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A Framework for Energy Optimization of Small, Two-Stroke, Natural Gas Engines for Combined Heat and Power Applications

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**A Framework for Energy Optimization of Small, Two-Stroke, Natural Gas Engines for
Combined Heat and Power Applications**

Mahdi Darzi

**Dissertation submitted to Benjamin M. Statler College of Engineering and Mineral
Resources at West Virginia University in partial fulfillment of the requirements of the
degree of Ph.D. in Mechanical Engineering**

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Keyword: Two-stroke, Natural gas, GENSETS, CHP, LPDI, Simulation

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ABSTRACT

A Framework for Energy Optimization of Small, Two-Stroke, Natural Gas Engines for Combined Heat and Power Applications

Mahdi Darzi

This research was focused on the development of a framework for the energy optimization a natural gas engine for small combined heat and power (CHP) applications operating with low-pressure natural gas (NG) available at homes. The required targets of the ARPA-E GENSETS program for 1 kW electric power generation and previous GENSETS simulation at West Virginia University, suggested a design space for the engine which is currently dominated by simple two-stroke designs. Hence this research focused on screening, modeling, and experimentally evaluation of cost-effective technologies to achieve a system design that maximized thermal efficiency and utilization factor, while reducing emissions. A baseline engine was selected which started with 8% brake thermal efficiency (BTE) on natural gas operation. By implementing intake and exhaust optimization BTE increased up to around 12% and with head design optimization and exhaust backpressure, the engine reached 15% BTE. Though the initial optimization methods almost doubled efficiency, it was realized that further increases in BTE must be achieved for a commercially competitive design. The engine was redesigned to utilize modified porting for enhanced breathing and scavenging and a method to deploy low-pressure direct injection (LPDI) was developed. With these enhancements, BTE increased to around 24%. A second round of optimization was performed then, by modeling the whole system in a 1D platform and using a genetic algorithm and experimental data to further optimize scavenging which increased the efficiency up to around 26%. Finally, a 3D computational fluid dynamics (CFD) was developed to investigate the stratification effects of LPDI and determine the optimal spark plug location. This effort increased the BTE to around 27.5%. To assess issues with commercial deployment, three different NG compositions and propane operation were investigated. With an energy balance and exergy distribution analysis for each fuel, fuel quality effects on the CHP system performance were determined. At the end, with combination literature review, experiments, 1D and 3D simulations, a framework for optimization of micro-CHP systems operating on gaseous fuels was developed that can serve industry to highlight methods that can more than triple brake thermal efficiency of small two-stroke engines while improving the energy distribution for CHP systems.

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Abbreviations

Acronyms	
AFR	Air-Fuel Ratio
AMR	Adaptive Mesh Refinement
ATDC	After Top Dead Center
BDC	Bottom Dead Center
BMEP	Brake Mean Effective Pressure
BSFC	Brake Specific Fuel Consumption
BTDC	Before Top Dead Center
BTE	Brake Thermal Efficiency
CA	Crank Angle
CAD	Crank Angle Degrees
cc	Cubic Centimeters
CFD	Computational Fluid Dynamics
CFR	Code of Federal Regulations
CH ₄	Methane
CHP	Combined Heat and Power
CNG	Compressed Natural Gas
CO	Carbon Monoxide
CO ₂	Carbon Dioxide
COV	Coefficient of Variation
CR	Compression Ratio
DI	Direct Injection
DME	Dimethyl Ether
DOI	Duration of Injection
DR	Delivery Ratio
ECE	Exhaust Chemical Energy
ECU	Engine Control Unit
EGR	Exhaust Gas Recirculation
EIA	Energy Information Administration
EPA	Environment Protection Agency
EPC	Exhaust Port Closing
EPO	Exhaust Port Opening
FC	Fuel Consumption
FTIR	Fourier-Transform Infrared Spectroscopy
g	Grams

