Otto cycle (spark-ignited) engine by:

$$\eta = 1 - \frac{1}{CR^{(\gamma-1)}} \quad (\text{Eqn. B1})$$

In lean fuel-air mixtures, the ratio of specific heats, $\gamma = (C_p/C_v)$, increases, thereby leading to higher efficiencies ($> 38\%$). Concurrently, the combustion temperatures decrease to a point where NO_x formation is mitigated and engine-out NO_x values are well below emission regulation levels (usually $< 0.5 \text{ g/kW-hr.}$) such that an aftertreatment device is not required. In extreme cases, as in the state of California, advanced aftertreatment systems such as urea-SCR (selective catalytic reduction) are used for regulatory compliance. However, these performance benefits are accompanied by a loss in specific power to the engine. To offset this low-energy density, intake air boost is employed with the use of a turbocharger.

Figure B2 shows the typical operation of a lean-burn engine. These engines are operated at the intersection of knock (auto-ignition) limit and misfire (lean-ignition) limit so as to attain maximum efficiency and simultaneously low NO_x emissions. Boost and pre-turbine temperature limits are imposed by the turbocharger materials. Also, as one advances the spark timing, combustion starts early in the compression stroke, and the knock limit is approached. On the other hand, as one retards the spark timing the gas density at the time of ignition tends to be higher, resulting in misfire. One stands to gain substantially by extending the misfire-limit through the judicious choice of a better ignition system.

B.1.1 Ignition Limits

Figure B2 recast in combustion terminology is shown in Figure B3. This figure represents the ignition limits of a typical fuel-air system for $\phi \leq 1.0$. For rich mixtures, self-ignition occurs above a certain pressure, thereby defining the self-ignition limit. Furthermore, for a given method of ignition, a lean limit exists (ϕ_l), for mixtures leaner than which ($\phi < \phi_l$) ignition cannot be achieved. For methane-air mixtures $\phi_l = 0.5$. For achieving maximum combustion efficiency and low NO_x emissions, lean-burn engines are operated at the intersection of lean-ignition limit and the self-ignition limit. Better performance can be achieved by extending the lean-ignition limit by choosing an advanced ignition system.

Figure B2. Operational Region of a Typical Lean-Burn Engine (Courtesy: SwRI).

Figure B3. Ignition Limits of a Typical Fuel-Air System.

B.1.2 Conventional Electrical Spark Ignition

In a typical spark plug, successful sparking is achieved when the potential drop across the spark gap exceeds the dielectric breakdown threshold of typical gases. The sparking voltage potential across the electrodes is given by Paschen's law:

$$V_b = f(p \cdot d)$$

(Eqn. B2),

where p is the pressure of the gas and d is the spark gap. The breakdown voltage, V_b , exhibits a linear dependence on the product pd . The electrode shape and material are also found to have significant influence, the details of which may be found in [2]. Once gas breakdown occurs and a plasma kernel is established, energy transfer occurs, mainly through diffusion on the surface to the surrounding gas. Whether such a diffusion process results in a successful combustion flame front depends upon the kernel energy exceeding Minimum Ignition Energy (MIE), the kernel size exceeding a certain size, turbulence, and gas speed [3]. In practice, factors influencing successful spark creation far outweigh those influencing its transformation into a flame front, and it is normally assumed that once a spark is created the mixture is successfully burned.

B.1.3 Why Laser Ignition?

In present turbocharged lean-burn natural gas engines, capacitance discharge ignition (CDI) systems are used. A schematic of one such system is shown in Figure B4. Although these systems are rated at 100–150 mJ per strike, after thermal losses, typically only 40–60 mJ is transmitted to the spark kernel at rates of voltage rise of 500 V/μs. In CDI systems, energy stored in a high-voltage capacitor (at ~175 VDC) is discharged through a high-voltage coil resulting in voltages in excess of 28k VDC across the spark plug gap.

Figure B4. Schematic of a CDI System.

With a push toward lean-engine operation, with a concomitant requirement to maintain engine specific power, the intake air pressure is increased. Lean operation along with high-intake air pressure results in very high charge densities at the time of ignition. Such high gas densities necessitate spark gap voltages in excess of 40 kV that cannot be achieved using current CDI systems. This often leads to increased misfiring, with subsequent loss of fuel efficiency and increased unburned hydrocarbon (UHC) emissions.

Furthermore, with the use of high-voltage ignition systems, the erosion of spark electrodes is accelerated (see Figure B5). Depending on the manufacturer, typical iridium- and platinum-tipped spark plugs are currently replaced every 1,000–3,000 hrs of operation. To reduce the maintenance burden, engine manufacturers are seeking to extend this interval to cover 8,000 hrs of engine operation.

Figure B5. Ignition Voltage vs. Engine Operational Duration [1].

To address such problems, various research organizations have been exploring alternate ways to achieve ignition [4–9]. Among these alternate methods, laser ignition proves attractive as it offers the following performance benefits:

- Successful ignition of mixtures at *high pressures* ensures reduced occurrence of misfire (see Figure B6), and consequently improved fuel efficiency and lower UHC emissions;
- *Lower maintenance* as the requirement to maintain a reasonable spark gap is eliminated;
- Extension of lean operating limits, thereby enabling lower NO_x emissions;
- Shorter ignition delays and enhanced combustion rates, which allow retarded timings and thereby *reducing NO_x emissions*; and
- Location of the ignition kernel away from the walls, thereby *enhancing overall efficiency* because of reduced heat loss to the cylinder head.

Figure B6. Pressure Dependence of laser Ignition (LI) and Conventional Spark Ignition (SI) (please note that BMEP is given to be representative of in-cylinder pressure [1]).

With such potential benefits, an attempt to use laser ignition for reciprocating engines was made by Dale and Smy as early as 1974 [10]. However, the size and cost of laser systems at that time proved too large and prevented the reduction of laser ignition to practice. Over the last two decades, however, on account of the developments in electro-optic systems, there is a renewed interest in laser ignition for reciprocating engines.

The present effort aims to:

- Conduct fundamental ignition studies of natural gas-air mixtures,
- Determine the benefits that accrue with the use of laser ignition, and
- Design, develop, and demonstrate an integrated laser ignition system on a production multi-cylinder engine.

In pursuit of these goals, researchers at Argonne National Laboratory (Argonne) initiated several activities that can be listed as follows:

- Fundamental ignition studies of NG-air mixtures,
- Single-cylinder ignition studies,
- Development of an Advanced Laser Ignition System (ALIS), and
- Performance evaluation of ALIS.

These are presented in greater detail in the following section.

B.2 IGNITION EXPERIMENTS ON NATURAL GAS–AIR MIXTURES

B.2.1 Rationale

With renewed interest in laser ignition, there have been quite a few studies recently evaluating laser-based ignition in static chambers [11, 12]. Results from one such study conducted at Argonne in a static chamber are summarized in Figure B7. As evident in the figure, lasers enable ignition of mixtures at pressures higher than those that can be ignited by conventional coil-based (CDI) ignition. However, no significant extension of the lean-ignition limit was found with

laser ignition. The lean ignition limits for both laser ignition as well as conventional ignition coincide at $\phi = 0.675$. Similar tests performed elsewhere by Kopecek et al. [13] report a lean-limit extension to $\phi = 0.417$ (with a useable range of $\phi = 0.456$). With most of the lean-burn engines operated close to the intersection of the lean ignition and self-ignition limits, such a spread in data warrants a systematic study under in-cylinder-like conditions. To attain this goal, researchers need to perform ignition tests in a rapid compression machine (RCM) that facilitates highly accurate measurements under in-cylinder-like conditions.

Valves	V1-V11	valves
Orifices	Air coarse	300 μm
	Air fine	30 μm
	Methane coarse	400 μm
	Methane fine	40 μm
	Bleed	50 μm
Pr. Trans.	P1	0-50 psia
	P2	0-300 psia
	Kistler 7061B	0-20 Mpa

Figure B7. Ignition Limits of Methane-Air Mixtures Established in a Static Chamber. Initial Mixture Temperature $\sim 22^\circ\text{C}$.

B.2.2 Experimental Setup

B.2.2.1 Design Features of Argonne's Rapid Compression Machine

As most of the current stationary power generation engines are operated at speeds of $\leq 1,800$ rpm, the RCM was designed with a compression time of < 17 ms. Overall, the system was designed to withstand conditions at the end of combustion of 362 Bar and 3,000 K. In addition, with compression ratios of typical gas engines being $CR \leq 12.5$, the RCM was designed for a $CR = 12$.

The design concept that was used is an improvement over the one developed by the Massachusetts Institute of Technology [14]. A schematic and a photograph of the RCM are shown in Figure B8. This RCM consists of two pistons which, when released, travel toward each other with extremely small resultant vibration. Each side of the RCM consists of three separate chambers that are each carrying a piston. All of the three pistons are mounted onto the same central Titanium shaft that forces their movement in unison. The outermost chamber is a pneumatic chamber carrying a 6-inch-diameter aluminum piston. The innermost is a compression chamber wherein a 2.5-inch-diameter aluminum piston compresses the experimental gases into the central ignition chamber. In the middle is a hydraulic chamber that contains hydraulic oil pressurized to 165 Bar. Special design features within the hydraulic chamber enable it to hold the piston in the retracted position even when pressurized air at 20.7 Bar was present in the pneumatic chamber. The same design features allowed release of the piston when synchronized with an external sparking event. Similar additional features in the hydraulic chamber enabled the piston to be held in the compressed position, thereby avoiding the piston bounce at the commencement of combustion. Various ports on the compression chambers allowed filling the RCM with dry compressed air and 99.99% pure methane. Fine orifices in the gas lines along with a high-resolution pressure transducer allowed establishing mixtures of the required pressures and equivalence ratios to be accurately established. A port on the combustion chamber supports ignition with a conventional spark plug (i.e., an 18-mm thread, J-style) that is powered by an Altronic PM-1 (CDI) ignition system. A second port was used to direct and focus a laser ($f = 13$ mm) to achieve ignition. A third port carrying a Kistler 4073A500 pressure transducer recorded the pressure traces. A fourth port carried an exhaust valve. A total of 22 pneumatically driven solenoid valves interfaced to a computer allowed remote operation of the RCM. A computer program written in NI-LabVIEW driving an NI-Field Point system enabled automation of most of the processes.

B.2.2.2 Laser Delivery and Ignition System

The optical train used in laser ignition is schematically shown in Figure B9. The output of a frequency-doubled Nd: YAG laser (a Spectra Physics GCR 170) was routed through a combination of a half-wave plate and a polarizer to vary the laser power. A beam-splitter and a power meter allowed monitoring of the laser power. A fast-shutter with a 3-ms response time allowed incidence of a single pulse from the laser pulse train. All of the timing was controlled by the NI-Filed point system.

Figure B8. (Upper) Schematic of the Rapid Compression Machine and (lower) a Photo of Argonne's Rapid Compression Machine.

Figure B9. Schematic of the Optical Setup.

B.2.3 Results and Discussion

B.2.3.1 Test Matrix

With the above setup, various tests were performed while varying the initial pressure of the mixture, P_1 , and the equivalence ratio, ϕ . The mixtures established in the RCM were limited to $1.0 > \phi > 0.4$, $3.0 > P_1 > 1.0$ Bar, and initial temperature, $T_1 = 298$ K. A typical pressure trace obtained during one such test run is shown in Figure B10. As the figure shows, when the pistons are released, the gaseous mixture is isentropically compressed to P_2 . Next, as the ignition (sparking) event is sequenced 20 to 30 ms following the end of compression, there is a small pressure drop that results from heat transfer to the combustion chamber walls, ($P_2 - P_2'$). Following an ignition delay after the incidence of spark, the pressure rises steeply to P_3 because of combustion. A subsequent pressure drop occurs primarily because of condensation of water vapor and heat transfer to the walls of the chamber.

From thermodynamics, we obtain the following relationships:

$$P_2 = P_1 \cdot (CR)^\gamma, \text{ and} \quad (\text{Eqn. B3})$$

$$T_2 = T_1 \cdot (CR)^{(\gamma-1)}, \quad (\text{Eqn. B4})$$

where CR = compression ratio and $\gamma = (C_p/C_v) = 1.4$ for air.

Figure B10. Typical Pressure Traces from RCM Operation; $P_1 = 1$ Bar, $\phi = 0.7$.

B.2.3.2 Ignition Limits

With the above setup, tests were conducted by varying the equivalence ratio, ϕ , between 0.5 and 1.0, and by varying the initial pressure of the mixture, P_1 , between 1.0 and 3.0 Bar. For each condition, typically 5 to 6 test runs were executed while varying the laser pulse energy. With each test, the window within which the threshold energy was present was halved until the final threshold value was determined within ± 2.25 mJ/pulse accuracy.

The ignition boundaries determined through such tests expressed as a function of pressure at the time of ignition, P_2' , are shown in Figure B11. A prominent finding is that self-ignition dominates for mixtures with $P_2' > 63$ Bar. In addition, it is of note that the lean ignition limit while using the CDI system is $\phi \sim 0.6$. On the other hand, by using laser ignition, this limit could be extended all the way to the flammability limit of $\phi \sim 0.5$. Such extensions are of significance as the current lean burn engines are operated at the intersection of the self-ignition and lean ignition limits.

Figure B11. Ignition Boundaries as Determined by Using an RCM. The Additional Operational Region Owing to Laser Ignition is shown in the Shaded Region.

B.2.3.3 Minimum Required Energy Scans

For the ignition boundaries established above, minimum required laser energy (MRE) values for successful ignition were determined for various mixture conditions. Values determined for a lens focal length of $f = 13$ mm and a laser beam of $M^2 \leq 5$ are shown in Figure B12. It is of note that, except for $\phi = 1.0$, MRE values decreased with an increase in pressure—finally resulting in self-ignition. For a variation of the equivalence ratio, note that a minima exists at $\phi = 0.85$ for these methane-air mixtures. A further result is that there is a sharp rise in the MRE values for mixtures leaner than $\phi = 0.7$. Such a trend was also noticed at other pressures. This result further implies that the laser energy demands of a future laser-based ignition system for lean-burn applications could be significantly high.

B.2.3.4 Ignition Delays and Rates of Pressure Rise

Lean natural gas-air mixtures ($\phi < 0.8$) are characterized by slow flame velocities and longer ignition delays that are of concern for lean-burn engine operation. As shown in Figure B13, similar tests performed in the RCM showed that ignition delays increased and combustion decelerated with lean operation for both CDI ignition as well as laser ignition. However, the benefits in terms of smaller ignition delays and accelerated combustion were only pronounced under lean conditions, $\phi < 0.8$.

Figure B12. Minimum Required Laser Energies (MRE) for a Lens Focal Length of $f = 13$ mm and a Laser Beam of $M^2 \leq 5$.

Figure B13. (left) Ignition Delays for CDI and Laser Ignition and (right) Rates of Pressure Rise for CDI and Laser Ignition.

B.2.3.5 Conclusions for RCM Tests

Tests performed in the RCM highlighted the performance benefits with the use of laser ignition over conventional ignition: (1) extension of lean ignition limits, (2) smaller ignition delays, and (3) faster combustion rates. More importantly, as shown in Figure B12, these set of tests provide an insight into the trends regarding the minimum required energies that help ensure successful ignition under the lean conditions typical of engine operation.

B.3 SINGLE-CYLINDER LASER IGNITION STUDIES

The objective of the present tests is to determine the impact of the altered combustion behavior that results from laser ignition on the trade-off between brake thermal efficiency and NO_x emissions in a natural gas-fired engine.

In a typical reciprocating engine, chemical energy during combustion is converted to mechanical work on the piston. The net shaft power is a result of such work performed on the pistons less the mechanical losses. Although the mechanical losses originate at various points on a working engine, the most significant of these (up to 50%) is the friction loss that occurs between the piston and cylinder liner. The impact of such losses, however, is diminished in a large-bore engine as the specific surface area is reduced. Furthermore, the reduced heat losses lead to additional efficiency improvements as the combustion cycle approaches the ideal Otto cycle. On account of such factors, the impact of using laser ignition varies in engines of different bore sizes. Field installations of natural gas-fired engines have bore sizes ranging between 130 and 380 mm. For large bore engines, either flame jet ignition or diesel pilot ignition is used to reduce the combustion time. Usually, use of open-chamber spark ignition is limited to bore sizes smaller than 165 mm.

By the time of these tests, Argonne's engine test cells were still under construction. The tests that the Argonne research team pursued in a small generator set [15] proved to be supportive of these trends; however, the chamber geometry was far smaller than the typical 3-liter displacement ARES engine. Consequently, Argonne researchers decided to conduct ignition tests in a Bombardier single-cylinder research engine (BSCRE) at Southwest Research Institute (SwRI), which has a 9.5-inch bore and a displacement of 11 Liters. This engine was equipped with a CDI system that is typical of most field-installed natural gas engines, which readily provided a baseline for performance comparison. In addition, the engine is controlled by a fully flexible control system, RPECS (developed by SwRI), which enables varying all operational parameters within the physical limits. Such flexibility allowed testing up to 18 bar BMEP. Furthermore, the instrumentation to monitor fuel quality and perform emissions measurement was already in place.

In the following sections, details of the experimental setup are presented first. Subsequently, experimental test results obtained over a range of ignition timings and equivalence ratios are discussed along with the noted benefits of laser ignition.

B.3.1 Experimental Setup for Single-Cylinder Engine Tests

B.3.1.1 The Bombardier Single-Cylinder Research Engine (BSCRE)

A large-bore, single-cylinder engine at SwRI was chosen as the experimental engine for the present ignition tests. The specifications of this engine are provided in Table B1. The engine was coupled to an eddy-current dynamometer and controlled by SwRI's proprietary RPECS control system. The dynamometer, in turn, was coupled to a synchronous motor that assisted engine startup. The control scheme and the data acquisition scheme are schematically shown in Figure B14.

Table B1. Specifications of SwRI's BSCRE Engine.

Feature	Specification
Engine Make	Bombardier BSCRE-04
Engine Type	Single-cylinder, 4-stroke
Bore (inches)	9
Stroke (inches)	10.5
Swept volume (liters)	11.5
Compression Ratio	9.3:1
Rated Speed (RPM)	900

Figure B14. Schematic of the Control Scheme of the BSCRE Single-Cylinder Engine Using SwRI's RPECS System.

In-cylinder pressure measurement was performed using a Kistler pressure transducer, and combustion heat release analysis was subsequently performed. Emissions measurements were performed using a Horiba emissions bench, and the data were analyzed following the standard

procedure suggested by Heywood [3]. Natural gas was injected into the intake manifold using an array of low-pressure injectors, and the air/fuel ratio was monitored using a UEGO sensor located on the exhaust manifold.

The conventional spark ignition system included an Altronic CD-200 module and an 18-mm STITT spark plug. The spark plug had three ground electrodes and was located at the same position as the laser plug identified in Figure B15. With this arrangement, the following operating variables were identified:

- Intake boost pressure,
- Air/fuel ratio, and
- Spark timing.

B.3.1.2 Open-Path Laser Ignition Setup

For the open-path laser ignition tests, a compact frequency-doubled Nd:YAG laser was directly mounted over the cylinder head. The output of the laser traveled through the valve cover into a laser plug; from there, it was focused into the combustion chamber by a sapphire lens. The sapphire lens was mounted flush with the fire deck and was subjected to combustion pressure and temperature. With this lens, the point of laser ignition was centrally located in the combustion chamber at ~13 mm from the lens face, and ~30 mm from the piston at top dead center. The piston, cylinder head, and laser plug are identified in Figure B15.

Figure B15. Photograph Showing the Installed Laser Plug in the Combustion Chamber.

Initial experiments showed that the engine cylinder head vibrated sideways at 15 Hz and ± 3 -mm amplitude. To minimize the undesirable effects resulting from these vibrations, the laser was mounted on the ground. The mounting scheme and the spark location are schematically shown in Figure B16.

For the present tests, Big Sky's frequency-doubled Ultra Nd:YAG laser was used. The Big Sky Ultra laser was capable of delivering 33.5 mJ of energy per pulse at 532 nm when operating at

10 Hz. The pulse duration for the Ultra was 8 ns. For the present engine tests, the laser output was adjusted to an energy setting of ~29 mJ per pulse. It should be noted that for an equivalence ratio (EQR) of 0.6 and a BMEP of 15 bar, a laser output of ~9 mJ per pulse is sufficient to ensure consistent ignition of the natural gas-air mixture at normal engine operating conditions. The present application required an operating frequency of 3.75 Hz during engine start-up and the ability to transition to a frequency of 7.5 Hz at rated speed (900 rpm). The external trigger of the Ultra was utilized in conjunction with the RPECS control system to synchronize the laser pulse to the engine cycle in an appropriate manner. Synchronization also provided the flexibility to adjust laser ignition timing during engine operation.

Figure B16. Setup for the Open-Path Laser Ignition Tests.

B.3.1.3 Fiber-Coupled Laser Ignition Setup

A fiber-coupled laser ignition system, shown in Figure B17, was developed for the present subtask. A compact laser, Model Tempest from New-Wave Research, that had high beam quality was used for this purpose. The output of this laser was injected into a 28-inch-long, 700- μ m core silver/polymer (Ag/COP) hollow glass waveguide (HGW) using a 250-mm focal length lens. At the distal end, the laser emission was collimated and refocused using a combination of lenses with focal lengths of 150 mm and 13 mm. A nitrogen purge was used to prevent sparking at the fiber input. A charge-coupled device (CCD) mounted in proximity to the fiber input allowed fine mechanical adjustments. All of these elements were mounted on a single ½-inch-thick plate for testing on the BSCRE engine. Prior to the actual engine tests, engine vibration was simulated in the laboratory using a shaker table, and laser ignition was observed. The fiber-coupled laser ignition system exhibited consistent sparking for more than 24 hours. Subsequently, the system was mounted on the engine at 15 degrees from the

vertical, as shown in Figure B18. A small port on the side of the cylinder head provided optical access for observing the spark kernel.

Figure B17. Layout of the Fiber-Coupled Laser Ignition System.

Figure B18. Fiber-Coupled Laser Ignition System as Mounted on the BSCRE Engine.

B.3.2 Test Matrix

The table below shows the test matrix used to compare the laser and conventional spark ignition systems at a BMEP of 15 bar; the matrix was duplicated at the lower load of 10 bar BMEP (~873 N-m of torque). The engine coolant temperature was maintained at 75°C, and the lube oil temperature was maintained at 85°C. The intake air temperature was maintained at 55°C for full-load operation and at 28°C for partial-load operation to simulate a turbocharged and intercooled intake charge induction system. The simulated turbocharger efficiency was set at 60% by controlling the pressure ratio across the cylinder head. The test matrix shown in Table B2 was expanded to include a comparison between the two ignition systems at a BMEP of 10 bar.

Table B2. Test Matrix for Single-Cylinder Laser Ignition Studies.