GA	Genetic Algorithm
GENSETS	Generators for Small Electrical and Thermal Systems
GHG	Greenhouse Gas
GWP	Global Warming Potential
H ₂	Hydrogen
H ₂ O	Water
HC	Hydrocarbon
HCCI	Homogenous Charge Compression Ignition
HPDI	High Pressure Direct Injection
HZ	Hertz
IC	Internal Combustion
ICE	Internal Combustion Engine
IEA	International Energy Agency
IMEP	Indicated Mean Effective Pressure
ITE	Indicated Thermal Efficiency
K	Degrees Kelvin
kHz	Kilohertz
kJ	Kilojoules
kWe	Kilowatts of Electrical Power
LFE	Laminar Flow Element
LHV	Lower Heating Value
LPDI	Low-Pressure Direct Injection
LPG	Liquefied Petroleum Gas
MBT	Maximum Brake Torque
MBTU	Thousand British Thermal Units
MFB	Mass Fraction Burned
MFB50	50% mass fraction burnt
MFC	Mass Flow Controller
MJ	Megajoule
mm	Millimeter
MN	Methane Number
NG	Natural Gas
NMHC	Non-Methane Hydrocarbons
NO _x	Nitrogen Oxides
O ₂	Diatomic Oxygen
OEM	Original Equipment Manufacturer
OTS	Off the Shelf

PCCI	Premixed Charge Compression Ignition
PI	Port Injection
PISO	Pressure Implicit with Splitting of Operators
PM	Particulate Matter
PSIA	Pound-force per Square Inch Absolute
RCCI	Reactivity Controlled Charge Ignition
RMSE	Root Mean Square Error
ROHR	Rate of Heat Release
ROI	Return of Investment
RPM	Revolution per Minute
SCFM	Standard Cubic Foot per Minute
SCR	Selective Catalyst Reduction
SI	Spark Ignited
SLPM	Standard Liter per Minute
SOI	Start of Injection
TBC	Thermal Barrier Coating
TDC	Top Dead Center
TE	Trapping Efficiency
THC	Total Hydrocarbons
TKE	Turbulent Kinetic Energy
TPA	Three Pressure Analysis
TPO	Transfer Port Opening
TR	Trapping Ratio
TSCI	Thermally Stratified Charge Ignition
UF	Utilization Factor
US	United States
VE	Volumetric Efficiency
VOC	Volatile Organic Compounds
WOT	Wide Open Throttle
Variables	
AFR_{stoich}	Stoichiometric Air to Fuel Ratio
a_i	Polynomial Constants
$\bar{C}_p$	Heat Capacity at Constant Pressure Molar Based
$\bar{C}_{p_{ex}}$	Heat Capacity of Exhaust
C_μ	Turbulence model constant
$\dot{E}_{ex}$	Exhaust Energy
$\dot{E}_{ex}^{fuel}$	Exhaust Fuel Energy

$\dot{E}_{ex}^{ub}$	Exhaust Unburnt Energy (CO and H ₂)
$\dot{E}_{ex}^{HC}$	Exhaust HC Energy
$\dot{E}_{in}^{fuel}$	Fuel energy
$\bar{h}_{f_i}^o$	Enthalpy Formation at Standard Reference State
$\bar{h}_i$	Sensible Enthalpy at Specified State
$\bar{h}_i^o$	Sensible Enthalpy at Standard Reference State
$\dot{H}_{products}$	Total Enthalpy Flow Rate of Products
$\dot{H}_{reactants}$	Total Enthalpy Flow Rate of Reactants
IMEP	Indicated Mean Effective Pressure
K _{wg}	Equilibrium Constant
LHV _{CO}	Lower Heating Value of Carbon Monoxide
LHV _{fuel}	Lower Heating Value of Fuel
LHV _{H₂}	Lower Heating Value of Hydrogen
LHV _i	Lower Heating Value
$\dot{m}_{air}$	Intake Air Mass Flow
$\dot{m}_{fuel}$	Fuel Mass Flow
N	Operating Speed
$\dot{n}_{exh}$	Exhaust Molar Flow Rate
P _{amb}	Ambient Pressure
P _{ex}	Exhaust Pressure
$\dot{Q}_l$	Heat Loss
$\dot{Q}_{ex}^{th}$	Exhaust Thermal Energy
$\bar{R}$	Universal Gas Constant
Sc	Schmidt number
$\dot{S}$	Entropy Rate
$s_{f_i}^o$	Entropy of Formation
T	Temperature
T _{ad}	Adiabatic Flame Temperature
T _{amb}	Ambient Temperature
T _{boundary}	Coolant Temperature
T _{exh}	Exhaust Temperature
T _{in}	Intake Temperature
T ₀	Reference Temperature
V _d	Displacement Volume
V _m	Molar Volume
ω _n	Natural Frequency
v _{CO}	Mole Fraction of Carbon Monoxide

v_{H_2}	Mole Fraction of Hydrogen
v_i	Component Mole Fraction
$\dot{W}_{\text{indicated}}$	Indicated Power
$^{\circ}\text{C}$	Degrees Celsius
$\Delta_r H$	Enthalpy of CO oxidation reaction
$\Delta_f H\{\text{CO}_{(g)}\}$	Enthalpy of CO formation
$\Delta_f H\{\text{CO}_{2(g)}\}$	Enthalpy of CO_2 formation
$\Delta H\{\text{O}_{(\text{Pt})}\}$	Heat absorption for releasing O radicals
Δt	Time step in 1D simulation
Δx	Discretization Length in 1D simulation
δ_{max}	Beam end deflection
δ_{ij}	Kronecker Delta
μ	Viscosity
μ_{mol}	molecular viscosity
μ_{tot}	Total Viscosity
μ'	Dilatational viscosity
λ	Air Fuel Equivalence Ratio
η_{II}	2 nd law efficiency
χ_1	Design Constant for Resonator
χ_2	Design Constant for Resonator
ϕ	Passive scalar

1 Introduction

With an industry shift towards clean energy, increasingly stringent regulations have driven energy researchers to create more energy efficient systems. While efficiency is of utmost concern, utilizing the available alternative energy resources may be more cost effective and, in some cases, offer emissions reductions. Natural gas (NG), due its abundance, low price, applicability to current power generation systems, and lower carbon content has become the dominant energy provider in power generation for the first time in 2016 surpassing coal [1]. NG utilization is primarily split between industrial purposes and electrical generation on large scales [2]. It has also been used for large displacement two-stroke engines and four-stroke engines in the transportation sector for decades, however this has not been widespread due to required, costly fuel supply infrastructure changes [3]. It has been used in dedicated NG engines and dual fuel engines to lower operating costs [4]. NG is available in over 61% of US homes [5]. Currently, it is a major source of energy for residential applications as shown in **Figure 1** [1]. It is used for heating (furnaces, boilers), appliances (stoves, water heaters), and backup power. Nearly 50% of US households utilize natural gas as an energy source for cooking or home heating [6]. However, its potential dedicated use for decentralized power generation has not yet been exploited

Figure 1. US energy consumption summary in 2017 [1].

Realizing the fuel availability and electrical generation and transmission efficiency issues, the Advanced Research Projects Agency – Energy (ARPA-E) conceived the Generators for Small Electrical and Thermal Systems (GENSETS) program to develop transformative generator technologies to enable widespread deployment of residential combined heat and power (CHP) systems [7].

This research was part of an ARPA-E GENSETS program at West Virginia University (WVU), which aimed to develop a high-efficiency and low-cost combined heat and power generation system, powered by a two-stroke engine fueled with low-pressure NG available at homes [7]. Based on a previous studies, the average daily electricity consumption per household in US is about 29.2 kilowatt-hours (kW-hr) setting the average power to around 1.2 kW [8, 9]. Therefore, the target electric power for GENSETS was set to 1 kWe to account for the move towards higher household efficiency [7]. This means the engine must produce more than 1 kW brake power, to offset any inefficiency in the mechanical to electrical conversion system.