Note	Load N-m	Speed rpm	Phi	Ign. Timing degBTDC	Boost/EBP	Ignition System	Piston
<i>EQR Sweep - 0.65- @ 15bar BMEP</i>	1307	900	0.650	PTT Lim***	15bar / 60%comp Eff.	CD200 / Open-path Laser	nominal
<i>EQR Sweep - 0.65- @ 15bar BMEP</i>	1307	900	0.650	+3	15bar / 60%comp Eff.	CD200 / Open-path Laser	nominal
<i>EQR Sweep - 0.65- @ 15bar BMEP</i>	1307	900	0.650	+6	15bar / 60%comp Eff.	CD200 / Open-path Laser	nominal
<i>EQR Sweep - 0.65- @ 15bar BMEP</i>	1307	900	0.650	+...Knock	15bar / 60%comp Eff.	CD200 / Open-path Laser	nominal
<i>EQR Sweep - 0.625- @ 15bar BMEP</i>	1307	900	0.625	PTT Lim	15bar / 60%comp Eff.	CD200 / Open-path Laser	nominal
<i>EQR Sweep - 0.625- @ 15bar BMEP</i>	1307	900	0.625	+3	15bar / 60%comp Eff.	CD200 / Open-path Laser	nominal
<i>EQR Sweep - 0.625- @ 15bar BMEP</i>	1307	900	0.625	+6	15bar / 60%comp Eff.	CD200 / Open-path Laser	nominal
<i>EQR Sweep - 0.625- @ 15bar BMEP</i>	1307	900	0.625	+...Knock	15bar / 60%comp Eff.	CD200 / Open-path Laser	nominal
<i>EQR Sweep - 0.6- @ 15bar BMEP</i>	1307	900	0.600	PTT Lim	15bar / 60%comp Eff.	CD200 / Open-path Laser	nominal
<i>EQR Sweep - 0.6- @ 15bar BMEP</i>	1307	900	0.600	+3	15bar / 60%comp Eff.	CD200 / Open-path Laser	nominal
<i>EQR Sweep - 0.6- @ 15bar BMEP</i>	1307	900	0.600	+6	15bar / 60%comp Eff.	CD200 / Open-path Laser	nominal
<i>EQR Sweep - 0.6- @ 15bar BMEP</i>	1307	900	0.600	+...Knock	15bar / 60%comp Eff.	CD200 / Open-path Laser	nominal
Lean Limit*	1307	900		MBT from 0.6	15bar / 60%comp Eff.	CD200 / Open-path Laser	nominal

* Lean Limit Determined by COV of IMEP > 5 at MBT timing
 ** Knock Limit Determined by Cylinder Pressure Analysis: Pressure fluctuations of 15 psi Peak to Peak for over 50% of the cycles
 *** Pre-Turbine Temperature (PTT) limit set at 720 degC

The engine was allowed to stabilize for 5 minutes at a given test condition before data were recorded. Ignition timing sweeps were performed to set a baseline vis-à-vis its effects on engine emissions and performance. The lean operating envelope was determined by advancing spark timing from the onset of misfire (at very retarded ignition timings) to an advanced ignition timing, which entailed an exhaust NO_x concentration greater than 2,000 ppm (a typical lean-burn engine would operate well below this NO_x concentration). Engine knock, rather than high exhaust NO_x concentration, often limits ignition advance: however, it was found that the Bombardier engine did not knock during any of these tests. The onset of the misfire regime was defined as an operating condition wherein the coefficient of variance (COV) of the indicated mean effective pressure (IMEP) over 100 consecutive cycles was greater than 5%. Single-cylinder engines will often exhibit higher COV of IMEP than their multi-cylinder counterparts because the charge induction process in the former is not continuous. Therefore, a COV of IMEP of 5% was used to identify the onset of misfire at retarded ignition timings; however, a complete lean misfire was defined as an operating condition wherein 1% of engine cycles are devoid of *any* heat release at maximum brake torque (MBT) timing. Indicated parameters and combustion metrics were calculated based on cylinder pressure data acquired with a Kistler piezoelectric pressure transducer that was flush-mounted on the combustion chamber.

With the test matrix described above, three sets of tests were performed:

- (i) Baseline tests using a conventional CDI spark ignition system,
- (ii) Tests using open-path laser ignition, and
- (iii) Tests using fiber-coupled laser ignition.

Results from tests are presented below. It should be noted that a large part of the discussion that follows focuses on results obtained with the open-path laser ignition system. In this regard, it should be mentioned as well that results from the fiber-coupled laser ignition system closely paralleled results from the open-path laser ignition tests.

B.3.3 Results and Discussion for Single-Cylinder Engine Tests

Common metrics for lean-burn engine performance include brake thermal efficiency (η) and brake-specific NO_x emissions (BSNO_x). Macro-operational settings that affect these metrics, *ceteris paribus*, include the fuel-air equivalence ratio, ϕ , and ignition timing. The EQR was controlled globally through a fuel-metering block and UEGO sensor feedback; however, the EQR values reported herein were calculated with a carbon-balance method based on exhaust gas analyses [3]. Crank-resolved engine parameters are plotted versus the crank angle (CA) after top dead center (ATDC), at which 50% of the total in-cylinder mass had burned (i.e., mass fraction burn [MFB] 50). This manner of representing the crank-resolved parameters minimized the ambiguity surrounding actual ignition timing in the two ignition systems. Through combustion analysis of average cylinder pressure (obtained by ensemble-averaging over 100 successive engine cycles), fundamental differences between the two modes of ignition were also compared. Flame development and propagation were quantified through a heat release (burn-rate) analysis. Specific parameters of importance include the CA duration for 10%, 10 to 50%, and 50 to 90% of the trapped mass to burn. These parameters are abbreviated as MFB 0–10, MFB 10–50, and MFB 50–90, respectively. Estimating these parameters required an accurate determination of the start of combustion (SOC). For the test results discussed here, SOC was defined as the CA where the heat release becomes non-zero. This method of determining SOC was employed herein because in the present laser ignition system, the delay between trigger and laser pulse was appreciable ($225 \mu\text{s} \pm 100 \mu\text{s}$). These parameters are delineated in Figure B19.

B.3.3.1 Full-Load Comparison (15 bar BMEP)

The engine was operated at a BMEP of 15 bar (or 1,307 N-m of torque) at 900 rpm, with both a conventional spark ignition system and an open-path laser ignition system for identifying the benefits that laser ignition could have on lean-burn natural gas engines. Laser ignition was found to extend the lean misfire limit from an ϕ of 0.55 with open-chamber spark ignition to 0.50. Laser ignition also improved combustion stability at retarded ignition timings. The combined effect of these two improvements was a 50% decrease in NO_x emissions while maintaining a constant level of efficiency. Figure B20 depicts how laser ignition was capable of extending the lean misfire limit. The various data points represent COV of IMEP over a range of ϕ for both laser and spark ignition at different ignition timings. In this plot, increased COV of IMEP correlates to more retarded ignition timings at a given ϕ .

Figure B19. Arbitrary Cylinder Pressure and Heat Release Comparison to Clarify Nomenclature of Combustion Parameters.

Figure B20. COV of IMEP vs. Equivalence Ratio at a BMEP of 15 bar.

When the engine was operated at increasingly lean ϕ values with open-chamber spark ignition, complete misfire occurred at a ϕ of 0.55 and was detected by a large COV of IMEP ($\sim 15\%$). Even when ignition timing was advanced to 40° before top dead center (BTDC), a steady torque could not be maintained. By comparison, complete misfire occurred at a ϕ of 0.50 with laser ignition. As ignition timing was retarded at a given ϕ , the COV of IMEP increased (shown by multiple points in the data set in Figure B20). For both ignition systems, Figures B21 and B22 show combustion stability as a function of MFB 50 at multiple ignition timings. Evidently, laser ignition improved combustion stability at any given MFB 50 for every ϕ tested.

Figure B21. Combustion Stability with Conventional Spark Ignition at a BMEP of 15 bar.

Other higher-energy ignition systems for natural gas engines are also capable of extending the lean misfire limit. These include pre-combustion chambers and high-energy spark ignition systems. However, they do not necessarily improve the overall performance of the engine. Although pre-combustion chamber ignition systems can ignite leaner mixtures in the main chamber, the combustion in the pre-combustion chamber may contribute significantly to the overall NO_x emission. High-energy spark ignition systems often accelerate the deterioration of the spark plug, thereby requiring increased maintenance and/or replacement. In addition, they also constrain the flame kernel to the chamber wall where flame growth is often stunted by heat transfer to the metal surroundings. By comparison, laser ignition extended the lean misfire limit, thus gaining the emission and performance benefits without any undesirable side effects or constraints.

Figure B22. Combustion Stability with Laser Ignition at a BMEP of 15 bar.

Lean-burn engine technologies are used to improve efficiency and decrease NO_x emissions. Figure B23 compares the trade-off between BSNO_x emissions and brake thermal efficiency for the two ignition systems. This method of comparing the trade-off between engine performance and BSNO_x emissions is consistent with other such comparisons of lean-burn technologies. As the engine ran leaner, the trade-off leaned toward lower BSNO_x emissions. Laser ignition allowed the engine to run leaner and extended the trend toward lower BSNO_x . With open-chamber spark ignition, a brake thermal efficiency value of 32% could be obtained, along with 17.7 g/kWh BSNO_x emissions when the engine was operated at 90% of the misfire limit (typical of lean-burn applications). Maintaining the same misfire margin and brake thermal efficiency, the BSNO_x emissions could be reduced to 5.4 g/kWh using laser ignition; this amounts to a 69% improvement. From an alternate viewpoint, while maintaining the NO_x emissions level at a constant of 10 g/kWh, efficiency improvements of up to 3 percentage points are likely using laser ignition.

Combustion characteristics of the two ignition systems were analyzed to examine the reasons behind the benefits observed with laser ignition. Figure B24 shows cylinder pressure data for 100 consecutive cycles for both open-chamber spark ignition (shown on the left) and laser ignition (shown at right). Spark ignition exhibited complete lean misfire whereas laser ignition provided relatively stable combustion even at a leaner ϕ .

Figure B23. BSNO_x-Brake Thermal Efficiency Trade-off at a BMEP of 15 bar.

Figure B24. Cylinder Pressure Comparison.

With laser ignition, the COV of IMEP was 5.2% at a ϕ of 0.52 compared to a COV of IMEP of 16.5% at a ϕ of 0.55 for conventional spark ignition. Figure B25 shows the ensemble-averaged (over the 100 consecutive cycles) pressure curves for both ignition systems and their corresponding heat release rate profiles. The initial heat release was accelerated with laser ignition, and consequently the total burn duration was decreased. As a result of these effects, combustion was more stable, and the engine could operate at a lean ϕ without misfiring. For

the same reasons, good brake thermal efficiency values were also sustainable at more retarded ignition timings with laser ignition as compared to spark ignition. This ability to employ more retarded ignition timings further reduced NO_x emissions. The considerable difference in peak pressures between the pressure traces for laser and spark ignition may be attributed to the higher boost pressure required to achieve the same BMEP value (15 bar) at a leaner equivalence ratio with laser ignition.

Figure B25. Cylinder Pressure and Heat Release Comparison.

B.3.3.2 Part-Load Comparison (10 bar BMEP)

The performance and emissions improvements shown at full load were also observed at part load. In addition, laser ignition was able to extend the lean misfire limit and improve combustion stability; as shown in Figure B26. These test results at a BMEP of 10 bar are comparable and consistent with work published by National Energy Technology Laboratory [16], in which laser ignition extended the lean limit and decreased ignition delay. Using conventional spark ignition, the engine experienced complete lean misfire (COV of IMEP of 15%) at a ϕ of 0.55. Laser ignition improved combustion stability at the EQR of 0.55 (COV of IMEP of 2.5%) and allowed the engine to operate down to a ϕ of 0.50, beyond which misfire was observed.

Figure B27 shows the BSNO_x-brake thermal efficiency trade-off at part-load and illustrates how laser ignition enabled the engine to operate at lower BSNO_x emissions without compromising efficiency. The BSNO_x emissions were reduced by 65% while maintaining the thermal efficiency constant at 32%.

Figure B26. COV of IMEP vs. Equivalence Ratio at a BMEP of 10 bar.

Figure B27. BSNO_x-Brake Thermal Efficiency Trade-off at a BMEP of 10 bar.

B.3.3.3 Fiber-Coupled Laser Ignition Results

Using the setup presented in Section 2.3, 100% ignition probability was achieved with laser ignition and with the engine operating at a ϕ of 0.6 and a BMEP of 10 bar. A comparison of the burn durations for different modes of ignition and different percentage mass fraction burns is shown in Figure B28. This plot shows that the apparent advantages with the use of fiber-coupled laser ignition are similar to those obtained using free-space laser ignition, that is, accelerated burn rates during all phases of combustion. This finding is consistent with the explanation provided by Bradley et al. [17] in that the increased energy content in the plasma kernel generated by laser ignition results in overly reactive species. These species result in the development of a flame front in “overdrive,” with the associated flame velocities much higher than those typical of conventional spark ignition. The overdriven flame speeds are advantageous to lean-burn engines as the reduced combustion durations can be used to retard ignition, thereby ensuring improved efficiencies and lower NO_x emissions.

Figure B28. A Comparison of Burn Durations for Different Modes of Ignition.

B.3.4 Conclusions for Single-Cylinder Engine Tests

Experiments were performed on a single-cylinder research engine comparing different ignition systems, including the following:

- (i) Conventional capacitance discharge spark ignition,
- (ii) Free-space laser ignition, and
- (iii) Fiber-coupled laser ignition.

Several benefits were observed with laser ignition, including the following:

- Extension of the lean misfire limit by about 10% at BMEP of 10 and 15 bar,
- Increase of the overall burn rate, and
- Improved combustion stability at all comparable test points.

The improved combustion combined with optimization of engine intake air pressure and ignition timing was found to result in:

- A reduction of BSNO_x emissions by ~70% for a given efficiency, or
- An increase in brake thermal efficiencies up to 3 percentage points, while maintaining BSNO_x emissions at a constant level.

Considering all of the noted benefits of using laser ignition, the Argonne's ongoing efforts aim to develop an Advanced Laser Ignition System for use with a multi-cylinder engine. These efforts are discussed next.

B.4 DESIGN OF ADVANCED LASER IGNITION SYSTEM (ALIS)

From an initial survey of possible configurations for a laser-based ignition system, two promising concepts were identified: (1) the laser-per-cylinder concept, and (2) the multiplexed laser concept.

Laser-Per-Cylinder Concept. In the laser-per-cylinder concept, shown schematically in Figure B29, a miniature laser is used per each cylinder for ignition purposes. Various agencies [16, 18, 19], spread throughout the world, have been trying to develop micro-lasers that fit in the sparkplug wells of standard engines and serve as igniters. A variant of this approach is the two-part laser system originally proposed by GE-Jenbacher [1] and later developed by Nippon Soken [19], wherein the pump laser is placed away from the heat and vibration of the engine. In such a case, the pump laser pulse is transmitted via a standard fiber to end pump a passively Q-switched micro-laser placed in the spark plug well. Although this approach facilitates electronic distribution of the signals among different cylinders, it can easily lead to a very expensive system as one laser is used per cylinder. Furthermore, because cylinder head temperatures can reach as high as 95°C, the effort to perform thermal management to maintain a stable lasing cavity becomes a challenge.

Multiplexed Laser Concept. Alternately, as shown in Figure B30, the output of a single laser can be distributed among the various cylinders of a multi-cylinder engine. This approach was pursued primarily by Argonne researchers. This configuration benefits from the cost savings that result from the use of a single laser. In addition, the laser system is isolated from the heat and vibration of the engine. However, this system requires the development of associated high-power components including laser plugs, an optical multiplexer, and fiber delivery system.

Figure B29. Schematic of the Laser-Per-Cylinder Concept.

Figure B30. Schematic of the Multiplexed Laser Concept.

For design of the ALIS, in addition to the data gathered in the earlier tasks of this effort, guidance in design was also derived from performance requirements of the ignition system as specified by engine manufacturers, as given in Table B3.

Table B3. Performance Requirements of an Advanced Ignition System
(Courtesy: Caterpillar, Cummins, and Waukesha).

1	Cost (current dollars)		
	First Cost (add \$1/kWe for CSA ^a requirement)	4.00	\$ / kWe
	Life Cycle Cost (including system replacement at major overhaul)	0.25	\$ / MWe-hr
2	Performance		
	Maximum Ignition Pressure (peak cylinder pressure)	220	bar
	Minimum Air/Fuel Ratio	0.9	λ
	Maximum Air/Fuel Ratio (with swirl)	2.5	λ
	Minimum Methane number (hydrogen capable)	0	
	Maximum Methane Number (landfill capable)	140	
	Ignition Timing Repeatability (non-mechanical)	0.08	° CA
	Ignition Timing Accuracy (non-mechanical)	0.08	° CA
	COV (ARES steady state, 0.5 g/bhp-hr NO _x , 25-bar BMEP)	<1.0	%
	COV (ARICE steady state, 0.015 g/bhp-hr NO _x , 25-bar BMEP)	<1.0	%
	RPM Maximum (overspeed)	125	% of rated
	RPM Minimum (cranking)	50	rpm
	Full Load Range (minimum–maximum)	10–25	bar
3	Ignition System Durability		
	Life to Replacement for Ignition Module and Harness	80,000	hrs
4	Reliability		
	Ignition System (continuous duty)	6,000	MTBF (hrs)

^a ARICE = Advanced reciprocating internal combustion engine; CSA = Canadian Standard Association; MTBF = mean time between failure.

B.4.1 Fiber Delivery System for ALIS

The original ALIS scheme as envisioned early in the program is shown schematically in Figure B30. As part of the current ALIS scheme, it was envisioned that the pulsed output of a laser would be transmitted via optical fibers to laser plugs installed in individual cylinders. The functional requirements specified by engine manufacturers for the optical fibers to be used in a multi-cylinder engine are given below:

- Length > 3 m.
- At least one 90° bend with a radius of curvature < 9 inches.

- Operating temperature > 130°C.

In addition, to achieve sparking at the distal end of the fiber, a laser flux density of $\sim 10^{12}$ W/cm² is necessary when refocused.

For a given fiber and the two-lens system shown in Figure B31, the Lagrange invariant yields the following:

$$a \cdot NA_e = s \cdot NA_s \quad (\text{Eqn. B5})$$

$$\text{As a result, the laser flux density at the focal spot} = \frac{I_{laser}}{s^2}, \quad (\text{Eqn. B6})$$

where:

- a = core diameter of the fiber (microns)
- s = focal spot size (microns)
- NA_e = numerical aperture at the fiber exit $\approx$ half cone angle at fiber exit
- NA_s = numerical aperture at the focal spot
- I_{laser} = intensity of laser (W [watts]).

Combining Eqns. B5 and B6, the following equation is obtained.

$$\text{Laser flux density at the focal spot} \approx \left(\frac{I_{laser}}{a^2} \right) \cdot \left(\frac{NA_s}{NA_e} \right)^2 \quad (\text{Eqn. B7})$$

In Eqn. B7, the first term is determined by the fiber core material damage threshold. In the second term, NA_s is determined by the space available for the laser plug. For fibers of short lengths (~ 3 m), the numerical aperture at the injection end is approximately equal to that at the fiber exit, that is, $NA_i \approx NA_e$; in other words, the exit cone angle is determined by the injection scheme used. Hence the laser flux density can be maximized by making a judicious choice of both the optical fiber and the injection scheme.

Figure B31. Schematic of Laser Refocusing Scheme at the Distal End of the Optical Fiber.

However, in deriving Eqn. B7, it has been assumed that the fiber is mode preserving. For the present case where transmission of high-laser powers is required, the use of large core diameter fibers is encouraged. As is usually the case, a large mode area excites higher-order

modes, whereby the energy is not equally distributed and is skewed toward the higher-order modes. These aspects of actual physical behavior are not captured by Eqn. B7. Nevertheless, this equation provides an acceptable basis that assists in the choice of the optical fiber and the injection scheme.

With the insight provided in the aforementioned arguments, a number of fibers were obtained and tested for sparking in the laboratory. The results of such efforts are discussed below.

B.4.1.1 Solid Core Fibers

Largely driven by advances in the telecom industry, there have been rapid developments in solid-core fiber technology over the past two decades. Currently, step-index (see Figure B33[a]) solid-core fibers with a 1-mm core diameter and a damage threshold of 5 GW/cm² are readily available. Initial efforts to inject such fibers limited the maximum laser energy transmission to 8 mJ/pulse. The primary mode of failure in such fibers was material damage at the entrance end of the fiber. Analysis showed that significant gains in terms of transmitted laser energy could be obtained by ensuring that the laser beam cross-section profile is incident on the face of the fiber as uniformly as possible. For instance, as shown in Figure B32(a), the beam cross-section incident on the fiber face with the use of a simple plano-convex lens had a peak-to-average (P/A) ratio of 15.6. However, a profile that distributed the energy more evenly on the fiber face was achieved using an appropriate axicon-lens combination (see Figure 32[b]). The P/A ratio in such a case was 3.9, and the transmitted laser energy was as high as 30 mJ/pulse.

Figure B32. Fiber Face Laser Intensity Distribution Profiles for an Injection Scheme Using (a) Plano-Convex Lens, and (b) a Combination of Axicon and Plano-Convex Lens.

Nevertheless, such advanced injection schemes introduce higher-order modes, and thus the quality of the beam exiting the fiber degrades. Despite the best efforts to counter these effects, the trade-off between the maximum transmittable laser energy and the generation of higher-order modes proved difficult to overcome, and sparking could not be achieved. In this respect, the gradient-index fiber shown in Figure 33(b) appeared promising as it had a better ability to preserve beam quality. Initial trials in the laboratory showed that these fibers suffer from low material damage threshold. Ultimately, it was decided to direct the present effort toward strategies with hollow-core fibers.

Figure B33. The Refractive Index Distribution in Two Solid Core Fibers: (a) Step-Index Fiber, and (b) Gradient-Index Fiber.

B.4.1.2 Hollow Glass Waveguides (HGWs)

Hollow glass waveguides have the structure illustrated in Figure 34(a). They are essentially glass capillary tubes coated on the inside with silver and a reflectivity-enhancing dielectric. The mode of transmission through HGWs is first surface reflection, whereas total internal reflection is the mode of transmission in solid core fibers. As a result of the transmission in air, the damage threshold of these fibers is 40 times larger, that is, $\approx 200 \text{ GW/cm}^2$. HGWs also tend to preserve the mode quality and exit the beam at a low cone angle, both characteristics rendering them ideally suited for spark generation. However, these fibers tend to have higher transmission losses compared to solid core fibers. In addition, they exhibit certain unique characteristics:

- (i) Transmission losses $\propto (\text{core diameter})^{-3}$.
- (ii) Bending losses $\propto (\text{bend radius})^{-1}$.

Initial evaluations in the laboratory showed that the 700- μm -core HGWs were the most ideally suited as they offered the best compromise between flexibility and transmission.

Subsequently, 700- μm -core HGWs were obtained from three different sources and tested in the laboratory. Their characteristics are as given below in Table B4.

Figure B34. (a) Schematic of the Cross-Section of a Hollow Glass Waveguide (HGW), and (b) a Photograph Showing Spark Generation Using HGW in the Laboratory.

Table B4. Hollow Glass Waveguides Tested for High-Power Laser Transmission.

Source	Coating	Wavelength Optimized for:
Polymicro Technologies	Proprietary	3.2 μm
Rutgers University	Ag/CdS	0.532 μm
Tohoku University	Ag/COP	0.532 μm

Sparking was achieved in the laboratory with all three fibers shown in Table B4. In all three cases, the injection was performed with lenses of $f > 250$ mm into fibers typically 1–2 m long. However, the fibers from Tohoku University [20] offered the lowest transmission losses (see Figure B34[b]). Subsequently, a fiber-coupled laser system was developed using these fibers, and the operation of a single-cylinder engine was demonstrated [21, 22]. However, the downside with these fibers was that they were very bend-sensitive; for bends $> 45^\circ$, sparking was severely affected [21, 23]. Consequently, advanced fibers that are relatively bend-insensitive are desirable, while retaining the favorable characteristics of the HGW fibers from Tohoku University.