Typically, engines of this power rating are dominated by two-stroke designs. These engines are simple, cheap to produce, and have higher power density compared to four-stroke engines [10]. On the other hand, this research was assumed to be transferred to a linear alternator driven by a single cylinder engine on one side and a spring mechanism on the other side [11]. This required having a power cycle on each oscillation which is achievable only with two-stroke engines. In addition, because of the absence of rotary motion in the linear alternator, it would be difficult to easily implement a four-stroke engine, based on the need for linear valve actuation.

My research was conducted under the broad objective of converting chemical energy in natural gas to useful work and heat locally in the home, seeking to minimize criteria pollutants and climate change emissions, while increasing efficiency and maximizing waste heat recovery. I found that little information was available on the performance of small two-stroke engines fueled by NG, which would serve as the prime mover of a small CHP system.

My objective was to evaluate recent technologies deployed in small two-stroke engines and to create a framework for energy optimization of small CHP systems operating on gaseous fuels. Such a framework combined extensive experimental design and evaluation, 1D and 3D modeling for optimization (with experimental validation), and a complete energy analysis. This framework can serve as a general guideline for researchers and industry to follow on the path towards

improved efficiency for small, decentralized power generation systems. To achieve this objective and align with project objectives, the following goals were targeted.

1.1 Project Goals

The ARPA-E GENSETS program efficiency target for NG to electric conversion was 37%. The electric power output target was 1 kW. NG was considered as the primary fuel and it was noted it was only available at low pressures as found in residential applications. Finally, an assessment of available energy for a complete CHP system was required. Long life and low cost were required for the application but were not the main drivers of my research.

1.2 Objectives

Based on NG being the only fuel for GENSETS required by ARPA-E and previous assessment of researchers at West Virginia University a two-stroke engine was selected for the GENSETS. The objective of this research is to develop a framework for energy optimization of a small two-stroke natural gas engine for micro-CHP application. Energy optimization mainly includes raising brake thermal efficiency, maximizing useable heat while maintain or improving combustion stability. To develop this framework a combination of experimental research, advanced simulation, and literature review was required. This resulting framework should clearly identify the path of energy efficiency evolution of the system. It should consider gaseous fuel variation effects on the GENSETS performance and provide cost and emission analyses for the micro-CHP system. The final framework can be used by researchers and industry as a set of “rules of thumb or guidelines” for the design or modification of small engines that could serve as the prime movers of micro-CHP systems.

2 Literature Review

This work was focused on various possible technologies that could have been deployed in advanced two-stroke engines operating on NG. CHP system evaluation also was set at the final stage of the project's goals. So, in this section, a variety of topics including two-stroke engine history, technologies, NG as an internal combustion engine fuel, and CHP systems are reviewed to assess the potential improvements from a variety of technology candidates.

2.1 Two-stroke Engines

2.1.1 History

The first two-stroke engine was designed in 1877, and was patented in 1881 [12]. Two-stroke engines were deployed in small vehicle transportation, marine engines, handheld equipment, and numerous other applications over the past 13 decades. There was a brief surge of interest in two-stroke engines for automotive applications during the 1980's-90's by many manufacturers with the focus of direct injection and electronic control, however deep market penetration was not realized except for marine applications [13, 14].

Most handheld lawn and logging equipment use gasoline fueled two-stroke engines operating with carburetors. However, industry has developed small four-stroke engines to replace conventional two-stroke engines in motorcycles and even some handheld equipment due to emissions regulations [15, 16]; however, fuel injection for two-stroke chainsaws is arriving in the marketplace [17]. By nature of operation, port scavenged two-stroke engines tend to have excessive hydrocarbon (HC) emissions due to short-circuited fuel and oil lost via the exhaust port during the scavenging process. These emissions are regulated and represent a significant efficiency penalty [18, 19]. In the past decade, research efforts primarily focused on redesign of the two-stroke engine for alternative fuel usage and power density, as well as to achieve higher efficiency via more complex porting systems [20–22].

2.1.2 Basic Design

Two-stroke engines operate with one power stroke and one compression stroke per cycle. For this reason, both the intake and exhaust ports are simultaneously open for some duration. A cycle begins with the piston moving towards top dead center (TDC). When the piston reaches TDC,

combustion expansion pushes it downward creating the power stroke until the exhaust port becomes exposed. After the exhaust is partially expelled, transfer ports become exposed which deliver fresh fuel and air charge that pushes additional exhaust out of the cylinder; however, in conventionally fueled designs this action also loses some fuel and air charge. Crankshaft inertia causes the piston to begin another upward stroke, which after the exhaust port is fully closed the piston compresses the remaining mixture for the next cycle [10]. **Table 1** shows a summary of advantages and disadvantages of two-stroke engines over four-stroke counterparts.

Table 1. Summary of two-stroke engines advantages and disadvantages.

Two-stroke Advantages	Two-stroke Disadvantages
<ul style="list-style-type: none"> Higher power density than four-stroke engines of the same displacement Valve train not required except for uniflow design No oil pump loss Higher operating speeds versus four-stroke engine counterparts Less output torque fluctuation per cycle than four-stroke engines [13] More cost effective to manufacture than four-stroke engines 	<ul style="list-style-type: none"> Increased hydrocarbon (HC) emissions due to typical carbureted engines scavenging with an air-fuel mixture Higher heat flux near TDC causing increased heat losses Pumping losses in the case of crankcase compression Misfires at low speeds due to poor scavenging Incomplete combustion

Two-stroke engine designs are normally differentiated by one of the various scavenging methods employed by the porting style. Common scavenging methods include cross-scavenging, loop scavenging, reverse loop scavenging, and uniflow scavenging as shown in **Figure 2**.

Figure 2. Scavenge flow patterns for the four basic scavenging approaches. Note the uniflow approach is the only one that uses an exhaust valve as opposed to an exhaust port [14, 23].

The most challenging part of designing two-stroke engines is determining the best scavenging method for the engine. The difficulty lies within the randomness of cycle-to-cycle variations of in-cylinder gas flow motion. Large uniflow diesel two-stroke engines have been the most thermally efficient engines ever constructed at over 50%. The uniflow scavenged type is the only one which relies on an exhaust valve, while all others are port controlled. Uniflow is commonly recognized as the best method but optimized loop/cross scavenging can be made to be nearly as efficient as uniflow [18]. However, due to the goal of implementation onto a linear system and lack of rotary motion for simple valve actuation, a uniflow scavenge design that included a valve was not selected.

Most two-stroke engines use the crankcase as a mixing chamber for the fuel and air intake prior to passage into the cylinder via transfer ports. This is known as crankcase compression. The pistons upward motion draws the fresh mixture into the crankcase and during the subsequent downward motion that follows it compresses the charge. Engines may use cylinder and piston porting to prevent back flow or have a reed valve in the crankcase to allow flow only into the crankcase and seal under pressurization. This reed valve method is quite common in medium displacement engines. For both cases, air induction occurs with the piston's upward motion; followed by compression and release of the fresh charge into the combustion chamber [10]. Crankcase compression engines rely on the piston's upward movement for breathing. However, pumping losses during the piston's downward motion are inevitable. Crankcase compression engines can reach brake specific fuel consumption of 450 g/kW-hr using gasoline in a 50 cubic centimeter (cc) engine [24].

2.2 Natural Gas in Internal Combustion Engines

Recent literature addresses fuel choices, but for engines that were different from the hardware considered. Chandra et al. converted a small diesel engine to run as spark-ignited (SI) using NG, biogas, and methane enriched biogas to show the benefits of alternative fuel usage. Under port fuel fumigation, the efficiency of pure biogas was higher than compressed natural gas (CNG) over a range of ignition timings [25]. Yousefi and Birouk performed research on a dual fuel NG and diesel pilot ignited engine where they showed reductions in oxides of nitrogen (NO_x) [26]. Other dual fuel research on NG-diesel operation showed the possibility to reduce carbon monoxide (CO) and hydrocarbon (HC) emissions by 38.3% and 34.7%, respectively when changing the intake air