B.4.1.3 Advanced Air-Core Fibers

For future on-engine laser ignition applications, two kinds of advanced fiber technologies appear promising: (1) multi-layer hollow glass waveguides, and (2) hollow-core photonic bandgap fibers. These are schematically shown in Figure B35(a) and B35(b). Both rely on multiple reflections to confine light to the central air core, and most importantly, both fibers are bend-insensitive. Manufacturing processes of both kinds of fibers are very involved and those that are commercially available—with core diameters $< 10 \mu\text{m}$ —are not suitable for the

present purpose. It is expected that fibers with core diameters $\sim 30\ \mu\text{m}$ will be required to achieve sparking [24–26]. However, fibers of this size are not readily available.

Later in the program, as a part of a Small Business Innovation Research grant awarded to Colorado State University, Argonne tested “Kagome fibers” (purchased from GO photonics of France), a variant of the air-core photonic band gap fibers. Although sparking could be achieved in 1 atm air and laser energies up to 8 mJ/P could be transmitted, the fibers did not prove to be reliable for long-term use.

Figure B35. (a) Schematic of the Cross-Section of a Multi-Layer Hollow Glass Waveguide, and (b) Photograph of an Air-Core Photonic Bandgap Fiber

With fiber technology proving to be a limitation, Argonne decided to use free-space transmission for further development of the ALIS. As shown in Figure B36, this version of ALIS relies on a high-power multiplexer to distribute the pulsed laser output among various cylinders of the engine.

Figure B36. Schematic of ALIS Using Free-Space Transmission.

B.4.2 High-Power Optical Multiplexer

The optical multiplexer performs a function similar to the traditional automotive distributor: it distributes the output of a pulsed laser among various laser plugs installed in different engine cylinders. The functional requirements of such a high-power optical multiplexer are listed below:

- Ignition timing variation of 0–48° CA BTDC.
- Laser trigger pulse generation.
- An individual cylinder ignition timing variation of $\pm 6^\circ\text{CA}$ (a requirement that the engine manufacturers prescribed late in the program).

In addition, the system needs to be of low-cost and must conform to the durability targets for the overall system of 80,000 hrs.

Though several potential schemes—hydraulically activated, pneumatically activated, piezo activated, etc.—are possible for the multiplexer, Argonne evaluated two potential schemes: (1) electro-optic switches, and (2) mechanically actuated systems. The results from the performance evaluation of prototypes of these systems are discussed below. It should be noted that the system designs considered below conform to a 6-cylinder, 1,800-rpm, 4-stroke engine. These can be extended to engines with more cylinders, if necessary.

B.4.2.1 Electro-Optic Modulator (Pockels Cell)

A Pockels cell acts as an electro-optic switch because it rotates the polarization of the laser light by 90 degrees when activated. As shown in Figure B37(a), a polarizing beam splitter can direct the beam one way or the other based on the polarization state of the laser beam incident on it from the Pockels cell. A linear array of such Pockels cell-beam splitter combinations can be used

(a)

(b)

Figure B37. Schematic of a Pockels Cell-Based Multiplexer and (b) Photograph of a Pockels Cell-Based Two-Channel Multiplexer.

for the present multiplexing purpose. For evaluation, a two-channel system was fabricated at Argonne, and it demonstrated the required performance (see Figure B37[b]).

This scheme facilitates manipulation of the laser beam without having any mechanical movement of the components. However, the number of required optical surfaces increases with the number of engine cylinders and eventually becomes too unwieldy. In addition, voltages as high as 5 kV are required for activating the Pockels cell. Under the present market conditions, it was estimated that the cost associated with this scheme amounts to about \$2,000 per cylinder, which is considered to be too high.

B.4.2.2 Electro-Mechanical Multiplexer

The electro-mechanical multiplexer consists of a linear array of mirrors. An individual mirror, when activated, moves into the path of the laser beam and deflects it into the respective fiber injection port. This system, shown schematically in Figure B38, facilitates the timing variation of individual cylinders. To test the performance of the flip-flop system, a rotary actuator (Model 5EM) was obtained from the Ledex Division of Johnson Electric, an automotive parts supplier. This actuator, when activated, rotates its shaft by 22.5° and moves the mirror into or out of the path of the beam. In a 4-stroke, 1,800-rpm, 6-cylinder engine, the target response time for such a system is 11 ms. The time response of a one-channel system was measured using the arrangement shown in Figure B39(a). As is evident in Figure B39(b), the system shows very little bounce and, in addition, exhibits a response time of less than 7 ms. Subsequently, efforts were undertaken to develop a six-channel system for use with a 6-cylinder engine.

As mentioned previously, with advances in actuators and micro-electromechanical systems (MEMS) technology, many other multiplexing schemes, other than those discussed above, are possible. However, because of the low-cost and fast response time, we have chosen mechanical multiplexing using rotary actuators.

Figure B38. Schematic of Electro-Mechanical Multiplexer.

Figure B39. (a) Schematic of Setup to Measure the Response Time of the Flip-Flop, and (b) a Typical Detector Response Curve.

B.4.3 Laser System for ALIS

From fundamental physics, it is well-known that when a high-power coherent laser beam is focused, multiple photons are absorbed resulting in the generation of free electrons. These electrons are further accelerated by the field gradients and generate more electrons and ions through an inverse *Bremsstrahlung* process. The plasma so generated serves as the ignition kernel for the combustible mixture surrounding it. The energy transfer to the surrounding gas mixture is primarily through diffusion, and depending on its magnitude may or may not result in successful combustion. Overall the process is not wavelength specific and is termed “non-resonant multi-photon ionization.”

An initial literature survey showed that Nd:YAG lasers are ideally suited for laser ignition applications. Based on the configuration of the laser, the output of an Nd:YAG laser can have wavelengths of 1,064 nm, 532 nm, or 266 nm. The focal spot diameter of a collimated laser beam focused by a lens is given by

$$w_o = \frac{W_o}{M} = \left(\frac{4\lambda}{\pi} \right) \left(\frac{f}{D} \right), \quad (\text{Eqn. B8})$$

where:

- w_o = focal spot diameter for ideal Gaussian mode laser (microns),
- W_o = focal spot diameter for a typical multi-mode laser (microns),
- M = is the mode quality,
- λ = laser wavelength (microns),
- F = lens focal length (cm), and
- D = laser beam diameter (cm).

As evident from Eqn. B8, smaller wavelengths result in smaller focal spot diameters. As a result, the use of smaller wavelengths is desirable to achieve a laser flux density of $\sim 10^{12}$ Watts/cm²,

which is required for sparking. Given that the harmonic generation process is, at best, 50% efficient, theoretically speaking, an advantage of factor of two is achieved by going to a higher harmonic. However, a compromise is necessary as system complexity increases. For the present purpose, a wavelength of 532 nm was chosen.

From a functional standpoint, the laser was found to need the following operational characteristics:

- Wavelength = 532 or 1,064 nm,
- Pulse width < 7 ns,
- Repetition rate = 90 Hz (equivalent to the firing requirements of a 6-cylinder, 4-stroke engine operating at 1,800 rpm),
- Laser energy per pulse = 65 mJ/pulse,
- Mode quality, $1.0 < M^2 < 5.0$,
- Operating environment temperature = 10–40°C,
- Compact laser head with low power requirement, and
- Lifetime > 10^9 shots.

A survey of laser technology, as of 2005, showed several potential candidates: (1) passively or actively Q-switched Nd:YAG lasers[27]; (2) diode-pumped, solid state lasers (DPSSLs); (3) disk lasers; and (4) fiber lasers [28]. The last two were nascent technologies, and commercially available lasers were designed with kHz to MHz repetition rates that are mostly suitable for machining applications. Solid-state lasers, either diode pumped or vertical cavity surface-emitting laser (VCSEL) pumped, promise long lifetimes of the order of 10^9 shots. In addition, with efficiencies of more than 30%, the cooling requirements were significantly reduced. Although this technology was following a trajectory amenable to laser ignition, for keeping the prototype costs low, a Q-switched Nd:YAG laser with a small laser head that was already available at Argonne was used. Except for the longevity of the pump source, the performance of this laser mimics that of solid-state lasers in all other respects.

B.4.4 Laser Plugs

Laser plugs are elements that are used instead of a standard spark plug. While confining the combustion gases to the combustion chamber through an appropriate seal, they introduce an optical window so that laser radiation can be focused to create a spark inside the cylinder. Additional requirements for their performance are given below; they must:

- Have the same thread size as a conventional spark plug, that is, M18 × 1.5,
- Provide pressure sealing to 3,000 psi,
- Withstand temperatures as high as 2,400°C,
- Minimize first and second surface reflections,
- Minimize overall laser energy requirements,
- Provide sufficient reliability while transmitting laser energies ~ 60 mJ/pulse,

- Be self-cleaning of any deposits, and
- Facilitate coupling to fiber-optic transmission.

After a couple of iterations, a design was selected that carries a single sapphire lens that also acts as a high-pressure window. In the arrangement shown in Figure B40, the thickness of the plano-convex sapphire lens was chosen to withstand pressures up to 300 bar. With such a thick lens, it is very important that the curved side of the lens be pointed toward the laser so that focusing of reflections at the sapphire-air interfaces are avoided within the sapphire material as it may lead to cracking of the lens. Subsequent tests showed that this lens design also withstood typical in-cylinder combustion temperatures.

Through tests performed by incorporating this laser plug in a 4-kW natural gas engine, it was observed that the laser flux density on the exit face of the sapphire lens was critical. At low laser flux densities, distinct carbon deposits were visible on the lens. Above a certain threshold, the laser radiation ablated such deposits and the lens was found to be self-cleaning. Caution needs to be exercised to keep the laser flux densities well below the material damage threshold of 5 GW/cm^2 .

Figure B40. Schematic Arrangement of the Laser Plug for ALIS.

B.4.5 Electronic Interface

In the case of natural-gas fired stationary engines, the engine control unit (ECU) performs two primary functions: it provides (1) ignition with feedback from a timing disk, and (2) speed control with feedback from a speed governor. In most of the gas-fired engines, these functions are performed by two separate units. Earlier in the program, as shown in Figure B36, it was envisioned that an electronic interface would be required for the ALIS to communicate with the ignition control part of the ECU for ignition timing coordination. After various iterations, a scheme shown in Figure B41 was ultimately used.

Figure B41. Schematic Diagram of the Electronic Interface.

In this electronic scheme, transistor-transistor logic (TTL) trigger signals from the shaft encoder—one per revolution—are fed to a field-programmable gate array (FPGA) programmed using LabVIEW. The FPGA, in turn, provides a TTL signal at a user-specified crank shaft position in crank angle degrees (CAD) from top dead center ($^{\circ}$ CAD ATDC). This signal is conditioned and parsed into six TTL pulses separated equally by 120 CAD. Each of those pulses is fed to a “golden box,” a circuit specifically developed for ALIS. Details of the “golden box” circuit are shown in Figure B42. Triggered by each of the incoming TTL signals, two signals are generated: (1) a 24-VDC signal so generated drives the rotary actuator, and (2) a TTL pulse generated after appropriate delay triggers the laser pulse. As shown in Figure B42, three of the laser triggers are OR gated and fed to each of the power supplies. Such a scheme proved to be robust and allowed us to follow the standard firing order for a 6-cylinder engine: 1-5-3-6-2-4.

In summary, on account of advantages such as low cost and simplicity of thermal management, a scheme was chosen wherein the pulsed output of a single laser is multiplexed to different cylinders of an engine. A thorough evaluation showed that reliable, high-power laser-beam transmission using optical fibers is not yet feasible. As a result, it was decided to rely on free-space transmission for ALIS. Subsequently, the needed components—laser plugs, electro-mechanical multiplexer, and a control system for ignition timing—were developed.

Figure B42. Circuit diagram of the control "Golden Box."

B.5 ALIS INTEGRATION ON A 6-CYLINDER ENGINE

B.5.1 The Test Engine

Early on in the program, the decision was made to use the Cummins QSK-19G engine as the test platform. The specifications of this engine are given in Figure B43. This base engine conforms to the ARES engine development platform at Cummins. This open-chamber, spark-ignited combustion geometry is somewhat similar to the combustion chamber designs at the other two engine manufacturers that are a part of the ARES program, namely, Caterpillar and GE-Waukesha. The QSK-19G engine was installed in an engine test cell and was coupled to a 465-kW dynamometer. Instrumentation installed at various points allowed acquisition of both slow-speed data of the various engine parameters, as well as high-speed cylinder pressure data. Emissions were measured using a Horiba 7100D emissions bench. Further details are provided in Appendix A of this report.

Inline-6, 4-Stroke, SI engine	
Turbocharged, Lean-burn	
Bore (mm)	159
Stroke (mm)	159
Comp. Ratio	11:1
Displacement	19 (Liters)
Power (kW)	350/469
Speed (rpm)	1200/1800

Figure B43. Specifications of the Test Engine.

B.5.2 ALIS Integration on the Engine

Functional requirements for the integrated ALIS system are as follows:

- (i) Vibration insensitivity,
- (ii) Electromagnetic insensitivity,
- (iii) Tolerance for operating temperatures up to 100°C, and
- (iv) Complete enclosure for the laser beam, thereby avoiding inadvertent exposure to operators.

To meet these requirements, the ALIS elements were laid out as shown in Figure B44. A Big Sky PIV Ultra (up to 90 Hz, 60 mJ/pulse, 532 nm) was introduced into a line of mirrors. Each of the mirrors was moved into position by a rotary actuator that moves by 22.5° when energized. In addition, the movement of the actuators and the firing of the laser were synchronized with the engine rotation. Mirrors M1 and M2 provided the Z arrangement to facilitate alignment. Mirror M3, with a hole in the center, allowed transmission of the laser pulse. M3 further relayed the white light emission from the ignition kernel to a photodiode for ignition monitoring. Laser plugs installed in each of the spark plug wells carried a sapphire lens ($f = 18$ mm, back focal length = 13 mm) that focused the incident laser pulse to create a spark.

For this design to be easily adaptable to the engines of different manufacturers, the overall system was designed to be modular to accommodate differences in cylinder-to-cylinder spacing. Each of these modules is interconnected using opaque gas-tight tubes. Besides providing adequate laser safety, they also provide easy installation. Figure B45 shows the ALIS assembly mounted on Argonne's QSK-19G engine.

Figure B44. Schematic of the Integrated ALIS Installed on One Cylinder of a Multi-Cylinder Engine.

Figure B45. Photograph of the ALIS Assembly Mounted on Argonne's QSK-19G Engine.

Initial tests performed on a bench-scale setup showed that ALIS had the durability for continuous operation of > 24 hrs. However, on-engine tests showed that the response time of the actuators varied slightly with temperature; this issue was addressed with sufficient water cooling. In addition, metal heat shields were placed to reduce heat transfer via thermal radiation.

Although there will need to be additional engineering development before ALIS can be commercialized, it provides a platform on which to conduct laser ignition tests on production multi-cylinder engines. Use of high pulse energies that are facilitated by ALIS, as compared to the ~ 2 mJ/pulse allowed by other laser ignition systems [16–19], accelerates the flame speed—a very desirable feature under lean-burn conditions—that, in turn, leads to higher engine efficiencies.

B.5.3 Control System Integration

The engine fluid flows are shown schematically in Figure B46(a). In this turbocharged engine, the fuel is introduced before the compressor section of the turbocharger, which ensures charge homogeneity before entering the intake manifold.

Figure B46. (a) Engine Flow Diagram, and (b) Engine Control Schemes.

Control of various parameters is achieved as follows:

Throttle position (load) control. The test cell software issues a 4–20 mA control signal to ProACT-II hardware, which, in turn, controls the throttle position.

Excess Air-ratio, λ . An air flow meter placed in the air intake stream and a UEGO sensor placed in the engine exhaust stream provide signals to the engine ECU, which, in turn, controls the fuel valve to achieve the user-supplied λ target.

Ignition timing. The engine ECU, while receiving a signal from a cam shaft encoder, supplies the ignition signal to the ignition coils to match up the ignition timing specified by the user in Calterm-II software.

For laser ignition, load control and λ control remained the same, whereas a LabVIEW program built in house and working in tandem with an NI-FPGA received a signal from the crank shaft and provided the ignition timing (see Figure B46[b]) at the user-specified time.

B.6 ALIS TESTING ON 6-CYLINDER ENGINE

B.6.1 Test Matrix

Early bench-scale tests showed that ALIS had the required time response and long-term durability. However, early on-engine tests showed resonance in the actuator driver circuits to make individual channels interfere with each other. As a result, engine testing was limited to a speed of 1,200 rpm. Furthermore, because of limitations of the dynamometer, the load at this speed was limited to 224 kW (300 hp). The laser was operated at ~ 33 mJ/pulse at 532 nm. Tests were conducted using laser ignition (LI), as well as conventional spark ignition (SI).

The test matrix consisted of gradually increasing λ values starting with $\lambda = 1.5$. For each λ value, ignition timing sweeps were performed. With each parameter change, sufficient time—usually 5 minutes—was allowed for the engine to stabilize. With ignition retard to approximately 13–15 CAD BTDC, the COV of IMEP values increased to substantially higher levels than the industry standard value of 5%. With ignition advance, engine efficiency increases but so do the NO_x emission values. Usually in engines, ignition advance is limited by the onset of knocking. In this engine, however, knocking was never encountered; however, the ignition advance was limited to 33 CAD BTDC.

With lean operation, the flame speed decreases, and as a result, the combustion duration increases. To offset the loss in efficiency, ignition is advanced. With this engine for lean conditions, $\lambda > 1.76$, when ignition was advanced beyond 33 CAD BTDC, steady control of engine load could not be achieved (see Figures B47–B49).

Figure B47. Screen Shot for One Case of Low COV of IMEP.

Figure B48. Screen Shot for One Case of High COV of IMEP.

Figure B49. Screen Shot for One Case of Advanced Ignition Timing. Although High Engine Efficiency was Achievable, Engine Load Control was Difficult.

B.6.2 Results and Discussion

The emissions data obtained in these set of tests were reduced using a code that follows the guidelines provided in SAE J1003. The processed data are provided in Figures B50 to B58.

In Figures B50 and B51, the COV of IMEP, which serves as a measure of ignition quality (the lower the COV of IMEP value, the better) is plotted as a function of efficiency for SI and LI cases, respectively. As will be noted, for a given λ value, with advanced ignition timing, efficiency increases and COV of IMEP decreases. Furthermore, with leaning (increasing λ), COV of IMEP values increase as cycle-to-cycle combustion deteriorates. A widely accepted standard used in the gas engine industry is to deem conditions with COV of IMEP $> 5\%$ as misfires. As a result, data points having COV IMEP above this limit were discarded. In addition, it is evident that with SI, the lean ignition limit is $\lambda = 1.68$. In the case of LI, we encountered engine instabilities, which limited lean operation to $\lambda = 1.76$.

Brake-specific NO_x values for different SI and LI test conditions are plotted in Figures B52 and B53, respectively. As is evident, for a given λ value, with ignition advance, efficiency increases. However, the associated BSNO_x values also increase monotonically. In the case of SI, the baseline point corresponds to an efficiency of 36.6% and a BSNO_x of 1.1 g/kW-hr. In contrast, with LI the best operational point corresponds to 37.4% efficiency and a BSNO_x of 0.47 g/kW-hr. That is a 60% reduction in NO_x with a concomitant efficiency increase of 0.8%. Please note that if we were to compare the best SI low- NO_x point, which has a similar BSNO_x emission value as the best LI point, LI yields an efficiency improvement of 1.6% points.

Figure B50. Ignition Quality (COV of IMEP) For Lean-Burn and Various Ignition Timings of Spark Ignition (SI).

Figure B51. Ignition Quality (COV IMEP) For Lean-Burn and Various Ignition Timings of Laser Ignition (LI).

Figure B52. BSNO_x vs. Break Thermal Efficiency for Spark Ignition (SI).

Figure B53. BSNO_x vs. Break Thermal Efficiency for Laser Ignition (LI).

With increasing lean operation, unburnt hydrocarbon (UHC) increases irrespective of the ignition timing (see Figures B54 and B55). As shown in Figures B56 and B57, the trend in the case of brake-specific carbon monoxide (BSCO) is somewhat less clear; however, increased CO emissions result from lean operation facilitated by LI. The UHC and CO emissions are less of a concern as they can be addressed easily using appropriate aftertreatment systems.

Figure B54. Brake-Specific Unburnt Hydrocarbon Emissions for Lean-Burn and Various Ignition Timings of Spark Ignition (SI).

Figure B55. Brake-Specific Unburnt Hydrocarbon Emissions for Lean-Burn and Various Ignition Timings of Laser Ignition (LI).

Figure B56. Brake-Specific CO Emissions for Lean-Burn and Various Ignition Timings of Spark Ignition (SI).

Figure B57. Brake-Specific CO Emissions for Lean-Burn and Various Ignition Timings of Laser Ignition (LI).

B.6.3 Summary of 6-Cylinder Laser Ignition Tests

Engine operation using the conventional spark ignition system was limited to $\lambda = 1.68$, whereas with laser ignition, it could be operated as lean as $\lambda = 1.76$. Table B5 further summarizes the findings of these tests. As shown by comparing the baseline NO_x emissions with that of best-point (LI), NO_x emissions reduce by 60% with a concomitant increase of 0.8% in break thermal efficiency. Although CO and UHC emissions increase, these can be reduced easily by using appropriate aftertreatment systems. Further improvements in performance/emissions are likely if the engine can be operated in a stable manner under lean operating conditions.

Table B5. Summary of 6-Cylinder Laser Ignition Tests Conducted at 1,200 rpm, 224 kW

		λ	Efficiency	BSNO _x	BSCO	BSHC
			%	(g/kW-hr)	(g/kW-hr)	(g/kW-hr)
SI	Baseline	1.6	36.6	1.1	2.47	7.67
	Best Low NO _x	1.68	35.8	0.43	3.25	11.7
LI	Best_pt	1.74	37.4	0.47	3.23	11.64
	Regulations			1	2	0.7
	ARES target		50	0.074		

B.6.4 Future Efforts

With help from Cummins, a thorough troubleshooting procedure was followed to identify the problem leading to engine oscillations observed for $\lambda > 1.76$. Finally, it was narrowed down to a faulty waste gate operation and has been corrected.

Currently, attempts are being made to reduce the interference among channels owing to resonance in the actuator driver circuits by appropriate electronic design. Once this is achieved, as a part of future efforts, SI and LI tests will be performed at rated speed of 1,800 rpm.

B.7 LASER-PER-CYLINDER DESIGN

Early in the program, Argonne decided not to pursue this design, as it could prove cost prohibitive. However, other organizations, such as Robert BOSCH Corporation and Nippon Soken/IMS consortium have had considerable success in designing a micro-laser that can be used as an igniter for each cylinder in an engine.