strategy to reduce the bulk quenching [27]. Navaro et al. conducted experimental research on NG blended with hydrogen in SI engines. They showed a reduction in carbon dioxide (CO₂) emissions and an increase in power output [28]. Djermouni and Ouadha investigated the impact of a turbocharger on the thermodynamic performance of a homogenous charge compression ignition (HCCI) engine fueled with NG. They indicated that both energy and exergy efficiency were enhanced with an increase of compressor and turbine efficiency [29]. Alamia et al. showed biomethane as a promising future fuel alternative, easily applied to engines [30]. Kan et al. performed fuel testing of biogas and syngas, which showed the benefits of the NG renewable alternative under premixed, SI engine operation [31]. Yang et al. examined injection timing impacts in a dual fuel NG piloted diesel. A pilot injection timing variation of 9 degrees crank angle was shown to improve the efficiency by up to 5% [32].

2.3 Two-stroke Engine's Air Handling (Breathing)

Tuning of two-stroke engines has occurred over the last 50 years mainly targeting increased power over a wide range of engine speeds, as applicable to performance two-stroke engines used in snowmobiles and dirt bikes. Tuning of such engines is nearly as much art as science due to the complex gas dynamics and numerous engine configurations [12, 18, 33]. Small handheld engines (e.g. chainsaws, lawn equipment) typically do not use intake and exhaust tuning because of packaging limitations, while larger engines such as performance dirt bikes are required to operate over a wide speed range, which reduces the impact of fixed geometry intake and exhaust systems. However, stationary two-stroke NG engines can benefit greatly since weight and packaging are not critical factors when compared to efficiency and stability. Current commercial designs include both two-stroke and four-stroke engines, fueled with gasoline, natural gas, propane, and diesel fuel. For back-up or temporary power generation, efficiency and stability are perhaps of less concern; however, for long term, independent power generation or sensitive applications like hospital's back-up power generation, both are critical. Air handling directly affects the power density and combustion stability and research on small diesel generators showed that stability of the electricity generated was directly proportional to combustion stability [34].

2.3.1 Intake Optimization

Intake optimization of two-stroke engines primarily consists of making geometrical changes to the intake system. The base geometry of the intake is characterized by overall length, volume, and taper angles of any Helmholtz resonator chambers. Mitianiec's experiment showed that by varying the overall length of the intake pipe, the delivery ratio of fresh charge was directly impacted. This was also true with variance of the diameter of the intake pipe. The addition of a side volume in the intake system also improved delivery ratio [35]. Delivery ratio is the ratio of intake air mass to the theoretical mass calculated based on engine total displacement. A study showed that by varying the length of inlet pipe at constant engine speed, a 17% gain in compression pressure was achieved [36]. Adding Helmholtz resonator cones to the intake pipe improved the delivery ratio [37]. A study showed that intake resonators, which operated at approximately twice the frequency of the piston, raised both power and inducted mass [38]. The primary pressure wave sought to be captured was that of the final closing of the intake port, which would be reflected at such a time that assists the next intake process. It is also noted that wave velocity increased with increased pipe diameter [36]. Intake systems with common rail type branching showed advantages over those with completely separated ducting [38, 39]. Overall, intake optimization must be tailored for each specific type and size of engine [33].

2.3.2 Exhaust Optimization

Understanding of the gas flow dynamics over the scavenging period is essential to improve the performance of any engine [40, 41]. Though many investigators have contributed greatly to the theoretical design, the complexity of the wave dynamics in the exhaust pipe still requires a deep understanding. Due to packaging considerations in most two-stroke engine applications, the exhaust pipe was designed to improve power density rather than the improving trapping ratio. A study considered the effects of exhaust's lead-in pipe length, expansion angles, and attachment of the muffler to the exhaust pipe of scooter type motorcycles and showed that the maximum power of the engine decreased linearly with increased angles of the first expansion [42]. A buildup of exhaust pressure prevented the escape of fresh mixture from the cylinder, hence proper arrangement of convergent cone and expansion length were required for timely arrival of the

reflected wave front. Blair reported the construction of the divergent cone was three to four times longer when compared to convergent cone for best results [18].