As part of the ARES Program, Argonne subcontracted with Princeton Optronics, Inc. (PO), of Mercerville, New Jersey, to build two prototypes of micro-laser igniters. Previously, as a part of a Defense Advanced Research Projects Agency (DARPA)-funded project, PO had developed high-power VCSEL lasers. Moreover, the company has in-house capability to design VCSEL-pumped micro-lasers. Figure B58 shows the schematic arrangement and a photograph of the Gen-I micro-laser the company supplied. Gen-I is a VCSEL end-pumped Nd:YAG laser with a Cr⁴⁺:YAG saturable absorber as a passive Q-switch. This laser uses a VCSEL source that is powered by a 20-VDC, 100-Amp power supply (Lumina power LDQCW-600-200-20-300 micro-

sec). For thermal management of this laser, it is also equipped with a thermo electric cooler (TEC). The TEC element is controlled by a controller (PTC5K-CH) using an embedded 100-Ohm thermistor as a temperature-sensing element. For additional thermal management, the unit is also equipped with a passive heat exchanger that carries a cooling fan.

Tests were performed in the laboratory using various detectors and optical elements. In addition, performance under engine-like conditions was determined using a block heater that can heat it up to 95°C.

Figure B58. (a) Schematic of the Gen-I Micro-laser Design, and (b) Inverted Gen-I.

The findings are summarized below:

1. **Emitted Power.** A 1,064-nm output was measured using a laser power meter (Molelectron). A laser diode driver (LDD) setting of 300 μ s, 20 Amp, at 10 Hz yielded two consecutive pulses of 4.1 mJ and 5.9 mJ separated by 111 μ s.
2. **Pulse width.** A 24 ns full width at half maximum (FWHM) was measured using Photodiode (Thorlabs SM05PD2A).
3. **Performance at high temperature.** Poor performance as temperature was varied from 20°C to 95°C. At some temperatures, the laser pulse energy dropped below 2 mJ.
4. **Ability to spark.** Barely achieved at 1 atm air, using a 10 mm aspheric lens.

Later in the program, PO supplied an improved GEN-II version, a photograph of which is shown in Figure B59. Its performance can be summarized as follows:

1. **Emitted Power.** Single-pulse emission, that is, not multiple pulses in a single-emission event: 8 mJ/P at 20°C, 6 mJ/P at 95°C.
2. **Pulse width.** 24 ns FWHM. Measured using Photodiode (Thorlabs SM05PD2A).
3. **Performance at high temperature.** Better temperature stability but dropped to zero at 45°C and 95°C.
4. **Ability to spark.** Could not spark in 1 atm air, using a 10 mm aspheric lens.

Figure B59. Photograph of (Inverted) Gen-II Micro-laser.

B.8 SUMMARY

Fundamental ignition studies performed in this effort have shown laser ignition to be able to ignite mixtures far leaner than those limiting ignition by conventional capacitance discharge ignition. In addition, ignition delays were shortened and combustion rates were enhanced. Such combustion behavior with laser ignition was found to reduce NO_x emissions in a single-cylinder engine by up to 70%. Alternately, for a given NO_x emission level, brake-thermal efficiency could be improved by up to 3 percentage points.

Although most of the required components for a successful laser ignition system were developed, suitable optical fibers for reliable high-power laser transmission were not found. As a result, an ALIS was integrated that primarily relies on free-space laser transmission. Tests conducted on a bench-scale system showed that the system has sufficient long-term durability. However, poor engine control and resonances in electronic driver circuits limited testing on a 6-cylinder Cummins QSK-19G engine to speeds lower than 1,200 rpm. These multi-cylinder engine tests showed a 60% reduction in BSNO_x with a concomitant 0.8% improvement in efficiency. Better performance can be envisioned with better engine control under lean conditions.

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C APPENDIX C: NITROGEN-ENRICHED AIR USING AIR SEPARATION MEMBRANES FOR NO_x REDUCTION IN STATIONARY GAS ENGINES

C.1 SUMMARY

Current reciprocating engines rely on exhaust gas re-circulation (EGR) and after-treatment to meet the regulatory limits for nitrogen oxides (NO_x) emissions. However, the EGR control scheme is beset with a wide range of issues owing to the induction of corrosive gases. In this study, the nitrogen enrichment of intake air (NEA) using air separation membranes (ASMs) has been proven to reduce NO_x because of lower combustion temperatures but without the undesired adverse ramifications of EGR.

This technology relies on using polymeric membranes to separate air into oxygen-rich and nitrogen-rich streams. The nitrogen-rich stream is used as combustion air in the engine. As nitrogen acts as a diluent, the combustion temperatures are reduced, thereby mitigating NO_x formation. Tests conducted in a single-cylinder engine have shown NO_x reductions of up to 70%. The associated efficiency penalty (excluding that attributable to work done to separate air streams) remains modest. This pretreatment technology is an alternative to EGR, and therefore can be applied in almost all engines implementing EGR. It is also suitable as an upgrade for older engines installed in the field for NO_x abatement.

This concept was demonstrated in three phases. Phase 1 included conceptual studies performed on a Kohler 4-KW natural gas generator using bottled nitrogen. A 50–70% reduction in NO_x was observed with a modest 2% NEA. Ignition timing was also optimized to account for best engine performance. Subsequently, after the Distributed Energy Research Center (DERC) was commissioned, a single cylinder research engine was utilized to evaluate this technology on state-of-the-art, research-grade equipment in Phase 2. Initially, bottled nitrogen was used to introduce NEA. Test results followed similar trends as the conceptual experiments. In Phase 3, experiments were performed using an ASM module to generate the NEA for engine operation. At all conditions of engine testing, NEA had a profound impact on the reduction of NO_x emissions. A new patent was awarded for this concept in 2009. In addition, Argonne National Laboratory (Argonne) has obtained a suite of patents of this technology, which are applied to various engine configurations.

Furthermore, several industrial partners have expressed interest in this technology. However, the membrane manufacturers do not currently have a business model to tap into the potential engine market. Nevertheless, Argonne's role in demonstrating the technology's benefits has been very successful.

C.2 BACKGROUND

The availability of clean, sustainable energy to fuel the ever-increasing use of energy-hungry prime movers is one of the most critical challenges encountered by mankind. Alongside concerns about fuel reserves, atmospheric pollution caused by anthropogenic activities especially as a result of energy consumption has become a topic of extensive discussion and deliberation. NO_x emissions are a major contributor to photo-chemical smog present in urban areas. It has severe health repercussions, which, if left unchecked, could potentially affect millions of people. The U.S. Environmental Protection Agency (EPA) estimates that 58% of NO_x emissions come from on-road and off-road vehicles; 24% from power generation (electric utilities); and the remaining 18% from industrial, commercial, and residential sources. Because of its serious health and environmental impacts, the reduction of NO_x in our atmosphere has become a major focus in the fight against air pollution. It is, therefore, no surprise that the EPA, California Air Resources Board (CARB), and several agencies mandate increasingly stringent emissions regulations given the magnitude of the problem. The 2010 NO_x emissions level is 0.1 g/kW-hr.

Several technologies are being actively pursued to make engines produce minimal NO_x without compromising thermal efficiency or power density. Some of the emissions-reducing combustion concepts currently being studied include homogeneous charge compression ignition (HCCI), alternative ignition systems such as pilot fuel ignition, laser ignition (LI), etc., as well as low-temperature combustion (LTC) strategies, each with inherent advantages and limitations [1–5]. Because NO_x varies exponentially with temperature, LTC in engines is currently being exploited to its full potential. However, a threshold temperature needs to be maintained to extract the intended power output from an engine. The general consensus in the engine research community is that future NO_x emissions standards can be met only when combustion temperatures are below 2,000 K (e.g., Flynn et al. [6]). While EGR is effective in helping to realize such a gain, engine durability is compromised because of the induction of corrosive gases into the engine. Urea-based selective catalytic reduction (SCR) technology, another proven NO_x reduction tool, is being promoted very aggressively in Europe and elsewhere, but its use features a major drawback in terms of the astronomical infrastructural costs associated with its implementation, besides filling and monitoring urea levels.

C.2.1 Motivation

Stationary, natural gas-fired reciprocating engines are used for electrical power generation and oil-field pumping applications, most of which are spark-ignited. These large bore engines are required to have high reliability levels because of their round-the-clock operation. EGR has proved to be a very effective tool for reducing in-cylinder temperature and hence NO_x emissions, given that NO_x emissions are a strong function of temperature. However, use of EGR has several built-in adverse ramifications that negate its advantages in the long term. Some of these include the following:

- Combustion contamination,
- Greater control system complexity,

- Application variability,
- Material durability,
- Decreased fuel economy,
- Lubricant contamination, and
- Increased particulate matter (PM) emissions.

NEA is an effective alternative to EGR because it reduces EGR's undesirable consequences. Use of NEA could be achieved by using a mature technology, which involves selective permeation of gases with an ASM [7]. Oxygen-rich and nitrogen-rich streams are produced by pumping air through a nonporous polymeric membrane. The basic principle of membrane operation and various designs and operating characteristics are described in Poola et al. [8]. Research work performed on a two-stroke locomotive diesel engine by Poola and Sekar [9] corroborate variable air technique to reduce emissions. Introduction of inert diluents like nitrogen into a fuel-air mixture slow down the reaction rates of participating chemical species, which eventually lower combustion temperatures and hence NO_x . This process provides an added control parameter to reduce combustion temperature in advanced engines.

C.2.2 Market Impact

CARB approved a regulation to reduce emissions from existing off-road diesel vehicles used in California in construction, mining, and other industries. Most off-road vehicles today have no emission controls and can last 30 years or longer. As a result, the vehicles covered by the regulation emit large amounts of soot or PM and NO_x , accounting for nearly a quarter of statewide mobile source PM and NO_x . These emissions are toxic, currently causing about 1,100 premature deaths per year. Further, federally imposed clean air standards necessitate emissions reductions from off-road vehicles, where punitive sanctions are in place for noncompliance. This lack of compliance, in turn, affects infrastructure improvement efforts. Out-of-state companies doing business in California are also subject to the regulation. The regulation requires fleets to apply exhaust retrofits that capture pollutants before they are emitted to the air, and to accelerate turnover of fleets to newer, cleaner engines. In the aftermath of California implementing such a regulation, there is high probability that states throughout the rest of the country will follow suit. Therefore, the market impact of the ASM technology could be phenomenal. In addition, according to recent studies performed for the California Energy Commission (CEC) and CARB, generator sets powered by internal combustion (IC) engines are 54% more cost effective than reliance on the grid. With the projected load growth in California estimated to reach 1,144 MW, the corresponding market share for these engines is projected to increase proportionately. Furthermore, with NO_x emissions regulations becoming increasingly stringent, engine manufacturers are hard pressed for novel cost-effective technologies. Another factor is that engine manufacturers pursuing urea SCR would welcome any alternative to avoid ammonia slip, a highly toxic compound with inherent deleterious health impacts. This technology could also target the retrofit market via the installed engines database. Because the nitrogen enrichment strategy does not involve routing corrosive exhaust gases into the intake manifold as with EGR and as it requires only minimal additional hardware, both engine reliability and durability will be improved. In terms of cost,

the proposed technology is expected to be less expensive (capital + operations and managements) compared with both EGR and the urea based SCR exhaust after-treatment system. Although urea SCR is very effective, monitoring another chemical adds to the maintenance costs notwithstanding concerns surrounding ammonia slip. In addition, by avoiding EGR, potential lube oil contamination will be prevented, thereby reducing the maintenance requirements. Finally, by embracing the proposed technology, infrastructure costs associated with the construction and maintenance of urea filling stations, which is projected to run into the billions of dollars, could be totally eliminated.

C.3 EXPERIMENTAL APPROACH

This section is categorized chronologically into four distinct phases, namely:

- Phase 1: Simulated NEA using bottled nitrogen on a 4-KW natural gas generator
- Phase 2: Simulated NEA using bottled nitrogen on a 1.8-L, single-cylinder natural gas engine
- Phase 3: ASM on a 1.8-L, single-cylinder natural gas engine

C.3.1 Phase 1: Simulated NEA Using Bottled Nitrogen Gas (N₂) on a 4-KW Natural Gas Generator

C.3.1.1 Experimental Setup

In this study, a single-cylinder Kohler natural gas generator was used to investigate nitrogen-enriched combustion and the effect of ignition timing on its performance and emissions characteristics. Figure C1 shows the Kohler generator setup for the proof-of-concept experiment.

The engine details are included in Table C1, and Figure C2 shows the schematic arrangement of the experiment.

A natural gas conversion kit (Type 3 for the Kohler M12 generator) supplied by U.S. Carburetion, Inc., was installed to operate the engine with natural gas. It consists of a regulator and a load block. The regulator supplies fuel according to the engine demand via the load block, which, in turn, controls the amount of gas flow into the engine. The vacuum line from the carburetor to the natural gas regulator triggers the gas flow.

Figure C1. Kohler Natural Gas Generator Setup.

Compressed methane (98%) at 2,500 psig was used with two-stage regulation to acquire the required intake pressure of the natural gas regulator (R3). The primary regulator (R1) steps down the gas pressure to about 15 psig, while the secondary regulator (R2) further reduces the pressure to 10–14 inches of water, which is a requirement for the natural gas regulator (R3). The secondary regulator can handle a maximum pressure of 250 psig, and hence, the outlet pressure from the primary regulator was below the maximum limit. N_2 was regulated to a pressure between 15–40 psig and introduced into the intake air tank. It was controlled by a needle valve (#53) as shown in Figure C1 to achieve the desired flow rate. Methane was introduced into the intake manifold downstream of the intake air tank where it was fumigated with air and N_2 before entering the engine. Sierra mass flow meters were used to measure the flow rates of methane, nitrogen, and air.

The load on the generator was applied using a 10-kW Simplex load bank. It has a number of resistors rated at 500, 1,000, and 2,000 watts. Using toggle switches, a combination of different resistors can be coupled to apply the required load.

Table C1. Kohler 4-kW Natural Gas Generator.

Generator	6 MM
Wattage, 60Hz	4,000
Voltage, 60Hz	120, 120/240
Amperage, 60Hz	50, 41.7/20.8
Engine	Single cylinder, 4 stroke, spark ignition (SI), air cooled
Bore/Stroke (mm)	85.85/82.55
Comp. Ratio	6.6:1
Displacement (cc)	476.5
Horsepower	12
RPM, 60Hz	3,600
Ignition System	Module controlled/electronic

Figure C2. Schematic of Experimental Setup

High-speed, in-cylinder pressure was measured using a Kistler 6013B pressure transducer, which was plugged into a specially drilled hole in the cylinder head. The pressure signal was phased with respect to crank angle using an optical shaft encoder (BEI), which was coupled to the engine crankshaft. The transducer was connected to a data acquisition system (Win600) to perform combustion analysis via charge amplifier (Kistler), which converts the charge signal to a voltage signal. A new CD200 ignition module supplied by Altronic, Inc., was mounted on the test stand to vary ignition timing with respect to top dead center (TDC) of the engine. The maximum operating range was 48 crank angle degrees (CAD).

The engine-out emissions were measured using an integrated assembly of analyzers (Pierburg 2000 emissions bench) controlled by a computer. Hydrocarbons were measured using a heated flame ionization detector (HFID), while a chemiluminescence detector was used for NO_x measurement. Oxygen concentration was measured with a paramagnetic analyzer, and carbon monoxide (CO) and carbon dioxide (CO₂) were measured using infrared analyzers.

C.4 RESULTS AND DISCUSSION

The test matrix consisted of the following:

- N₂ enrichment,
- Variation of spark or ignition timing, and
- Combination of N₂ enrichment and ignition timing.

N₂ enrichment was obtained by mixing nitrogen and air in the intake manifold upstream of the intake air tank. The intake air temperature and pressure were not conditioned or altered. The ignition timing in Phase I was fixed at –20 after TDC (ATDC). The rated engine speed (3,600 rpm) was reduced to 3,000 rpm by changing the sensitivity of the governor in order to avoid harsh operating conditions. Further, engine speed dropped considerably for a combination of different load, ignition timing, and N₂ enrichment conditions. Load was applied by a combination of different resistors using toggle switches. Accurate load measurement was beyond the scope of this experiment, and hence the applied load was assumed to remain constant for every test condition despite the decrease in engine speed. It is believed, however, that the actual load could vary depending on the test conditions. Engine testing could not be performed at constant speeds as it was controlled by the sensitivity of the governor and was beyond the scope of this experiment. The rated load of the generator, before conversion to operate with natural gas, was 5 kW. However, with natural gas, fueling the engine could not produce the rated power efficiently, and hence full load was modified to 4 kW. Most of the discussion and analysis in this study was performed with respect to full load (4 kW). Additional results can be found in [10].

C.4.1 Nitrogen Enrichment

Figures C3a and C3b show fuel conversion efficiency (FCE) and engine speed as a function of N₂ enrichment for different loading conditions. FCE is defined as the ratio of the applied load to the fuel energy feed rate based on the lower heating values of natural gas. The FCE curves for all loads exhibit a decreasing trend with N₂ enrichment. N₂ enrichment was attained by controlling the N₂ flow rate from 0 to 50 standard liters per minute (slpm) with 10 slpm increments. However, acceptable engine operation was limited to 40 slpm of N₂. The equivalence ratio (Φ) defined as the ratio of actual fuel/air to stoichiometric fuel/air mass flow rates varied from 0.9 to 0.85 with N₂ enrichment. The engine-generated FCE values were of 7%, 13%, 18%, and 22% for the corresponding loading conditions of 1, 2, 3, and 4 kW. The ignition timing for Figures C3, C4, and C5 was fixed at –20 ATDC. Engine speed decreased with N₂ enrichment for all loads. This behavior is attributable to combustion inefficiency or lack of sufficient oxygen (O₂) for complete combustion of the fuel. Furthermore, the drop in engine

speed with N₂ enrichment suggests that FCE trends would decrease far more than results show in Figure C3a.

Figure C3a. Effect of NEA on FCE.

Figure C3b. Effect of NEA on Engine Speed.

On the other hand, NO_x reduction (Figure C4a) for higher loads was very aggressive, which amounts to 88% for 50 slpm (81.8%) of N₂ enrichment and 70% for 40 slpm (81.16%) of the same. N₂ enrichment was limited to 50 slpm at full load (4 kW) owing to engine misfire and poor operating conditions, which explain the abnormal rise in FCE at that point. It was observed that N₂ enrichment (0–50 slpm) had a moderate (35% reduction at 2 kW) or no effect (1 kW) on NO_x reduction at lower load conditions. However, unburned hydrocarbons (UHCs), as shown in Figure C4b, increased significantly at low loads and for higher nitrogen enrichment conditions. At low load (1 kW), the UHCs were higher compared to other loading conditions because of combustion inefficiency and poor throttle control.

Figure C4a. Effect of NEA on NO_x.

Figure C4b. Effect of NEA on total hydrocarbons (THC).

C.4.2 Ignition Timing

Figures C5a and C5b show the effect of both N₂ enrichment and ignition timing (IT) on the performance of the engine. FCE increases from 18.5% at TDC IT, to 22.5% at –30 ATDC IT. However, by further advancing ignition timing, FCE drops to 21% at –48 ATDC IT. A similar FCE trend was observed with N₂ enrichment (81.2%) but with lower FCE values compared to no N₂ enrichment. Engine speed displayed similar trends with change in ignition timing and N₂ enrichment. Ignition at TDC was almost impossible with nitrogen enrichment (81.2%). FCE was the highest (21.4 %) at –30 ATDC. It was found that the rate of increase in FCE with an ignition timing change from –20 to –30 ATDC was greater with N₂ enrichment than normal air. This behavior promotes the importance of advanced ignition timing with N₂ enrichment. However, advanced ignition timings produce consistently increased NO_x numbers because of higher cylinder gas temperatures as mentioned earlier. With the combination of N₂ enrichment and advanced ignition timings, NO_x emissions decrease significantly. Unburned hydrocarbons with normal air (79.05% N₂) were less than 0.5 g/kW-hr for most of the ignition timings except at TDC, which was one of the extreme operating conditions. However, with N₂ enrichment, it was found that advanced timings produce significantly more UHCs because of O₂ depletion and combustion inefficiency coupled with poor flame development and propagation speeds. Retarded ignition timing also resulted in higher UHCs owing to the occasional engine misfire and partial burn conditions.

Figure C5a. Effect of Ignition Timing on FCE and Speed.

Figure C5b. Effect of Ignition Timing on NO_x and THC.

C.4.3 Phase 2: Simulated NEA Using Bottled N₂ on a 1.8-L Single-Cylinder Natural Gas Engine

A single-cylinder ETech (RSi130Q) spark-ignited natural gas research engine was used to investigate nitrogen-enriched combustion coupled with the effect of ignition timing on its performance and emissions characteristics [11]. The engine details are included in Table C2, and Figure C6 shows the schematic arrangement of the experiment.

Figure C6. Schematic of Experimental Setup.

Table C2. ETech Engine Details.

Engine	Single cylinder, 4 stroke, SI
Bore (mm)	130
Stroke (mm)	140
Comp. Ratio	11:1
Displacement (L)	1.857
Power (kW)	33
Speed (rpm)	1,800
Ignition System	CDI (Altronic, Inc.)
Intake Valve Open	10 BTDC (before top dead center)
Intake Valve Close	50 ABDC (after bottom dead center)
Exhaust Valve Open	50 BBDC (before bottom dead center)
Exhaust Valve Close	14 ATDC

The air supply for the engine originated from an ATLAS COPCO laboratory air compressor. Compressed air was routed via an air receiver tank, a sonic flow measurement device, and an intake surge tank to the engine. A pneumatic intake pressure control valve is controlled by the operator to achieve the desired intake pressure. Intake air was unconditioned in that there was no temperature controller, and therefore its study was beyond the scope of this test.

The engine exhaust was expelled out of the building routed through an exhaust surge tank. The exhaust surge tank was used to maintain the required exhaust back-pressure and also to dampen pressure oscillations in the exhaust manifold. A pneumatic exhaust pressure control valve placed downstream of the tank was used to control exhaust back pressure.

Natural gas was supplied to a manifold from an array of gas bottles and routed through a two-stage pressure regulator, which reduced to an operating pressure of 120 psig. A series of valves, which include a service valve, a safety shut-off valve, a manual pressure control valve, and a fuel enable valve, controlled fuel flow. Both the safety shut-off valve and the fuel enable valve are solenoid-operated and digitally controlled to shut off natural gas supply and to enable natural gas supply to the fuel injector, respectively. The natural gas flow rate was measured with a Micro Motion Coriolis-type (ELITE), 1/10-inch, 316-L stainless steel flow meter coupled to an MVD single variable flow transmitter. This flow meter provides mass flow measurements over a flow rate range of 5–250 slpm at 150 psig and 70°F maximum process operating conditions to within $\pm 0.35\%$ (of actual flow rate) accuracy.

Natural gas was introduced into the engine intake manifold using an injector block consisting of two electronically controlled gas injectors manufactured by Clean Air Power, Inc. These stainless steel injectors (Model SP-010) can operate up to the rated pressure of 125 psig. Gas delivery is adjusted by a pulse-width, modulation-controlled solenoid.

Figure C7 shows expected gas injection, spark timing, and intake and exhaust valve events for the test engine. The opening and closing of the injector was triggered by the timing disc and was controlled so as to ensure natural gas injection only after the exhaust valve was closed and only for the intake valve's open duration. This prevented natural gas from being "short-circuited" to the exhaust during the valve overlap period, which reduced UHC emissions and improved FCE.

High-speed in-cylinder pressure was measured using a Kistler 6013B pressure transducer, which was plugged into a specially drilled hole in the cylinder head. The pressure signal was phased with respect to crank angle using an optical shaft encoder (Kistler), which was coupled to the engine crankshaft. The transducer was connected to a data acquisition system (Win600) to perform combustion analysis via charge amplifier (Kistler), which converts the charge signal to a voltage signal. A CD200 ignition module supplied by Altronic, Inc., was mounted on the test stand to vary ignition timing with respect to TDC of the engine.

Figure C7. Gas Injection Timing with Respect to Engine Cycle.

The research engine was instrumented with thermocouples, pressure sensors, flow meters, proportional-integral-derivative (PID) controllers, and CellAssistant software to control the equipment. Full control of spark timing, fuel flow, air flow, and exhaust back pressure allowed simulated turbo-charged conditions. Although boost air temperature control was not incorporated, it was believed that an intercooler (after the compressor in a production engine) could mimic inlet charge conditions observed in this study. The test matrix was developed based on typical stationary engine operating conditions, that is, a constant speed of 1,800 rpm and full load of the engine measured as brake mean effective pressure (BMEP), which in this case was 12 bar.

Exhaust emissions are measured downstream of the exhaust surge tank after the back pressure valve located in the path of the engine exhaust gases. A sample of hot exhaust gas is filtered and routed through a heated sample line to a Horiba MEXA-7100D integrated five-gas emissions bench, which uses separate analyzers to determine exhaust concentrations of CO, CO₂, NO_x, UHC, and O₂. The MEXA-7100D broadly consists of a 19-inch rack of analyzers with a raw sample line, an oven (OVN-723A) containing NO_x and hydrocarbon (HC) analyzers, the main control unit, the interface controller, the sample handling system, the solenoid valve system, the power supply system, and cables and miscellaneous tubing.

Housed in the oven are a heated flame ionization detector (HFID Model FIA-725A) and a heated chemiluminescence detector (HCLD Model CLA-720MA) for HC and NO_x emissions measurements, respectively. On the other hand, CO, CO₂, and O₂ were measured using rack-mounted “cold analyzers.” Oxygen concentration was measured with a paramagnetic analyzer, and CO and CO₂ were measured using infrared analyzers.

C.5 RESULTS AND DISCUSSION

The Advanced Reciprocating Engine Systems (ARES) Program of the U.S. Department of Energy (DOE) has established a Distributed Energy Research Center (DERC) at Argonne to achieve high FCE and low pollutant emissions, especially NO_x . The present research is an initial step toward meeting the ARES goals. The objectives of this effort were to:

- Identify the maximum NEA that an engine could potentially accept without compromising its performance,
- Quantify the NO_x reduction benefit through NEA,
- Evaluate the effect of spark or ignition timing with NEA, and
- Evaluate the best mode of engine operation vis-à-vis lean burn or stoichiometric.

N_2 enrichment was obtained by mixing nitrogen and air in the intake manifold upstream of the intake air tank. The boosted intake air temperature was not heated to typical compressor outlet conditions and was left unconditioned with the assumption that an intercooler could perform such a task. The ignition timing for initial tests was 20° BTDC. All results presented in this section of the report were obtained at 1,800 rpm, which is a typical stationary engine speed for most generator and combined heat and power (CHP) applications even though the rated speed of the engine was 2,200 rpm. The full load for this engine is defined as 12 bar BMEP or 33 kW. Ignition timing could be changed dynamically between 10° and 40° BTDC, with the aid of Altronic's CD200 software. Intake air pressure and exhaust back pressure were adjusted using two pneumatically controlled valves and PID controllers. The tolerances for the set points were within $\pm 1\%$. The turbocharged conditions for the engine were simulated assuming 60% turbocharger efficiency. Compressed natural gas via a Coriolis mass flow meter was delivered to the engine with timed port fuel injection. The fuel flow rate was controlled by changing the pulse width of the gas injectors to a maximum time limit based on inlet valve closing.

Traditionally, the equivalence ratio (Φ) is defined as the ratio of the actual (measured) fuel flow to air flow ratio to the stoichiometric fuel flow to air flow ratio. However, because the experiments in this work made use of nitrogen as a diluent, we introduced a new parameter called the O_2 -based equivalence ratio (ψ) that is defined as the ratio of the actual (measured) fuel flow to O_2 flow ratio to the stoichiometric fuel flow to O_2 flow ratio [12]. It is believed to be a more accurate parameter in performance comparison because of the introduction of nitrogen, which alters the conventionally accepted Φ .

C.5.1 Nitrogen Enrichment

NEA is the air containing N_2 in excess of 79.05% (by volume). N_2 enrichment was attained by controlling the N_2 flow rate upstream of the intake surge tank. This approach allowed for thorough mixing of air and N_2 before being inducted into the engine. All NEA-related data presented in this paper was acquired by using bottled N_2 . Use of an ASM integrated with the research engine will be discussed in the next section.

Figures C8a and C8b show NO_x as a function of N_2 enrichment at an ignition timing of 20° BTDC. It was observed from previous research that engine load has a direct effect on the NO_x reduction characteristics using NEA. NEA yields greater reductions in NO_x emissions at higher engine loads. This result occurs primarily because of the prevalent higher flame temperatures for higher engine loads. Hence, the present work was limited to evaluating the engine performance and behavior at full load, which in this case was 12 bar (BMEP). The N_2 flow was controlled so as to achieve the desired enrichment levels varying from 0 to 3.5%. However, acceptable engine operation was limited to below 3% NEA. There is a significant drop in NO_x emissions as NEA is increased. NO_x emissions reduce primarily because the “diluent effect” of N_2 yields lower combustion temperatures when coupled with O_2 depletion in the charge. According to previous NO_x studies, NO_x emissions are strongly correlated as a function of combustion temperatures. Bulk gas temperature is an exponential component in the NO_x formation mechanism. Even a slight reduction in the bulk gas temperature can significantly alter NO_x formation. NO_x reductions between 0% and 2% NEA are more pronounced than beyond 2%. The bar chart shows NO_x emission reductions as a percentage. All N_2 enrichment levels yielded excellent NO_x emissions reductions reaching as high as 90% at 3.5% NEA.

Figure C8a. NO_x Reduction as a Function of NEA.

Figure C8b. Effect of NEA on NO_x.

However, FCE decreased simultaneously, as shown in Figure C9. FCE is defined as the ratio of the brake power produced by the engine to the fuel energy feed rate based on the lower heating values of the fuel (natural gas). Although FCE and brake thermal efficiency (BTE) are essentially similar, FCE is the preferred measure, as the quantity is described precisely and is also differentiated from other engine efficiencies such as available conversion efficiency, thermal conversion efficiency, combustion efficiency, etc. [12]. The drop in FCE for the 2% NEA condition was rather modest, amounting to less than 1.5 percentage points (< 4% fuel penalty) compared to the other enrichment levels, which rose to an unacceptable 5 percentage points (13% fuel penalty).

Therefore, N₂ enrichment beyond 2% is not considered an ideal approach to mitigate NO_x emissions because of the high fuel penalty. This limit benefits engine manufacturers in that an NEA-producing device such as an ASM could be used with reduced parasitic losses and is more economical to implement than otherwise. In addition, the stability of engine operation suffers exponentially after 3% NEA. The coefficient of variation of indicated mean effective pressure (COV_{IMEP}), a parameter used in the industry to measure engine stability, exceeded the accepted value of 5%. This behavior results from combustion inefficiency or the lack of a sufficient supply of O₂ to complete combustion of the fuel. The O₂-based equivalence ratio (ψ) as shown in Figure C5 varied from 0.91 (normal air) to 1.03 (3.5% NEA). As mentioned earlier, when N₂ was introduced into the intake manifold, it was found that ψ increases proportionately because it displaces a portion of the air that would have otherwise been utilized during combustion.

Figure C9. Specific NO_x and ψ as a Function of FCE

Figure C10 displays the cylinder pressure, heat release rates, and the mass fraction burn (MFB) trends for different N₂ enrichment conditions at full load (12 bar) and 20° BTDC (IT). Cylinder pressure was averaged over 100 consecutive engine cycles for combustion analysis. Clearly, the peak pressures decrease with N₂ enrichment, resulting in lower bulk gas in-cylinder temperatures, which explains the reduction in NO_x emissions. The phasing of the peak pressure relative to TDC increases with N₂ enrichment, along with a drop in peak pressure, amounting to lower FCE. Both the heat release rates and the MFB rates decrease with N₂ enrichment. Mass fraction burn is defined as the instantaneous burned mass normalized by the total mass of charge in the cylinder. The phasing of the heat release curves is shifted (away from TDC) more into the expansion stroke of the engine cycle, which leads to a loss in FCE. N₂ enrichment delays the 10% burn rate considerably, which is often referred to as the flame development angle or sometimes as ignition delay. The difference in the crank angle of MFB at the extreme conditions (0% and 3% of NEA) increases from 3 CAD at 10% to 5 CAD at 50%. This behavior implies that N₂ enrichment results in lower burning rates and a longer combustion duration. The lower burning rates are attributed to the slower flame development and propagation speeds caused by N₂-enriched air. Therefore, it was understood that the lower heat release rates, longer combustion duration, and the shift of the phasing of heat release rates all contribute to the drop in FCE and NO_x emissions.

Figure C10. Combustion-Related Data as a Function of Engine Cycle.

C.6 PHASE 3: NEA USING AN AIR SEPARATION MEMBRANE ON A 1.8-L, SINGLE-CYLINDER NATURAL GAS ENGINE

The investigation in this section was performed with an ASM capable of delivering at least 3.5% NEA to a single-cylinder, spark-ignited natural gas engine. Low-temperature combustion is one of the pathways to meet the mandatory ultra-low NO_x emissions levels set by regulatory agencies. In this study, a comparative assessment is made between natural gas combustion in standard air and 2% NEA. Enrichment beyond this level degraded engine performance in terms

of power density, BTE, and UHC emissions for a given equivalence ratio. The ignition timing was optimized to yield maximum brake torque for standard air and NEA. Subsequently, conventional SI was replaced by LI to extend the lean ignition limit. Both ignition systems were studied under a wide operating range from ϕ : 1.0 to the lean misfire limit. It was observed that with 2% NEA, for a similar fuel quantity, the equivalence ratio (Ψ) increases by 0.1 relative to standard air conditions. Analysis showed that lean-burn operation, along with NEA and an alternative ignition source such as LI, could provide the pathway to realizing lower NO_x emissions with a slight penalty in BTE. Additional results can be found in [13–16].

C.6.1 Experimental Setup

A single-cylinder ETech (RSi130Q) spark-ignited natural gas research engine was used to investigate nitrogen-enriched combustion via an air separation membrane. Figure C11 shows the schematic arrangement of the experiment.

The major change in the experimental setup compared to that of the previous section involved the installation of a CompAire natural gas compressor, which compressed the Argonne site-wide natural gas supply pressure from 5 psig to 130 psig. Previously, an array of natural gas bottles was used to fuel the engine whose composition was slightly different from the current supply source. Therefore, the stoichiometric air/fuel ratio changed from 16.2 to 16.39. Furthermore, gas injection pressure dropped by about 15 psig. The natural gas flow rate was measured with a Micro Motion Coriolis-type flow meter. Natural gas was introduced into the engine intake manifold using an injector block consisting of two electronically controlled gas injectors (CAP, Inc.). Gas delivery was adjusted by a pulse-width, modulation-controlled solenoid. In order to reduce UHC, the injection event was triggered by a timing disc to prevent natural gas from being “short-circuited” to the exhaust during the valve overlap period. Because of the drop in injection pressure, the pulse width duration was adjusted to attain previously observed fuel flow rates.

High-speed in-cylinder pressure was measured using a Kistler 6013B pressure transducer mounted on the cylinder head. The pressure signal was phased with respect to crank angle using an optical shaft encoder (Kistler) coupled to the engine crankshaft. The transducer was connected to a data acquisition system (Win600e) to perform combustion analysis via a charge amplifier (Kistler), which converted the charge signal into a voltage signal.

A Horiba MEXA-7100D, an integrated five-gas analyzer emissions bench, was used for CO , CO_2 , NO_x , UHC, and O_2 measurements. A heated flame ionization detector and a heated chemiluminescence detector were used for HC and NO_x emissions measurements, respectively. O_2 concentration was measured with a paramagnetic analyzer, whereas CO and CO_2 were measured using infrared analyzers.

Variation of the O_2 -enriched air, as shown in Figure C11 (Permeate), created partial pressures in ASM, which facilitated separation and produced the desired NEA (Retentate). This NEA was supplied to the engine. The O_2 concentration within the NEA supplied to the engine was measured by an O_2 analyzer to adjust nitrogen enrichment levels systematically.

Figure C11. Schematic of Experimental Setup.

An Altronic CD200 ignition module helped vary ignition timing between 10° and 40° BTDC. Baseline SI tests were followed by LI for the given test matrix presented in Table C3. An ultra-compact folded resonator (CFR) Nd:YAG laser (the Big Sky Laser) capable of delivering a 532-nm laser pulse with energy of 31 mJ/pulse was used as the laser source for the experiment. The Altronic system was used to trigger the laser ignition system. High-power laser pulses were transmitted directly to a “laser plug” installed on the cylinder head. The laser plug focuses the transmitted laser pulses to generate fluences of $\sim 10^{12}$ W/cm² in order to achieve gas breakdown [17]. The focal distance was 13 mm away from the laser plug tip.

C.6.2 Results and Discussion

The objectives of this effort were to:

- Quantify the NO_x reduction benefit by supplying NEA with an ASM,
- Compare engine performance between standard air and NEA supplied through an ASM, and
- Study the effect of alternative ignition sources such as lasers both with and without NEA.

Table C3. Test Matrix (BMEP: 12 bar, Speed: 1,800 rpm).

Parameter	NEA	IT	ψ
	%	BTDC	
Spark Ignition	0	MBT (35-23)	0.65–1.01
	2	MBT (37-27)	0.72–1.12
Laser Ignition	0	MBT (38-23)	0.62–1.01
	2	MBT (38-27)	0.68–1.10

The test matrix (shown in Table C3) was developed based on typical stationary engine operating conditions for most generator and CHP applications, that is, a constant speed of 1,800 rpm and full engine load measured as BMEP at 12 bar (33 kW at 1,800 rpm).

Complete control of ignition timing, fuel flow, air flow, and nitrogen enrichment allowed judicious choice of operating conditions. Intake and exhaust back pressure control facilitated simulated, turbo-charged conditions assuming 60% turbocharger efficiency. Intake air pressure and exhaust back pressure were adjusted using two pneumatically controlled valves with PID controllers. Although the test did not incorporate a boost air temperature control, it was believed that an intercooler (downstream of the compressor in a production engine) could mimic the inlet charge conditions observed in this study.

$$\psi = \frac{[\text{Oxygen}/\text{Fuel}]_{\text{Stoic}}}{[\text{Oxygen}/\text{Fuel}]_{\text{Actual}}} \quad \text{Eqn. C1}$$

ASM installation alters the composition of standard air based on the level of partial pressures maintained across the membrane fibers. O₂, being relatively more permeable than N₂, permeates through the membrane fibers (coated with a polymeric material) to yield a permeate flow (O₂-enriched air, or OEA) and retentate flow (nitrogen-enriched air, or NEA). This parameter is varied by opening or closing the permeate flow valve shown in Figure C2. In order to make an accurate comparison between the two technologies under study (i.e., standard air and NEA), the conventional definition of Φ was redefined to reflect only the O₂-to-fuel ratio. Traditionally, the equivalence ratio (Φ) is defined as the ratio of the actual (measured) fuel flow to air flow ratio to the stoichiometric fuel flow to air flow ratio. However, because the experiments in this work modified the chemical composition of air, we introduced an O₂-based equivalence ratio (ψ) that is believed to bring clarity to our performance comparison because of the variation in the O₂/N₂ ratio in air. It is represented by the following formula.

According to this definition, the O₂/fuel ratio for stoichiometric conditions remains constant at 3.794 (based upon the natural gas, C_{1.02943} H_{3.9925} that was supplied to Argonne). However, if the traditional equivalence ratio (Φ) were to be used, the air/fuel ratio for stoichiometric conditions would change from 16.3922 (standard air) to 18.072 (2% NEA) owing to the amount of O₂ depletion in the intake air. The O₂ flow rate was obtained by multiplying the O₂ mass fraction in the charge with the measured air flow rate. A correction factor of 0.9975 was used to compensate for the change in NEA density with respect to standard air for the 2% NEA condition.

C.6.2.1 Engine-Out Emissions

NEA is the air containing N₂ in excess of 79.05% (by volume). N₂ enrichment was attained by controlling the O₂ flow rate as shown in Figure C2. Previous research showed that with NEA, NO_x reduction is proportional to engine load—NO_x reduction was greater for higher engine loads [19]. This result occurs primarily because of the prevalent higher flame temperatures for higher engine loads. Hence, the present work was limited to evaluating the engine performance and behavior at the full load of 12 bar (BMEP). In addition, acceptable engine operation was

limited to below 3% NEA for near stoichiometric operation. In this study, only the 2% NEA condition is discussed. The engine operating regime vis-à-vis the equivalence ratio, Ψ , was varied from $\psi = 1.0$ to the lean misfire limit. The lean misfire limit was defined as the limit when the COV_{IMEP} exceeded 5%. This result is discussed at length in the following sections.

Figure C12 shows NO_x as a function of ψ at MBT ignition timing for standard air and 2% NEA. Results for both conventional SI as well as LI are shown to depict the benefits and limitations of the respective systems. LI indeed offered the benefit of leaner operation and hence the lower NO_x emissions compared to SI. For standard air, NO_x emissions increased steadily going from $\psi: 1.0$ to 0.81 and changed course when the charge was made leaner. However, NO_x emissions peaked at $\psi: 0.9$ with 2% NEA for both SI and LI. Both of these peak conditions for NO_x production occur at similar fueling rates. This phenomenon can be explained by considering the fact that the NEA case becomes “richer” (i.e., with a higher equivalence ratio, ψ) for a given fueling rate. For $\psi: 0.81$, the drop in NO_x emissions was 13 g/kW-hr for SI and 19 g/kW-hr for LI. The trends are fairly similar in both the SI and LI cases. LI, however, extended ψ from 0.65 to 0.62 with standard air and from 0.72 to 0.68 with 2% NEA.

When 2% NEA is supplied with a similar fueling rate as used for stoichiometric standard air, ψ becomes fuel rich and loses power, BTE, and NO_x emissions owing to insufficient O_2 available to complete combustion of the fuel. This treatment reduces the bulk gas temperatures and therefore decreases NO_x emissions. According to previous NO_x studies, NO_x emissions are strongly correlated as a function of combustion temperatures. Bulk gas temperature is an *exponential component* in the NO_x formation mechanism. Even a slight reduction in bulk gas temperature significantly alters NO_x formation. Another factor that affects NO_x formation is the O_2 content in a given mixture. Because nitrogen enrichment effectively depletes the net O_2 concentration, NO_x formation is significantly reduced. With nitrogen enrichment, the lean limits decrease considerably because of excessive and unacceptable misfires, as shown in Figure C12.

Attempts were made to maintain a constant BMEP while varying Ψ and nitrogen enrichment. This was accomplished by varying the fuel flow and air flow proportionately to attain a specific Ψ for 12 bar BMEP. When 2% NEA was supplied to the engine for a given operating condition, the combustion reaction rates were decreased and delayed in the engine cycle. This step led to loss in power and BTE. In order to attain MBT for a given operating condition, the heat release peak or 50% MFB has to occur close to TDC. Therefore, the ignition timing was judiciously advanced, as shown in Figure C13, to compensate for the delayed combustion phasing. SI and LI curves followed very similar trends. With NEA, ignition timing had to be advanced by 3° at $\Psi: 1.0$ and close to 10° at $\Psi: 0.7$.

Figure C12. Specific NO_x as a Function of ψ .

Figure C13. Ignition Timing as a Function of ψ .

Figure C14 shows BTE as a function of ψ for both standard air and 2% NEA using SI and LI. It could be used effectively to compare the effect of NEA on BTE for both ignition systems. BTE is defined as the ratio of the brake power produced by the engine to the fuel energy feed rate based on the lower heating values of the fuel (natural gas). The power required for compressing intake air from ambient to engine intake pressures (103–250 kPa) was not accounted for in the BTE calculations and is beyond the scope of this study.

Figure C14. BTE as a Function of ψ .

It was assumed that a turbocharger could accommodate these conditions. It would be fairly reasonable to expect BTE corrections amounting to as high as 10% based on ASM installations on other engine platforms. It is therefore acknowledged that the actual BTE numbers would be lower from a practical standpoint. The pressure losses associated with using an ASM are shown in Figure C15. The pressure drop across the ASM varied from 5.5 to 7 kPa for passing standard air between ψ : 0.65–1.0 (with the O_2 valve closed; see Figure C11) and from 7 to 9 kPa while passing 2% NEA between ψ : 0.65–1.0 (with the O_2 valve opened appropriately). It must also be acknowledged that higher nitrogen enrichment would result in higher pumping losses.

Although Figure C14 shows that for a given ψ , say 0.81, BTE for 2% NEA is higher than for standard air, after accounting for parasitic losses (i.e., a relative pressure drop of 2.5 kPa; see Figure C15), the trend lines would shift lower than the standard air conditions.

Figure C15. ASM Pressure Drop as a Function of ψ .

As previously mentioned, nitrogen enrichment beyond the stoichiometric condition resulted in excessive power and a BTE penalty because of the unavailability of O_2 for complete combustion of the fuel. This result is reflected very clearly in total UHCs, CO, and CO_2 emissions in Figures C16, C17, and C18, respectively. CO emissions increased beyond the analyzers' measurement range for $\psi > 1$, which could be higher than shown (60 g/kW-hr) because of the incomplete oxidation of CO to CO_2 . UHC (Figure C16) increased slightly between ψ : 0.8–1.0 with 2% NEA for both SI and LI. However, UHC increased significantly as the mixture approached lean limits. The trends were similar for both ignition systems, with LI extending the lean limit further to 0.62 (air) and 0.68 (2% NEA), respectively. This behavior also explains the drop in BTE at lean conditions for both ignition systems. BTE with LI was lower than SI, as shown in Figure C14. It could be surmised that in the case of LI, the ignition kernel is forming at a non-optimal location. Earlier LI studies at Argonne showed improvement in combustion and therefore better BTE. However, in the scope of the present study, there is a clear benefit associated with LI in terms of extension of the lean limit. CO emissions (Figure C17) also increased slightly with leaner mixtures, accounting for unburned fuel in the exhaust and lower BTE.

Figure C16. Specific UHC as a Function of ψ .

Figure C17. Specific CO as a Function of ψ .

It was observed (see Figure C18) that CO₂ emissions were reduced significantly with use of NEA as compared to standard air; leaner operation is more attractive given current concerns about climate change. CO₂ emissions reduced from 12% at stoichiometric conditions to less than 7% under the lean burn condition.

Figure C18. Exhaust CO₂ as a Function of ψ .

Figure C19 shows the amount of O₂ available in the exhaust as a function of ψ . This chart explains the need for an O₂-based equivalence ratio, ψ , compared to the standard definition. It indicates that regardless of change in engine control variables such as ignition timing, percentage of NEA, etc., for a given fuel-to-O₂ ratio, there can only be a proportionate amount of excess O₂ in the exhaust. Therefore, all data points for both standard air and 2% NEA follow a very consistent trend and confirm this approach.

Figure C20 is a chart showing trade-offs between brake-specific fuel consumption (BSFC) versus NO_x emissions for different ψ and comparing the effect of a combination of NEA and LI with its SI counterpart. Clearly, NEA reduces NO_x for all ψ . However, BSFC increases considerably with richer than stoichiometric conditions, as expected. Leaner mixtures, for example, ψ : 0.65, decreases BSFC and NO_x simultaneously for both SI and LI. In addition, the LI system lowered NO_x emissions from a peak of 44 g/kW-hr to 5 g/kW-hr (an 89% drop) for similar BSFC levels (205 g/kW-hr). This benefit was significant considering that SI could only lower NO_x from 39.5 g/kW-hr to 12 g/kW-hr (a 70% decrease). Therefore, we deem it necessary to optimize LI to realize these benefits. LI coupled with ASM technology holds significant promise once developed for production engines.

Figure C19. Exhaust O₂ as a Function of ψ .

Figure C20. BSFC versus Specific NO_x at Different ψ .

C.6.2.2 Combustion Characteristics

High-speed, in-cylinder pressure data were acquired to analyze the combustion process for ASM-supplied NEA with SI and LI. Cylinder pressure was averaged over 100 consecutive engine cycles for this purpose. A “Rev-R” commercial combustion analysis program was used to calculate the parameters such as ignition delay, combustion duration (5%–50% MFB), peak cylinder pressure, and COV_{IMEP} .

Figure C21 shows the ignition delay, represented in crank angle degrees, as a function of ψ . Ignition delay is defined as the time between the start of ignition (IT) and the start of combustion. The start of combustion was chosen to be 5% MFB, or mass fraction burn, which is defined as the instantaneous burned mass normalized by the total mass of charge in the cylinder. As shown in the figure, ignition delay increases from 14° to as high as 30° as ψ approaches the lean limit. Natural gas inherently has a long ignition delay as compared to other fuels. As a result of NEA slowing the chemical reaction rates, observed ignition delays were prolonged even further with 2% NEA as compared to standard air.

Figure C21. Ignition Delay as a Function of ψ .

Combustion duration, the time between 5% and 50% MFB, provides insight into the nature of heat release rates for a given fuel/ O_2 mixture. Figure C22 shows combustion duration as a function of ψ . As expected, the combustion duration increases exponentially with leaner mixtures. Leaner mixtures result in slower burn or heat release rates for extended periods of time. The lower burning rates are attributed to the slower flame development and propagation

speeds caused by NEA. The lower heat release rates and longer combustion duration reduce peak temperatures and hence NO_x emissions.

Figure C22. Combustion Duration as a Function of ψ .

Figure C23 shows trends for peak cylinder pressures at different ψ . Both extreme conditions result in pressure drops because of misfires at the lean end and incomplete combustion beyond stoichiometric condition. COV_{IMEP} , a parameter used in the industry to measure engine stability, was maintained below the accepted value of 5% as shown in Figure C24. However, even though LI extends the lean limit to 0.62, COV_{IMEP} just begins to increase relative to other conditions.

Figures C25 and C26 are very similar in that both display the variation in BMEP and IMEP from a constant value. However, BMEP was calculated based on actual brake torque measurement, whereas IMEP was calculated from in-cylinder pressure measurement. The trends in both figures match well, confirming the analysis discussed above. A significant drop in power was observed when ψ exceeded 1.0. It is highly unlikely that engines will be able to operate at this condition for any period of time. Toward the lean end, it was observed that occasional misfires have to be checked by either shifting to a slightly richer or advancing ignition timing even further.

Figure C23. Peak Cylinder Pressure as a Function of ψ .

Figure C24. COV_{IMEP} as a Function of ψ .

Figure C25. Variation in Load, BMEP, as a Function of ψ .

Figure C26. Variation in Load, IMEP, as a Function of ψ .

C.7 RECOMMENDATIONS FOR FUTURE WORK

The development of this technology was primarily limited to a single cylinder research engine platform. Although attempts were made to apply this technology on a Cummins multi-cylinder natural gas engine, lack of hardware availability coupled with fuel-air premixing precluded engine experiments. The membrane technology is most effective when operated under pressure gradients. For example, in the Cummins engine, air and natural gas are premixed before entering the turbocharger. Because natural gas was part of the intake charge, the membrane could not be used downstream of the turbocharger, which would result in a dangerous mix of fuel and oxygen-rich air. If future advanced stationary power engines use port injection of fuel, this technology can be applied seamlessly. This technology could also be used for in-cylinder charge stratification to achieve more efficient management of energy transfer.

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D APPENDIX D: OPPORTUNITY FUELS/GAS BLENDING SYSTEM

D.1 INTRODUCTION

Ever-increasing global energy demands, shrinking conventional resources, and political atmosphere have been driving fuel prices higher and into more unstable. This scenario, along with environmental regulations and concerns, has driven renewed interest in alternative sources of energy. Apart from the solar and wind energy, the waste- and biomass-derived gases, short carbon-cycle fuels such as gasified coal, and by-product gases from manufacturing processes are all potential alternatives. However, as recent findings of natural gas resources have eased the situation for the time being, the increased demands is likely to increase natural gas prices worldwide. A U.S. Energy Information Administration report predicts prices for natural gas will increase by an average of about 2.4% per year, up to \$7.83 per million Btu (2011 dollars) in 2040.

Various opportunity fuels (Op-fuels)—digester gases and syngases—offer the potential to displace up to 20% of the United States' natural gas use. However, this source remains untapped as many of these gases have nonstandard consistency and further have very low energy content ($< 350 \text{ Btu/ft}^3$).

The disposal of ever-growing amounts of waste from industries and communities, small as well as large, is of major concern on a global basis. Untreated waste contributes to land, water, and air pollution. Many of the agricultural and community waste treatment facilities simply flare-up the gases generated. Opportunity-fuels and energy derived from various waste streams address these challenges in a sustainable manner. Thus, opportunity fuel development is of utmost interest to industries, government, and local municipalities.

These alternative gaseous fuels are derived from a variety of feedstocks such as biomass, waste products, and coal. Different feedstocks introduce variations in fuel composition, properties, and performance, the effects of which have not been fully investigated. Opportunity fuels comprise those generated via anaerobic digestion (such as biogas, digester gas, landfill gas, etc.), and those resulting from pyrolysis of biomass (such as syngas, wood gas etc.). Gases resulting from anaerobic digestion of biomass have methane (CH_4) and carbon dioxide (CO_2) as primary constituents, whereas those resulting from pyrolysis have Hydrogen (H_2) and Carbon Monoxide (CO) as primary constituents. In both types of gases, nitrogen gas (N_2), ethane (C_2H_6), and oxygen (O_2) are present in minor quantities.

Argonne National Laboratory's (Argonne's) Distributed Energy Research Center (DERC) is engaged in conducting research on reciprocating engine and micro-turbine platforms and has endeavored in developing technologies to improve efficiency and reduce the emissions and maintenance requirements of systems that use gaseous fuels. Working with fuels obtained directly from the original sources is certainly an option; however, coordinating with remote locations and dealing with the logistics of collection, compression, and transportation of opportunity fuels from the source are usually difficult. Argonne's approach is to blend the

individual component gases in representative proportions to simulate the targeted opportunity fuel to develop end-user technologies.

An advanced gas blending system (GBS) was designed and constructed that allows simulating the various opportunity gaseous fuels and their compositional variations by blending individual gases to the required concentrations. Apart from opportunity fuels, this system also allows evaluation of the expected variances in natural gas consistency on engine and micro-turbine platforms.

D.2 DESIGN CRITERION

D.2.1 Composition of Gaseous Opportunity Fuels

Gaseous opportunity fuels comprise those generated via anaerobic digestion (such as biogas, digester gas, landfill gas, etc.) and those resulting from pyrolysis of biomass (such as syngas, wood gas, etc.). Gases resulting from anaerobic digestion of biomass have CH₄ and CO₂ as primary constituents, whereas those resulting from pyrolysis have H₂ and CO as primary constituents. In both gases, N₂, C₂H₆, and O₂ are present in minor quantities. Table D1 shows typical compositions of opportunity fuels considered for the design of Op-fuels system at DERC.

Table D1. Typical Composition of Opportunity Fuels Considered for the Design of Op-Fuels System.

Fuel	Contents of (%):					
	N ₂	O ₂	CO	CO ₂	H ₂	CH ₄
Natural Gas	0	0	0	0	0	100
Syngas	0	0	50	0	50	0
Wood Gas	50	6	27	4.5	14	3
Bio Gas (1)	0	0	0	50	0	50
Bio Gas (2)	0	0	0	25	0	75

D.2.2 Gas Storage and Flow Requirements

The two test platforms to be used with the blended gas supply are DERC's single-cylinder test engine (33 kW, 1800 rpm, full load, 35% efficiency) and the Capstone C65 micro-turbine (full load of 65 kW, 30% efficiency). On the basis of typical compositions of opportunity fuels given in Table D1, the amount of individual gases required to ensure a blended fuel supply for at least 16 hours of testing is provided in Table D2. The sizing of tanks and trailers was based on the C65 micro-turbine's requirement. Natural gas and propane (C₃H₈) were also included in the system so that tests can be performed using these as standalone fuels. Table D3 provides the approximate capacity needed for storage tanks and trailers in the Op-fuel system.

Table D2. Approximate Gas Quantities and Flow Rates at STP (20°C at 1 atm) Needed for 16 Hours of Uninterrupted Fuel Supply Based on Compositions in Table D1.

Component Gas	For Single-Cylinder (5,431 MJ needed)			For the C65 (12,480 MJ needed)			Desired Range of Flow Rates (SCFH) ^a	
	kmol	kg	SCF ^a	kmol	kg	SCF	Lower	Upper
N ₂	19.6	549.6	16,664	45.1	1,262.9	38,293	50	4,000
O ₂	0.2	7.5	200	0.5	17.3	460	–	–
CO	10.6	296.8	8,999	24.4	682.0	20,678	25	2,000
CO ₂	7.5	331.9	6,404	17.3	762.7	14,716	20	1,500
H ₂	10.4	20.8	8,820	23.9	47.7	20,267	25	2,000
CH ₄	7.5	120.7	6,404	17.3	277.3	14,716	20	1,500
C ₃ H ₈	2.7	117.0	2,258	6.1	269.0	5,190	5	600
C ₂ H ₆	0.9	27.0	765	2.1	62.2	1,759	0.5	175

^a SCF = square cubic feet; SCFH = square cubic feet per hour.

Table D3. Storage Tank and Trailer Capacities.

Gas	Storage Phase	Storage Type	Approximate Tank/Trailer Capacity			
			Gallons	Kg	Lb.	SCF
N ₂	Liquid	Tank	1,490	4,552	10,035	128,486
CO ₂	Liquid	Tank	1,867	5,443	12,000	97,245
CO	Gas (Comp.) ^a	Trailer	–	1,592	3,510	50,000
H ₂	Gas (Comp.)	Trailer	–	114	252	45,000
C ₃ H ₈	Liquid	Mini tank	500	1,100	2,425	20,638
C ₂ H ₆	Gas (Comp.)	Cyl. Bank (8×300)	–	86	189	2,400

^a Comp. = Compressed

D.3 OPPORTUNITY FUELS SYSTEM OVERVIEW

The Op-fuel system blends individual gases to the desired composition and supplies the gas blend to the DERC engine/micro-turbine test cells at the required pressure and flow rate. Figure D1 shows an overview of the Op-fuel system. It has two main components:

(1) Gas Storage and Delivery System (GSDS)

(2) Gas Blending System (GBS)

The GSDS constitutes the storage tanks and tube-trailers that store individual gases, supply lines, pressure regulators, valves, and safety systems. GSDS collectively feeds individual (component) gases to the GBS.

The GBS consists of various electromechanical elements—flow controllers, valves, pressure regulators, etc.—that collectively provide a gas blend with a composition that matches one specified by the user via computer. Furthermore, the flow rate and supply pressure of the gas blend was designed to meet the requirements of a 33-kW, single-cylinder research engine and a 65-kW micro-turbine. The following sections detail various aspects of the system.

Figure D1. Overview of the DERC Op-fuel System.

D.3.1 Gas Storage and Delivery System (GSDS)

D.3.1.1 Gas Storage Farm

Prior to designing the storage farm and delivery system, Argonne's Facilities Maintenance Service and consulting firms HDR and KJWW performed a detailed review of codes and standards to determine the codes' requirements as they relate to the piping systems; heating, ventilation, and air conditioning (HVAC) requirements; and safety. The following codes and standards were reviewed:

- 2009 International Mechanical Code
- 2009 International Fire Code
- National Fire Protection Agency (NFPA) 30 – Flammable and Combustible Liquids Code

- NFPA 31 – Installation of Oil-Burning Equipment
- NFPA 37 – Stationary Combustion Engines and Gas Turbines
- NFPA 54 – National Fuel Gas Code
- NFPA 55 – Compressed Gases and Cryogenic Fluids Code
- 2011 National Electric Code

The gas storage farm shown in Figure D2 has four bays partitioned by 12-foot-high and 12-inch-thick concrete walls. The flammable gases are stored in separate bays, whereas the carbon dioxide and nitrogen share one of the middle bays. Figure D3 shows an aerial view of the storage farm's location with respect to surrounding structures. Following are brief descriptions of the gas storage equipment/vessels.

Figure D2. Photograph of the Gas Storage Farm.

Figure D3. Aerial View of Gas Storage Area (Source: Google Maps. Imagery ©2014 DigitalGlobe, U.S. Geological Survey; Map data ©2014 Google).

D.3.1.2 Carbon Monoxide and Hydrogen

Carbon monoxide and hydrogen are stored as compressed gas in a 50,000-SCF and 45,000-SCF capacity tube trailers in the first and second bays, respectively, of the storage farm. The fill pressures of the trailers are in the range of ~2,200–2,400 psig. Using a flexible hose, the outputs from the trailers are hooked up to unloading stanchions and connected to the underground stainless steel (SS) delivery tubing via pressure-reducing manifolds, purge ports, and solenoid valves (see Figure D1). The pressures are reduced to operating pressure of GBS (~150 psi). The process flow and pressure reduction manifold diagrams for the CO and H₂ are shown in Figure D4. After passing through the solenoid valves, the gases proceed to the 1-inch SS underground tubing, which has manual valves at both of the ends. The manual valves at stub-up in the gas storage farm are normally left open. The operators can start and stop the flow of gases by closing and opening the solenoid valves and the manual valve at the stub-up behind the gas blending main skid. There are additional valves (manual as well as pneumatic) in the GBS before the flow meters and mixing cylinder that provide additional control points.

D.3.1.3 Carbon Dioxide and Nitrogen

Carbon dioxide (CO₂) is stored in the third bay (co-located with the N₂ tank) as a refrigerated gas/liquid in a 6-ton-capacity horizontal tank. The CO₂ condenser/refrigeration unit maintains the tank pressure and temperature at ~300 psig and 0°F, respectively. As shown in Figure D5, the gaseous CO₂ travels through the main valve of the tank, the pressure reducing manifold, and the solenoid valve to the underground SS tubing.

The condenser/refrigeration unit for CO₂ is a semi-hermetic, air-cooled system that is powered by a 480-VAC/3-phase/100-A power line. The CO₂/N₂ bay is separated by 12-foot-high, 12-inch-thick concrete walls on both side from the flammable gas storage bays and meets the fire safety standards for electrical code. Figure D6 shows the CO₂ tank and related components.

Figure D4. Process Flow and Pressure Reduction Manifold for CO and H₂.
(MV: Manual Valve, PI: Pressure Indicator).

Nitrogen (N₂) is stored as cryogenic liquid in a 1,500-gallon horizontal tank. The liquid N₂ from the tank travels first to an ambient vaporizer (Figure D7) and then to a pressure-reducing manifold, as shown in Figure D5. The maximum working pressure of the nitrogen tank is 250 psi at 100°F.

D.3.1.4 Propane (C₃H₈)

Propane is stored in a 500-gallon commercial tank in the southernmost bay of the storage tank (Figure D8). The allowable working pressure of the propane tank is 250 psi. Propane is delivered as liquid to the propane mixing skid in TC #1 of the 362 Hi-bay. Compressed nitrogen at ~150 psi is introduced at the top of the propane tank, which pushes the liquid propane out to the underground piping delivering the propane to the propane mixing box. The propane mixing box has a propane vaporizer to convert it into a gaseous state before mixing with the other gases occurs. Figure D9 shows the propane process flow diagram (PFD) at the storage farm.

Figure D5. Process Flow and Pressure Reduction Manifold for CO₂ and N₂.
(MV: Manual Valve, PI: Pressure Indicator).

D.3.1.5 Ethane

Ethane (C₂H₆) is stored in standard 300-SCF cylinders within a bank of eight cylinders (shown in Figure D10). The ethane cylinders are hooked up to a manifold that has a two stage pressure regulator and solenoid valve.

D.3.1.6 Natural Gas

The onsite pipeline is the source of the methane and natural gas, which is compressed to ~160 psi using the NG compressor located in TC #1 and stored in a 20-gallon buffer tank rated to 200 psi. The compressed NG is piped to the GBS main skid where it can be mixed with other gas components as desired. Figure D1 shows the NG flow diagram schematically. Figure D11 shows the NG compressor and tank in TC #1.

Figure D6. Carbon Dioxide Tank and Pressure-Reducing Manifold.

Figure D7. Nitrogen Tank and Vaporizer.

Figure D8. Propane Tank and Compressed N₂.

Figure D9. Propane Process Flow
(MV: Manual Valve, PI: Pressure Indicator, R: Regulator, RV: Release valve).

Figure D10. Ethane Cylinder Bank.

Figure D11. Natural Gas Compressor and Tank.

D.3.2 Gas Blending System (GBS)

D.3.2.1 Overview of the System: Process Flow and Main Components

The gas blending system provides the capability of producing a multi-component homogenous gas blend. This blend can be delivered as fuel at varying flow rates to the stationary engine in TC #1 or the micro-turbine in TC #2. The system is capable of producing a mixture with varying compositions of hydrogen, carbon monoxide, carbon dioxide, nitrogen, methane (natural gas), ethane, and propane.

The system is composed of two separate assemblies, a Main Assembly (Figure D12) and a Propane Sub-Assembly (Figure D13). The Main Assembly is a skid-mounted package that includes the main supervisory control and data acquisition (SCADA) input/output (I/O) panel (Figure D14), gas feed lines, mass flow controllers/transmitters, pressure gauges, a mixer, and a Coriolis mass flow meter. This skid is mounted on an open chassis suitable for outdoor environments. A process and instrumentation diagram of the system is shown in Figure D15.

Figure D12. GBS Main Skid.

Figure D13. Propane Sub-Assembly.

Each gas feed line is connected from the gas storage tanks to the main skid through the manual ball valves. These manual valves must be open in order to supply the gases to the system. Pressure gauges after the ball valves indicate supply pressure. Following the pressure gauges there are pneumatically actuated and normally closed ball valves, which allow/disallow the gas supply to the rest of the gas feed lines. The SCADA system manipulates the pneumatic valves through the system's control program.

The gases then proceed through an inline filter to a pressure indicator/transmitter located after the inline filter before reaching the mass flow controllers (MFCs) or mass flow transmitters (MFTs) [except for propane and nitrogen]. The MFCs/MFTs measure and control the gases' flow rates.

The propane proceeds directly to a second pressure gauge, which indicates the propane line supply pressure being delivered to the propane sub-assembly. A second manual ball valve on the propane feed line allows the propane to flow from the main assembly to the propane sub-assembly.

Figure D14. SCADA I/O Panel.

Nitrogen supply for instrument control (pneumatic valve control) is tapped before the main nitrogen feed line's pneumatic ball valve and routed through a manual regulator, pressure indicator, and a manual valve (Figure D16) to the SCADA panel enclosure. The nitrogen in the main feed line proceeds to a pressure-reducing regulator and then to a second manual valve for isolation. After the second manual valve, a pressure indicator/transmitter provides the SCADA system with the inlet pressure level prior to feed into the MFC. The ethane feed line contains an MFT followed by a flow control valve (FCV). The propane line also has this setup, although the devices are found in the propane sub-assembly.

The carbon dioxide and methane feed lines contain two MFCs each for a greater degree of control; the rest of the gas lines have only one MFC/MFT. Because the Main Assembly is found outdoors, all of the MFCs/MFTs that are on the main assembly are mounted together and housed in an enclosure containing a Class 1/Division 2 space heater that maintains the interior temperature above 0°C. The minimum operating temperature of the MFCs/MFTs is 0°C. Therefore, the thermostat controlling the cabinet heater is set to turn on the heater at a temperature of 10°C.

Figure D15. Main Gas Blending Skid Process and Instrumentation Diagram.

Figure D16. Instrument and Nitrogen Feed Lines.

Following the MFCs/MFTs, another set of pressure indicators/transmitters provides feed pressures flowing into Mixer #1. The manual isolation ball valves and the spring-loaded check valves for every gas feed line upstream of Mixer #1 prevent the undesirable reverse flow of gases from the mixer. Each gas passes through its respective check valve and enters Mixer #1. The mixing vessel (Mixer #1) has a set of vanes that generate vortex to help ensure that a homogeneous mixture exits downstream.

The Blended Gases Line #1 (after Mixer #1) has a pressure indicator/transmitter, a Coriolis mass flow meter that provides the control system with blend mass flow and pressures. The Coriolis meter also provides internal temperature and volumetric flow at actual pressure. A pneumatic ball valve then allows or disallows the gas supply into the building and Propane Sub-Assembly through the Blended Gases Line #1.

The Propane Sub-Assembly is mounted inside a sealed enclosure inside of Test Cell #1 of the DERC. The propane feed line and the Blended Gases Line #1 from the Main Assembly provide the feed for the sub-assembly. Propane flows through an inline strainer followed by a propane vaporizer, which keeps all of the propane flowing through it in the gas phase. The propane gas then flows past a pressure indicator/transmitter before entering the MFT-FCV setup, which provides control and flow rates of propane stream. A manual isolation valve and a check valve before Mixer #2 prevent any reverse flow from Mixer #2.

The mixed gas (without propane) feed line from the Main Assembly also has a pneumatic ball valve, the pressure indicator/transmitter, a check valve providing the system with control, and the blend feed pressure into Mixer #2. Final blend from Mixer #2 is supplied to Test Cell #1 (the E-tech single-cylinder engine) and Test Cell #2 (C-65 Micro-turbine). In addition, output is

tapped after Mixer #2 that goes through a single-stage regulator and a flash back arrester to GC-2014 in Test Cell #2 for compositional analysis.

D.3.3 Mixing Tests Using Nitrogen and Carbon Dioxide

Mixing experiments were performed using bottled nitrogen and carbon dioxide to check the functionality and initial performance of the system. During initial tests, the inlet pressures were limited to < 50 psig because of the unavailability of an appropriate carbon dioxide cylinder regulator. Subsequently, a regulator rated to 150 psig was acquired and further tests were carried out. The composition of N₂-CO₂ was varied in GBS control program and was sampled using a gas chromatograph (GC). Table D4 contains the GC results.

Table D4. Blended Gas Composition Test Results Using Gas Chromatography.

Raw Concentration GC Analysis		Normalized Concentration (GC)		Set Points (% N ₂ -% CO ₂)	Comments
N ₂ Peak	CO ₂ Peak	% N ₂	% CO ₂		
113.67	28.89	79.74	20.26	80.00-20.00	(Standard calibration bottle)
68.64	7.11	90.62	9.38	80.00-20.00	Input pressures ~20 psi
43.65	2.56	94.46	5.54		
57.36	14.48	79.84	20.16		
60.66	12.39	83.04	16.96		
60.00	11.78	83.59	16.41	80.00-20.00	Input pressures ~30 psi
97.55	21.29	82.09	17.91		
77.14	19.44	79.87	20.13		
65.56	39.38	62.47	37.53	60.00-40.00	Input pressures ~30 psi
63.66	41.08	60.78	39.22		
76.09	49.95	60.37	39.63		
46.89	84.83	35.60	64.40	50.00-50.00	Input pressures ~30 psi (CO₂ becomes wild stream, unstable flow control)
47.97	81.82	36.96	63.04		Unstable (CO ₂ flow)
44.95	71.20	38.70	61.30		
56.23	56.84	49.73	50.27	50.01-49.99	Input pressures ~30 psi (N ₂ becomes wild stream)
50.67	68.73	42.44	57.56	49.99-50.01	N ₂ ~55 psi: CO ₂ ~50 psi
63.66	53.98	54.11	45.89	50.01-49.99	

Table D4. (cont.)

Raw Concentration GC Analysis		Normalized Concentration (GC)		Set Points (% N ₂ -% CO ₂)	Comments
N ₂ Peak	CO ₂ Peak	% N ₂	% CO ₂		
26.96	96.89	21.77	78.23	49.99-50.01	
58.80	53.26	52.47	47.53		
77.68	9.30	89.31	10.69	90.00-10.00	
92.50	19.98	82.24	17.76		
83.79	25.85	76.42	23.58	80.00-20.00	
77.08	20.58	78.93	21.07		
71.96	19.56	78.63	21.37		
68.38	30.79	68.95	31.05	70.00-30.00	
68.76	33.77	67.06	32.94		
65.42	33.83	65.91	34.09	60.00-40.00	
58.81	42.74	57.91	42.09		
66.99	39.36	62.99	37.01		
64.64	47.51	57.64	42.36	50.01-49.99	
63.68	50.99	55.53	44.47		
51.42	46.66	52.43	47.57		Input pressures ~ 100 psi
48.41	44.49	52.11	47.89		
44.71	45.95	49.32	50.68		
47.07	46.71	50.19	49.81		
45.99	46.30	49.83	50.17		
30.52	63.30	32.53	67.47	49.00-51.00	
26.54	66.51	28.52	71.48	30.00-70.00	
28.75	65.88	30.38	69.62		
24.75	67.38	26.86	73.14		Input pressure ~140 psi
26.23	62.82	29.46	70.54		
25.46	66.10	27.81	72.19		
28.18	64.93	30.27	69.73	35.00-65.00	
16.35	77.75	17.38	82.62	40.00-60.00	
35.47	56.20	38.69	61.31		

Table D4. (cont.)

Raw Concentration GC Analysis		Normalized Concentration (GC)		Set Points (% N ₂ -% CO ₂)	Comments
N ₂ Peak	CO ₂ Peak	% N ₂	% CO ₂		
38.79	56.34	40.78	59.22		
22.29	71.57	23.75	76.25	10.00-90.00	
4.20	90.86	4.42	95.58		
21.65	69.74	23.69	76.31	25.00-75.00	

These factors affect the mixing tests:

- When bottled CO₂ is used, the large pressure drop from bottle to regulator output results in a cooling effect at high flow rates, forming dry ice that results in erratic flow. For pressures < 100 psi, CO₂ flow was erratic. This was not the case when CO₂ from a large tank was used.
- The distance between the GBS main skid and GC located in TC #2 adds to delayed blended gas sampling.
- The “master”/wild stream pressure must be lower than that of the “slave” components, otherwise it results in hindered flow from the slave components.
- The percentage of the wild stream component is always the highest-percentage component.

Figure D17 shows the percentage set point and measured percent (based on volume flow rate) derived from GBS raw data. It shows very good flow control of the two components. Figures D18 and 19 show mixing response of MFT/FCV combination when CO₂ was fed through propane and ethane lines, respectively.

D.4 SINGLE-CYLINDER ENGINE OPERATION THROUGH GBS

The single-cylinder engine was operated using natural gas as the main fuel along with nitrogen and carbon dioxide as diluent. The purpose of this test was to make sure that the GBS meets the specified flow control and total flow requirement for engine operation. Figure D20 summarizes the results of the test.

GBS was operated in auto mode, that is, the flow rate was controlled by engine demand. The engine was brought gradually to a full load of ~44 hp by supplying natural gas only. Full load operation was achieved with NG flow rates at 6.3 kgph/5.9 kgph as provided, respectively, by the Coriolis flow meter/NG thermal mass flow meter. Once full load operation was achieved, the GBS control was set to manual and the NG flow was set at 6.5 kgph. Subsequently, nitrogen and

Figure D17. Mixing Test Results of GBS: Percentage Set Point and Measured Percentage (Based on Volume Flow Rate) Derived from GBS Raw Data.

Figure D18. Mixing Response of MFT/FCV Combination in a Propane Line When CO₂ Was Fed through the Propane Line.

Figure D19. Mixing Response of MFT/FCV Combination on the Ethane Line When CO₂ Was Fed through the Ethane Line.

Figure D20. Single-Cylinder Engine Operation Using Natural Gas, Nitrogen, and Carbon Dioxide Blends and 100% Natural Gas through the GBS System.

carbon dioxide were introduced at incremental flow rates of 1.0–2.0 kgph for both gases. As inert gas was added, the NG flow rate and engine power both dropped. The engine fuel injector was adjusted to increase the total flow rate and bring the power level to full load.

The tests have generated the following observations:

- There is a discrepancy between the Coriolis's flow meter values and the sum of the thermal mass flow meter values.
- The error appears to be systematically at ~6.0% of the total flow rate.
- Total flow is controlled by engine throttle and meets the flow rate requirement of the single-cylinder research engine.

D.5 SUMMARY

The gas blending system at DERC has been completed and tested to meet the specifications. Further tests with NG, N₂, and CO₂ are planned to calibrate and validate the performance of the system with an external Coriolis flow meter. Plans for the next set of experiments include performing NG compositional variations and determining its knock properties on a single-cylinder engine.

E APPENDIX E: IN-CYLINDER OPTICAL DIAGNOSTICS DEVELOPMENT

E.1 INTRODUCTION

The laser ignition system described earlier in this report provides a unique opportunity to study in-cylinder combustion and use optical diagnostic techniques that it is conventionally not possible to employ in real engines because of optically inaccessible system structures. Most of the research in the field of combustion using optically accessible engines is limited to low loads and speeds owing to the very nature of optical engines. Optically accessible engines are typically modified to accommodate large quartz windows/mirrors and or a piston/ring assembly. Further, these engines cannot use lubricants; as a result, they can only be operated for very short intervals. Typically, there is not enough time for engines to warm up properly and to be run in a stable mode before data are collected. Thus, the information obtained does not represent normal engine operation. The sapphire lens/window used in the laser ignition setup enabled the collection of an optical signal that originated inside of the cylinder while operating the engine at full speeds and loads; it also enabled devising the diagnostic methods described in this appendix.

In reciprocating internal combustion (IC) engines, the global heat release rates (GHRRs), combustion temperatures, and equivalence ratios (EQRs) are important metrics as they provide valuable insights into the efficacy of various combustion strategies and their influence on the overall engine efficiency. Two types of spectral signals (chemiluminescence and optical emissions attributable to laser-induced breakdown) were investigated [1–5].

E.2 CHEMILUMINESCENCE: HEAT RELEASE RATE AND COMBUSTION TEMPERATURE

In turbulent premixed flames, numerous studies [6–11] have correlated local heat release rate (LHRR) and GHRR with local and global flame luminosities, respectively. The widely used practice to derive HRR and temperature in IC engines is based on the simple thermodynamic treatment of cylinder pressure as measured by using a piezoelectric pressure transducer placed flush with the combustion chamber walls. However, the most significant part of combustion occurs away from the cylinder walls. Optical and spectral methods present a potential opportunity to obtain the information more pertinent to combustion volume and the time frame corresponding to active reactions. The recent advances in fiber optics make it possible to access the combustion chamber in IC engines optically, and the use of flame chemiluminescence as a diagnostic tool is easy to implement and thus highly desirable.

As natural gas is clean burning, the radiant emission is predominantly attributable to chemiluminescence. The early reviews by Gaydon [12, 13] associate chemiluminescence in the visible and near ultraviolet (UV) to be from four main electronically excited species formed through chemical reactions: hydroxyl (OH^*) (306.4 nm); carbyne (CH^*) (431.5 nm); diatomic carbon (C_2^*) (516.5 nm) and carbon dioxide (CO_2^*) (where the broadband emission is 340 to

more than 650 nm). These species are believed to exist in high concentrations in the immediate vicinity of the flame front. Figure E1 shows a typical combustion spectrum obtained from a natural gas reciprocating engine. As is evident, the emissions contribution from C_2^* is insignificant. The emissions from the CO_2^* species alone accounts for more than 90% of the signal integrated over the entire spectrum. Lee and Santavicca [8] conducted experimental studies on premixed turbulent flames to find that the global CO_2^* chemiluminescence intensity varies linearly with fuel flow rate (and hence with the global heat release rate), and the linearity coefficient itself was found to be an exponential function of the equivalence ratio. On further analysis, they allude to the fact that the CO_2^* emission is primarily governed by temperature rather than by equivalence ratio (EQR).

Figure E1. A Typical Luminescence Spectrum Obtained in a Natural Gas-Fired Engine.

Molecular spectra have often been used for temperature measurements, wherever direct methods are not feasible or are difficult, especially flame temperatures in the range 2,000–8,000°K [14]. OH^* spectra near a 310-nm wavelength form an excellent basis for estimating gas temperatures in IC engines and were previously used for hydrogen internal combustion engines (H_2 ICEs) [15]. However, hydrogen combustion is ideally placed in this regard as no interferences from other chemical species are present in the wavelength range of OH^* spectra near 310 nm. In the case of carbonaceous fuels, certain conditions and light emissions from carbon-based species interfere with the OH^* signal, making it difficult to obtain reasonable results. However, natural gas combustion spectrum obtained from an IC engine

(Figure E1) shows a distinct OH* peak, which can potentially be used to estimate gas temperature.

E.2.1 Experimental

E.2.1.1 Engine Setup

The four-stroke, spark-ignited, single-cylinder EngineTech (RSi130Q) natural gas research engine at the Distributed Energy Research Center (DERC) was used to conduct the diagnostics experiments. Details about the engine are provided in Appendix A of this report. Figure E2 shows the schematic arrangement of the engine setup. The engine was fueled with compressed natural gas at 160 psig, which was injected into the intake manifold using electronically controlled natural gas injectors (from CAP, Inc.). The engine was coupled to intake and exhaust surge tanks to dampen the flow pulsations and to help simulate turbocharged conditions.

Figure E2. Schematic of the Engine Setup
(Note: ECU: Engine Control Unit, FM: Flow Meter)

In-cylinder pressure was measured using a piezoelectric pressure transducer (Kistler 6013B) mounted on the cylinder head. The pressure signal was phased with respect to crank angle using an optical shaft encoder (Kistler 2614A) coupled to the engine crankshaft. The pressure transducer was connected to a high-speed data acquisition system (Hi-techniques Win600) that performed a one-dimensional, thermodynamic analysis to deduce bulk gas temperatures and heat release rates in addition to other engine combustion metrics.

E.2.1.2 Exhaust Gas Recirculation Setup

As the engine test cell was set up to simulate a turbocharged engine, the test conditions that were used necessitated intake pressures that were higher than the exhaust pressures. To overcome this pressure gradient while facilitating the needed levels of exhaust gas recirculation (EGR) (up to 29%), a system was designed utilizing a reciprocating compressor and a positioning valve. Care was taken to avoid water condensation through appropriate insulation and by using electric heaters. Carbon dioxide concentrations were measured in the intake plenum, exhaust plenum, and in the ambient air, and the EGR values were calculated according to the relation [2]:

$$\text{EGR\%} = 100 \times \frac{(\text{CO}_{2\text{exhaust}} - \text{CO}_{2\text{air}})}{(\text{CO}_{2\text{intake}} - \text{CO}_{2\text{air}})}, \quad (\text{Eqn. E1})$$

where the CO_2 concentrations used are on a wet basis.

E.2.1.3 Ignition and Spectral Collection Setup

The output from an Altronic CD-200 ignition system coupled to the engine encoder system was conditioned and used to trigger a frequency doubled Nd:YAG laser (the Big Sky Ultra CFR) that was capable of delivering 532-nm wavelength pulses with energy levels of up to 31 mJ/pulse. The high-power laser pulses were transmitted directly to a “laser plug” installed on the cylinder head. The laser plug carries a plano-convex sapphire lens in close proximity to the fire deck, which focuses the transmitted laser pulses to result in laser fluencies $\approx 10^{12} \text{ W/cm}^2$. This configuration leads to gas breakdown and subsequently to ignition. Figure E3 shows the schematic of the laser plug and light collection optics. The sapphire lens that was used to focus the laser pulses for igniting the charge was also used to collect the spectral signature from the ignition kernel as well as from the gas combustion.

The sapphire lens provided a field of view with a 50-degree cone angle that facilitates collection of a major portion of the flame luminescence. A broadband mirror with a central hole placed at 45° to the laser line path served the purpose of transmitting the laser pulses while deflecting the broadband emission from the combustion chamber onto a fiber optic cable. The distal end of the fiber was coupled to a 0.3-m spectrometer (Acton model 2300i) carrying an intensified charge-coupled device (ICCD) camera (Princeton Instruments IMAX with a 512×512 CCD array). The spectrometer used 150, 300, and 600 lines/mm gratings that enabled capturing a 263-, 127-, and 64-nm-wide spectra at spectral resolutions of 1.92, 0.94, and 0.53 nm, respectively.

Figure E3. Schematic of Laser Plug and Light Collection Optics:
 1: Mirror with Central Hole,
 2: Cylinder Head, 3: Laser Plug,
 4: F=13 Mm Sapphire Lens,
 5: F=50 Mm Quartz Lens, and
 6: Optical Fiber.

E.2.2 Co^*_2 Chemiluminescence: Heat Release Rates

E.2.2.1 Test Matrix

Tests were conducted by running the engine at a constant speed of 1,800 rpm. The equivalence ratio was varied between 0.6 and 1.0 by varying the fuel flow and boost pressure to maintain a constant brake mean effective pressure (BMEP) of 12 bar while the exhaust pressure was adjusted appropriately to simulate turbocharged conditions. The ignition timing was adjusted to achieve maximum brake torque (MBT) under all cases. To investigate the effect of charge dilution, exhaust gas recirculation up to 19% was carried out at a fixed equivalence ratio of 0.8. To improve the signal-to-noise ratios at lean equivalence ratios and high EGR levels, the signals had to be ensemble averaged over 100 combustion cycles.

E.2.2.2 Time Evolution of the Spectral Signal

The crank angle (CA)-resolved emission spectra for one engine operating condition, with an ignition timing of 22 CA degree (CAD) before top dead center (BTDC), are shown in Figure E4. The very first spectrum captures some of the atomic emission signal that lasts up to 8 μs following the ignition event. This signal is followed by a period of ignition delay, wherein no optical emission is observed. Subsequently, a broadband light emission primarily from electronically excited combustion species follows.

Figure E4. Typical Spectral Scans Obtained at 1 CAD Intervals.
Each Spectral Scan Was Averaged over 100 Shots at Each Crank Position [1, 2].

As widely accepted in the literature [8, 10], the chemiluminescent emission in the visible and near UV is attributed to three main species: OH^* with a peak at 306.4 nm, CH^* with a peak at 431.5 nm, and CO_2^* with a broadband emission over approximately 350–650 nm [16]. In all of the spectra that were collected, the emission from C_2^* (at 516.5 nm) was insignificant. The contribution from CO_2^* , however, remained dominant, accounting for more than 90% of the signal integrated over the entire spectrum.

The time evolution of flame luminosity (integrated over a narrow band near the peak of the CO_2^* luminescence) and interlaid with other engine combustion metrics is shown in Figure E5. For MBT timing, the peak of the flame luminosity was coincident with the measured peak cylinder pressure within ± 2 CAD. The calculated HRR precedes the flame luminosity, whereas the peak in the calculated bulk gas temperature peaks at a later time. This sequence was observed in all of the test cases, with the peaks in HRR occurring at 3.8–9.5 CAD before the peak optical intensities and the peak combustion temperatures occurring later at 5.8–15.6 CAD. Such an observation precludes CA-resolved correlations of HRR and bulk gas temperatures with optical emission intensities.

Figure E5. Flame Luminosity, Engine In-Cylinder Pressure, Heat Release, and Bulk Temperature as a Function of CAD. Ignition Timing = 22.73 CAD BTDC.

One plausible explanation for the temporal distribution of signals comes from the fact that the CO_2^* chemiluminescence can be attributed to a set of three elementary reactions [2]:

where M is the third body. Reaction 2 above predicts a pressure dependence and somewhat explains the coincidence of the peak flame luminosity with that of cylinder pressure.

In addition, with appropriate assumptions, the above reactions can be reduced to a single step reaction:

whose rate constant has been given by Baulch et al. [17] as:

$$K_1 = 2.5 \times 10^6 \exp[-1600/T(\text{K})] \text{ cm}^3/\text{mol/s}. \quad (\text{Eqn. E6})$$

As a result, the chemiluminescent intensity owing to CO_2^* can be expressed as:

$$I \propto \text{constant} \cdot e^{\left(\frac{-1600}{T(K)}\right)} \cdot [\text{CO}] \cdot [\text{O}]. \quad (\text{Eqn. E7})$$

With the value of activation temperature in the above expression being low relative to that of oxidation and pyrolysis reactions, Samaniego et al. [9] through kinetic simulations found an almost linear variation of luminosity with temperature. Lee and Santavicca [8] additionally acknowledge the temperature dependence through their experimental studies. Such a dependency, in the present case, results in a luminous intensity weighted toward the later parts of the combustion event: after the top dead center, increased in-cylinder charge temperature attributable to continued combustion is offset by the temperature decrease resulting from volume expansion, thereby resulting in a temperature peak that occurs toward the latter parts of the combustion cycle.

In a similar manner, Kim and co-workers [18] have argued that during the initial stages of the combustion cycle, CO is produced as the flame front progresses. As the combustion cycle progresses, the charge temperature increases, leading to increased levels of oxidation of CO by water (H_2O) and oxygen (O_2). This sequence leads to chemiluminescence from CO_2^* peaking at a later stage as compared to the HRR calculated from the pressure signal.

E.2.2.3 Spectral Shift and Intensity Variation of CO_2^* Chemiluminescence with EQR and EGR

Figure E6 shows the location of a broad peak as a function of EQR. The peak was observed to shift toward larger wavelengths for leaner combustion: the peak spectral signal shifted from 420 nm to 510 nm as the equivalence ratio was varied from 1.0 to 0.6. A similar shift was observed but was less pronounced with increased levels of exhaust gas recirculation. The exact reason for such a shift is not well documented in the literature. However, we speculate that it can be associated with the combustion temperature (i.e., lean conditions result in lower temperatures).

The CA-resolved peak spectral intensities for various equivalence ratios are shown in Figure E7. In addition, similar intensities for increasing values of EGR at a fixed equivalence ratio, $\phi = 0.8$, are shown in Figure E8. The trends evident in these two figures conform to the notion that low flame temperatures owing to lower equivalence ratios or increased levels of EGR lead to low levels of CO_2^* chemiluminescence.

Ranalli et al. [10] have observed higher levels of chemiluminescence from a lab-scale, premixed turbulent combustor upon dilution with CO_2 . For the present cases of EGR (see Figure E8), where the exhaust gases constituted up to $\sim 12\%$ CO_2 , such effects remain small as compared to the influence of decreased temperatures. Further, both with leaner equivalence ratios as well as increased EGR levels, the luminous intensity trends indicate larger ignition delays as well as decelerated combustion.

Figure E6. Peak Spectral Intensity Location for Various Equivalence Ratios.

E.2.2.4 Correlation of Spectral Intensities with Peak HRR and Peak Bulk Gas Temperatures

The temporal evolution of the spectral signal, as shown in Figure E4, makes it difficult to correlate with HRR and temperature on a CA-resolved basis. However, the strong dependence of the CO_2^* chemiluminescence intensity with EQR and EGR, as shown in Figures E7 and E8, suggest that at least on a global basis, it correlates with combustion temperatures and heat release rates. This dependence is manifested in Figures E9 and E10, where the temporal maxima of the peak spectral intensities show a monotonic variation with peak heat release rates and peak bulk gas temperatures calculated over the combustion cycle, with R^2 values of 0.96 and 0.92, respectively.

For practical uses, the CO_2^* chemiluminescence signal is likely to be collected with a photo detector used in conjunction with an optical filter. By using an optical window that spans over 400 and 550 nm, a range that can be easily accommodated with commercially available glass filters, the caveat due to spectral shift in the peak chemiluminescence signal can be minimized.

Although such correlations are very encouraging, caution needs to be maintained for the following reasons: (1) the species that are dominant in contributing to flame chemiluminescence— OH^* , CH^* , C_2^* , and CO_2^* —are believed to exist in close proximity to the combustion flame front, and the field of view has to be large enough to capture a major portion of flame luminescence; and (2) for premixed turbulent combustion, which is mostly the case for natural gas engines, high turbulence levels as well as flame strain rates [11] are reported to

Figure E7. Peak Spectral Intensity Variation with Equivalence Ratio.

Figure E8. Peak Spectral Intensity Variation with EGR.

Figure E9. Correlation of the Peak CO₂* Spectral Intensity Maxima with Peak Cycle HRR.

Figure E10. Correlation of the Peak CO₂* Spectral Intensity Maxima with Peak Cycle Gas Temperature.

influence the local chemiluminescence emissions. However, as evident in the present study, temperature effects instituted through EGR or the equivalence ratio remain highly dominant [2].

E.2.3 OH* Chemiluminescence: Combustion Temperature Estimates

Natural gas combustion from the single-cylinder engine shows the distinct peaks corresponding to OH* emission in the 306–310-nm range (see Figure E1). UV spectral bands of OH* emissions have been thoroughly measured and analyzed by Diecke and Crosswhite [19], and have been used as the reference spectrum to calculate gas temperature in plasma [14] and in flames [20]. There are four main band heads: R1, R2, Q1, and Q2 at 306.537 nm, 306.776 nm, 307.844 nm, and 308.986 nm, respectively, corresponding to the molecular transitions ($A^2\Sigma, v = 0 \rightarrow X^2\Pi, v' = 0$) in this wavelength region. The relative intensities of unresolved groups of lines in these bands can be utilized to extract the gas temperature [15, 20].

E.2.3.1 Simulation of Spectral Profiles

Following the references [1, 15, 19, 20], the intensity of a spectral line I_{nm} (a transition from the initial energy state “n” to energy state “m”) at temperature T with respect to the same transition (I_{nmref}) at a reference temperature T_{ref} can be represented as Dirac Impulses (i.e., lines with zero spectral widths), which is given by the following expression:

$$I_{nm} = I_{nmref} \frac{Z(T_{ref})}{Z(T)} \exp\left(-\frac{E_n(T_{ref}-T)}{T_{ref}T}\right) \quad (\text{Eqn. E8})$$

where $Z(T)$ represents particle partition function and E_n , the energy of the upper energy level of the transition. In order to generate synthetic spectrum, it was convoluted with “apparatus function” given by a normalized Gaussian profile, as follows:

$$G(\lambda) = \frac{2}{\Delta\sqrt{\pi}} \exp\left(-\frac{(\lambda - \lambda_0)^2}{(\Delta/2)^2}\right) \quad (\text{Eqn. E9})$$

where Δ represents the full width at 1/e of the maximum at the wavelength λ_0 of the spectral line broadened as a result of instrumental response. The apparatus function was obtained by measuring a sharp line at 632 nm from a He-Ne laser and fitting it with a Gaussian profile as a function of wavelength λ . The synthetic spectrum is finally obtained by first calculating the Dirac Impulse spectrum for the given temperature using Eqn. E8 and the convoluting with apparatus function. The final equation takes the form:

$$B(\lambda) = \int_0^\infty G(\lambda) \left(\sum_{i=1}^N I_i \delta(\lambda - \lambda_i) \right) d\lambda = \sum_{i=1}^N I_i G(\lambda_i) \quad (\text{Eqn. E10})$$

Here, it is assumed that the term $Z(T_{ref})/Z(T)$ in Eqn. E8 is unity. The reference spectrum at a temperature of 3,000°K is taken from [19]. To estimate the in-cylinder flame temperature, the spectral signal obtained from the engine is compared to the synthetic spectrum using a least square sum-error minimization routine with temperature as a variable parameter. Figure E11

shows an experimental and a synthetic spectrum ($T=3219$ K). The measured apparatus function of the setup used for this study was 0.53 nm.

Figure E11. Experimental and a Synthetic Spectrum ($T=3219$ K, apparatus function 0.53 nm).

E.2.3.2 Temperature Deduced From OH* Spectra

In order to minimize the effect of interference from the other species, only a narrow spectral region (304–310 nm) was used to estimate the in-cylinder flame temperature [1]. For an engine running at 1,800 rpm, 1° CA is roughly $92.56 \mu\text{s}$. The entire combustion process typically lasts for about 2.31 to 2.78 ms (~ 25 to 30 crank angles). However, in order to improve the signal-to-noise (S/N) ratio, a gatewidth of 200 μs was used.

Figure E12 shows OH* signal intensity as a function of the equivalence ratio. As observed by other experiments, the peak signal intensity increases exponentially with an increasing equivalence ratio [15]. However, for ϕ higher than 1.0, the emission intensity declines. For leaner operation, the S/N ratio decreases significantly, resulting in poor temperature estimates. In addition, plotted in Figure E12 are temperature values calculated from the cycle averaged in-cylinder pressure data (T_{pr}) and average temperature estimated from OH* spectra (T_{OH}). The average temperature from OH* spectra is the average of CA-resolved temperatures obtained from the cumulative OH* spectra over 100 cycles and which were distinctly above noise level. Therefore, it does not represent the time or spatially resolved flame temperatures. The main purpose of these measurements was to see whether T_{OH} thus obtained would show a trend. Figure E12 clearly shows that the T_{OH} trends as a function of ϕ are similar to that of T_{pr} .

However, T_{OH} values are much higher than the corresponding T_{pr} . This result is not surprising as T_{OH} ideally should represent the temperature in the reaction zone and in close proximity to very hot gases surrounding the flame, unlike T_{pr} , which is the global ensemble average temperature of the bulk gas based on an approximate calculation using the ideal gas law with inherent assumptions made for simplicity. The adiabatic temperature calculated for a stoichiometric mixture of methane (CH_4) and air for initial temperature of 300 K in a constant volume was 2,853 K.

Figure E12. Integrated Peak Intensity of OH* Spectra, T_{OH} , and T_{pr} as a Function of Equivalence Ratio without EGR.

Figure E13 shows the T_{oh} (crank angle resolved), T_{pr} , and HRR for $\phi = 0.88$ and 0% EGR for half load (6 bar BMEP). The range of temperatures during the extent of the combustion event was measured to be approximately between 800 K and 3,200 K. The large variations in the deduced temperatures are most likely the result of very low signal intensity resulting in poor S/N at both ends of the combustion event. The phasing of the peak T_{oh} and HRR occur simultaneously; however, T_{oh} does not follow the HRR curve.

Figure E13. Heat Release Rate, T_{oh} , and T_{pr} for Naturally-Aspirated Engine Operation.

Although conclusive remarks cannot be made with the available data, it is certainly possible to speculate. Chemical reactions, and hence the thermally excited OH^* , may continue emitting photons much beyond the peak HRR. HRR is a function of pressure and temperature, whereas OH^* spectral intensity is a function of pressure, temperature, ϕ , and field-of-view (FOV) [15]. The latter part the spectra show strong interference from the other species, OH^* peaks become featureless, and hence, the deduced temperatures may have a very large error. Further, for obtaining the OH^* spectra, the same lens that was used to focus the laser pulses for ignition was used to collect the light emitted in the combustion chamber. The short focal length of the lens and small aperture limit the captured and imaged volume at the face of optical fiber. This constraint implies that a portion of the combustion chamber did not contribute significantly to the observed signal. Because the combustion event is initiated at the focal-point of the laser spark plug, the initial part of the data is clearer and free from interference. Owing to the highly transient and turbulent nature of the flame front in the cylinder, the spectrum from consecutive cycles is likely to be very different. Further, the contributions from the other chemical species start interfering with the OH^* spectra during the later portion of the combustion cycle. It is very likely that the OH^* signal at the end of the combustion event is a local phenomenon that does not contribute significantly to the process. There may be other contributing factors to this discrepancy that need to be explored. However, during the initial part of combustion, the captured signals show somewhat structured OH peaks, and the S/N ratio is also reasonable.

Figure E14 shows specific NO_x emissions as a function of T_{OH} . The specific NO_x shows exponential dependence as a function of the T_{OH} with an excellent correlation ($R^2 \approx 98\%$) for $\phi > 0.8$. For the cases with $\phi < 0.8$, this dependence shows a different trend. It is well known that NO_x is a function of temperature, oxygen concentration, and equilibrium time [21]. EGR and ignition timing, two commonly applied techniques for NO_x abatement in IC engines, directly affect these variables. The literature also denotes that the peak NO_x yields occur at slightly leaner fuel-air mixtures (i.e., $\phi = 0.9$) where the O-atom (and OH^*) availability is the maximum for similar initial conditions. However, in this study, the engine's initial conditions (boost pressure, ignition timing, and fuel flow) were varied to attain constant load (12 bar BEMP) for different ϕ . The boost pressure and ignition timing were systematically increased/advanced for leaner conditions while readjusting fuel flow rates to obtain an appropriate ϕ . This treatment affects the initial temperature increase significantly until $\phi = 0.8$, after which the excess air within the charge increases the heat capacity and reduces the bulk gas temperature. However, at stoichiometric and fuel-rich conditions, NO_x yield drops dramatically because of the reduced availability of the O-atom, even though the flame temperatures are considerably higher. Therefore, NO_x peaked at $\phi = 0.8$ and decreased significantly from this point of inflection.

Figure E14. Specific NO_x as a Function of T_{OH} .

These trends bolster the methodology followed to estimate the combustion temperature using the OH-based technique. Finally, it could be inferred from this exercise that OH spectra and the temperature deduced from it could potentially be used for in-cylinder combustion diagnostics. This method can be improved by enhancing the S/N ratio and by finding ways to reduce and/or

account for the interference from other chemical species encountered during the combustion cycle in IC engines.

E.3 LASER-INDUCED BREAKDOWN SPECTRA: LOCAL EQUIVALENCE RATIO

Driven by the concurrent, and often conflicting, requirements to meet low NO_x emissions (< 0.1 g/bhp-hr), high specific power, and high fuel efficiency (> 50%), novel strategies are sought in natural gas-fueled stationary engines. So far, two strategies for effective operation have come to be in vogue within the gas engine industry: (1) lean-burn, turbocharged operation; and (2) stoichiometric operation with exhaust gas recirculation, turbocharging, and the use of a three-way catalyst (rich-burn). The performance under either strategy is limited by the ignitability of the combustion charge, either with increased levels of lean-operation or an increased fraction of EGR. In the open-chamber, spark-ignited engines, pressure, temperature, the level of turbulence, mean gas velocity, and primarily the equivalence ratio of the in-cylinder charge determine the ignitability of the in-cylinder charge. In addition, with an ability to monitor local equivalence ratios in real time, feedback strategies can be devised that enable stable combustion and help achieve even better performance. In this section, attempts toward developing a diagnostic based on laser-induced breakdown spectroscopy (LIBS) for use with lean combustion or exhaust gas recirculation that enables real-time monitoring of in-cylinder equivalence ratio are described [3, 4].

The use of LIBS for the measurement of elemental concentrations in solids, liquids, and gases has been well documented by the several review articles [22–25]. In LIBS applied to gaseous media, at the incidence of a very short high-power laser pulse, a plasma kernel having very high temperatures (10,000–25,000 K) is created. The molecules in the plasma are dissociated into constituent atoms, thereby creating a pool of radicals, ions, and atoms. The electrons in these atoms are elevated to higher energy levels and result in photonic emission as they relax back to ground states [26]. As a result, for time scales > 1 μs, the plasma reaches a quasi-thermodynamic equilibrium with surrounding gases, and the ensuing photo emission constitutes a broadband contribution overlaid with spectral lines characteristic of atomic transitions. While the atomic spectral line intensities and their time histories are dependent upon the laser power and the quenching environment, the ratio of intensities for specific elements are somewhat insensitive. Ferioli et al. [27] have evaluated the use of spectral features corresponding to C (711.3 nm), O (776.6 nm), N (746.3 and 743.8 nm), and cyano (CN) (broadband emissions of 707–734 nm) for equivalence ratio measurements in the exhaust of a gasoline engine. Phuoc and White [28] have advocated the use of a ratio of spectral lines corresponding to H_α (656.3 nm) and O triplet (near 777 nm) and performed equivalence ratio measurements on a methane-fueled lab-scale burner. Extending such a technique to in-cylinder measurements in a laser-ignited natural gas-fired engine, Joshi et al. [29] have demonstrated excellent correlation with equivalence ratios measured by using a UEGO sensor in the engine exhaust stream. The present investigation further extends such efforts for use with a natural gas-fueled engine equipped with exhaust gas recirculation.

Before proceeding further, it behooves to develop the flow relations, which form the basis for the development of a diagnostic to measure equivalence ratios and EGR rate using LIBS.

E.3.1 Flow Relations in A EGR Equipped Engine

Figure E15 shows a schematic representation of flows in an EGR equipped engine.

Figure E15. Schematic Representation of Engine Flows.

The combustion in an engine that consumes fuel of the form C_xH_y for cases where EGR is not used can be represented by:

where $z = x + (y/4)$. In cases where the engine indicated mean effective pressure (IMEP) and speed are held constant, for $\phi \leq 1.0$, with the introduction of EGR, this transforms to:

where $\alpha < 1$ and $\beta > 0$. For the present treatment, Eqn. E12 can be further simplified to:

$$C_x H_y + \alpha \cdot \left(\frac{z}{\phi}\right) \cdot (O_2 + 3.76 \cdot N_2) \rightarrow (1 - \beta) \cdot (a \cdot CO_2 + b \cdot H_2O + c \cdot N_2 + d \cdot O_2). \quad (\text{Eqn. E13})$$

By performing C, H, N, and O balance on Eqn. E13, the following is obtained:

$$a = \frac{x}{(1-\beta)} \quad (\text{Eqn. E14})$$

$$b = \frac{y}{2(1-\beta)} \quad (\text{Eqn. E15})$$

$$c = \left(\frac{z\alpha}{\phi}\right) \cdot \frac{3.76}{(1-\beta)} \quad (\text{Eqn. E16})$$

$$d = \frac{z}{(1-\beta)} \cdot \left(\frac{\alpha}{\phi} - 1\right) \quad (\text{Eqn. E17})$$

From the definition of the exhaust gas fraction in the inducted charge,

$$EGR = \frac{m_{EGR}}{m_f + m_a + m_{EGR}} \quad (\text{Eqn. E18})$$

By substituting the values of a, b, c, and d into the above relation and rearranging, the following is obtained:

$$\left(\frac{1}{EGR} - 1\right) = \frac{m_f + m_a}{m_{EGR}} = \left(\frac{1}{\beta} - 1\right) \cdot \left[\frac{MW_f + MW_a \cdot \left(\frac{z\alpha}{\phi}\right)}{x \cdot MW_{CO_2} + \left(\frac{y}{2}\right) \cdot MW_{H_2O} + 3.76 \cdot \left(\frac{z\alpha}{\phi}\right) MW_{N_2} + z \cdot \left(\frac{\alpha}{\phi} - 1\right) MW_{O_2}} \right] \quad (\text{Eqn. E19})$$

The term in the square brackets = 1 on account of mass balance in Eqn. E11, thereby yielding:

$$\beta = EGR \quad (\text{Eqn. E20})$$

Furthermore, owing to the fact that the total volume of the oxidizer, on the left hand side of Eqns. E11 and E12 should remain the same, the following is obtained:

$$4.76 \left(\frac{z\alpha}{\phi}\right) + \beta(a + b + c + d) = 4.76 \left(\frac{z}{\phi}\right), \quad (\text{Eqn. E21})$$

which, upon rearranging and substituting for β , results in:

$$\alpha = 1 - EGR \cdot \left[1 + \frac{y}{4} \cdot \frac{\phi}{4.76 \cdot z}\right]. \quad (\text{Eqn. E22})$$

In addition, on the LHS of Eqn. 12, the molar concentrations of O, H, and N atoms yield:

$$[O] = \frac{2z\alpha}{\phi(1-EGR)}, \quad (\text{Eqn. E23})$$

$$[H] = \frac{y}{(1-EGR)}, \text{ and} \quad (\text{Eqn. E24})$$

$$[N] = \frac{7.52 \cdot \left(\frac{z\alpha}{\phi}\right)}{(1-EGR)}. \quad (\text{Eqn. E25})$$

Therefore,

$$\frac{[H]}{[O]} = \left(\frac{y}{2z}\right) \cdot \left(\frac{\phi}{\alpha}\right), \text{ and} \quad (\text{Eqn. E26})$$

$$\frac{[H]}{[N]} = \left(\frac{y}{7.52z}\right) \cdot \left(\frac{\phi}{\alpha}\right). \quad (\text{Eqn. E27})$$

It becomes evident that $([H]/[O])$ and $([H]/[N])$ are $\propto fnc(\phi, \text{EGR})$.

The oxygen-based equivalence ratio, which is a measure of the local equivalence ratio, can be expressed as:

$$\psi = \frac{(m_f/m_{O_2})}{(m_f/m_{O_2})_{st, \text{EGR}=0}} = \frac{(1-\text{EGR})}{\left(\frac{\alpha}{\phi} - \text{EGR}\right)}, \quad (\text{Eqn. E28})$$

which essentially is a function of ϕ and EGR. The interdependency between ψ and ϕ for various levels of EGR is shown in Figure E16 and E17, which indicates a shift toward richer combustion with increased levels of EGR. In addition, such an effect is more pronounced under richer conditions than under leaner conditions.

Figure E16. Relation between ψ and ϕ for Various Levels of EGR.

Figure E17. Relation between ψ and EGR for $\phi = 0.6$ and $\phi = 1.0$.

E.3.2 Results and Discussion

With a view to avoid capturing the laser signals, as well as to allow the plasma kernel to achieve quasi-equilibrium with surrounding gases, the data collection was delayed by $1\ \mu\text{s}$ from the incidence of laser pulse. The time history of line intensity of H_{α} at 656.3 nm collected over a time window of $1\ \mu\text{s}$ and for different delays is shown in Figure E18. As the signal intensities for H, N, and O atoms were negligible for time delays $> 6\ \mu\text{s}$, the signal collection was limited to 1–6 μs time window. One such spectra obtained for a typical engine operation is shown in Figure E19. The wavelength regions of interest are the peaks that result from H_{α} at 656.28 nm; the N atom at 742.36, 744.22, and 746.83 nm; and the O atom at 777 nm. The laser pulse energies used were well above the 20 mJ/pulse threshold identified by Phuoc and White [28], and as a result, the spectral intensity ratios remain independent of the laser power even though the spectral lines by themselves vary linearly with laser power.

Figure E18. H Atom Signal Intensity Averaged over a 1-μs Time Window at 656.3 nm.

Figure E19. LIBS Signal Obtained with a 1-μs Delay and a 5-μs Exposure.

The engine was operated for a range of conditions, $0.6 < \phi < 1.0$ and EGR up to 29%, and the intensities of H α , N, and O spectral intensities were obtained by integrating under the corresponding peaks. In such cases, the global equivalence ratios, ϕ , were determined through intake air and fuel flow measurements.

As shown in Figure E20, for cases with $EGR = 0$, the intensity ratios (H_α/O) and (H_α/N_{746}) correlated to a very high degree with ϕ ; the corresponding $R^2 > 99\%$. Similar correlation for (H_α/N_{sum}), wherein N_{sum} is the sum of the intensities for the three peaks corresponding to N, correlated with $R^2 = 90\%$ (see Figure E20). These results are in agreement with the recent observations by Joshi et al. [29] and are a confirmation of the fact that the measured line intensities truly reflect the atomic concentrations.

According to Eqns. E26 and E27, for cases where $EGR \geq 0$, the line intensity ratios should be proportional to (ϕ / α) . The corresponding correlations are shown in Figure E21. The high degree of correlations, with $R^2 \approx 0.96$, is very encouraging and further points toward the possibility of estimating other combustion-related quantities.

For the test cases of this study, values of local oxygen-based equivalence ratios, ψ , were calculated per Eqn. E28. The line intensity ratios again correlated extremely well with such values (see Figure E22). Phuoc [30] has correlated equivalence ratio with line intensity ratios to obtain the relation, $\phi = a(H_\alpha/O) + b$, where the coefficients a and b were shown to vary with the combustion environment pressure. For the present cases, where the ignition timing was adjusted to obtain maximum torque (MBT timing), the effect of such pressure dependence remains relatively small. Provided the quantum efficiency of the detector remains relatively constant over the spectral range of interest, the correlations with spectral intensity ratios as shown in Figures E20, E21, and E22 could be carried over to other engine platforms as well. However, for other hydrocarbon fuels like gasoline, caution needs to be maintained as broadband contribution from CN radicals could lead to undesirable errors.

Figure E20. Correlation of Line Intensity Ratios (H_α/O), (H/N_{746}), and (H/N_{sum}) with ϕ for Cases with $EGR = 0$.

Figure E21. Correlation of Line Intensity Ratios (H_{α}/O), (H/N_{746}), and (H/N_{sum}) with (ϕ/α) for Cases with $EGR \geq 0$.

Figure E22. Correlation of Line Intensity Ratios (H_{α}/O), (H/N_{746}), and (H/N_{sum}) with ψ for Cases with $EGR \geq 0$.

E.3.3 Potential Uses of LIBS Measurement

Four uses are identified as follows:

- (i) For low-temperature combustion strategies where high levels of EGR are used, the local equivalence ratio, ψ , plays a very important role. It determines the local ignitability and subsequent flame speed in addition to emissions formation. The present diagnostic enables monitoring such an important parameter close to the spark plug and could prove valuable in strategies aiming to develop a locally stratified charge.
- (ii) Quite often, production engines are already equipped with instrumentation to measure the air flow rate and fuel flow rate, thereby enabling deduction of the global equivalence ratio, ϕ . Knowledge of ϕ can be used along with estimates of ψ obtained from LIBS line intensity ratios to further estimate the EGR rate (see Eqns. E22 and E28). Alternately, should the EGR rate be known, the present diagnostic enables estimation of the global equivalence ratio, ϕ .
- (iii) In most of the current natural gas engines, the fuel is introduced upstream of the compressor stage of the turbocharger. Although it is assumed that a very homogenous mixture is distributed among the cylinders, slight variations are inevitable. The current diagnostic enables estimation of such non-uniformities.
- (iv) In some of the large bore engines, usually for bore diameters > 163 mm, with a view to improve breathing efficiencies, the fuel is injected directly into the cylinder. In such cases, the present LIBS diagnostic can be used to estimate the homogeneity of the combustion charge for various injection parameters.

E.4 SUMMARY AND CONCLUSIONS

The goals of these experiments were to determine the potential of employing spectral measurements to deduce combustion metrics such as HRR, combustion temperatures, and equivalence ratios in a natural gas-fired reciprocating engine. A laser-ignited, natural gas-fired single-cylinder research engine was operated at various equivalence ratios between 0.6 and 1.0, while varying the EGR levels between 0% and maximum to thereby ensure steady combustion. Crank angle-resolved spectral signatures were collected over 266–795 nm, encompassing chemiluminescence emissions from OH*, CH*, and predominantly by CO₂* species. Further, laser-induced gas breakdown spectra were recorded under various engine operating conditions.

The peak spectral intensities for CO₂* (those defined over a narrow wavelength band centered at the peak signal) temporally exhibited a maxima coincident with the peak cylinder pressure to an accuracy of ± 2 CAD. For each combustion cycle, the maxima of heat release rate, peak spectral intensity, and temperature occurred in that sequence and were temporally well separated. The peak heat release rates preceded the peak chemiluminescence emissions by 3.8–9.5 CAD, whereas the peak temperatures trailed by 5.8–15.6 CAD depending upon the engine operational conditions. Although crank angle-resolved correlations were not possible, both peak cycle heat release rates as well as peak cycle temperatures correlated well with the

maxima of the chemiluminescence emission from CO_2^* . The correlations were retained to a high degree when a transmittance (400–550 nm) of a virtual optical filter was imposed on the collected spectra. Such observations point toward the potential use of flame chemiluminescence to monitor peak bulk gas temperatures, as well as peak heat release rates in natural gas-fired reciprocating engines.

The UV emission corresponding to the OH^* radicals in the 306–310-nm range was used for the calculation of combustion gas temperature. A computer simulation that predicted the spectra of OH^* at various gas temperatures was used to compare the measured spectrum. The simulated spectra were iterated until they closely matched with the measured spectra. This approach can be used to assess gas temperature whenever a reasonably isolated OH^* signal is present. Although it was not possible to obtain good single-shot measurements, the averaged data show the trends as expected. These preliminary results show that the current technique can be further improved to obtain more accurate and reliable measurements, which, in turn, will help develop NO_x reduction strategies in reciprocating engines.

The emission from the spark kernel immediately following the spark event was spectrally resolved, and the peaks corresponding to H_α , N and O atom were measured for a range of conditions with global equivalence ratios ranging between 0.6 and 1.0, and for EGR fractions up to 29%. The $(\text{H}_\alpha/\text{O})$ and $(\text{H}_\alpha/\text{N})$ peak intensity ratios from the spectral scans correlated extremely well ($R^2 > 0.97$) with local oxygen-based equivalence ratios. Appropriate relations were developed to relate such values to global equivalence ratios and the EGR rate. By using LIBS measurements, the current diagnostic enables estimation of one of the two values, global equivalence ratio or the EGR rate, with the knowledge of the other. As the present diagnostic is based on the ratio of line intensities, it can be transferred to other engine geometries and potentially to other fuels amenable to spark ignition.

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