Scavenging efficiency showed improvements by proper timing of the downstream, low-pressure wave during the overlap period via lowering the concentration of trapped residual gases inside the engine cylinder [42]. Tuning the exhaust pipe demonstrated better emptying of the burnt matter from the cylinder, better combustion of fuel, and less required throttling for a given engine speed [43]. Experiments on tuned exhausts increased engine power by 15.8% and reduced brake specific fuel consumption (BSFC) by 12% when compared to the Original Equipment Manufacturer (OEM) exhaust system [44]. Designing a tuned exhaust system for an opposed piston two-stroke HCCI engine led to a more efficient and smoother engine operation with 15% improvement in trapping efficiency when compared to an untuned pipe [45]. Exhaust tuning of the small two-stroke engines in handheld power tools was studied by Gustafsson to meet emissions regulations without effecting the power density [46]. Computational modeling of diverse designs of exhaust manifolds for multi-cylinder, two-stroke, NG engines with the objective of reducing NO_x emissions, showed possible reductions of 10-30% in those emissions [42]. Additional studies regarding exhaust tuning of single cylinder two-stroke engines are found in literature [47–49].

2.4 Effect of Compression Ratio

As for the effects of compression ratio (CR) on engine performance, thermal efficiency, BSFC, brake torque (BT), air-fuel ratio (AFR), and exhaust emissions have been mainly investigated [50, 51]. Research carried out on a two-stroke engine at Yamaha Motor Company showed 1-3% improvement in fuel consumption for each unit increase in CR between 6.6 and 13.6 at an engine speed of 4500 revolutions per minute (RPM) [52]. Another study investigated the effects of CR ranging from 8 to 14 on a four-stroke, SI, and direct injection NG engine. They reduced penetration distance of the fuel jet and had relatively strong mixture stratification due to higher CRs, which led to faster burn rate and higher thermal efficiency at low to medium engine loads. Their experiments showed maximum BTE at a CR of 12 for higher engine loads [53]. In a study focused on a single-cylinder, two-stroke, SI engine using methanol as fuel, researchers showed that a CR of 8.56 provided high BTE within the entire engine load range from 20% to 100% [54]. A two-stroke engine was tested to compare the effects of CR on different fuels including diesel fuel, hydrogen, gasoline, and NG. Results showed an increase in efficiency of the engine with the

exception of hydrogen due to its faster combustion. It was added that higher CR would result in higher frequency and power density [55]. The effect of an increase in CR from 7 to 8 was tested in a two-stroke engine with direct injection of gasoline under motoring conditions. The results showed a decrease in turbulent kinetic energy (TKE) and tumble ratio by 13% and 26%, respectively [56].

2.5 State-of-the-Art

In previous investigations using a port-injection (PI) configuration, I observed that two-stroke engines, even those with improved breathing and CR, suffered from fuel slip losses[57–60]. That is why direct injection was found to be necessary for energy optimization.

2.5.1 Injection Strategies

To overcome deficiency of PI, a direct injection strategy was evaluated in a small NG two-stroke engine which resulted in a more than 60% relative improvement in BTE [61]. A study conducted in Japan investigated the effects of low-pressure CNG injection into the transfer (scavenging) ports of a two-stroke SI engine. The thermal efficiency of the engine increased by 25% at best as compared to the baseline gasoline operation. Injecting into a secondary transfer port had better performance than injection in the main transfer port due to better scavenge/fuel jet interactions [62]. Hatakeyama et al. compared small two-stroke engine performance between NG manifold and in-cylinder injection, and carbureted gasoline operation. The peak BTE achieved was slightly under 20% for in-cylinder injection of NG [63]. A computational fluid dynamics (CFD) model by Bozza et al. showed insufficient removal of burnt gases near the center of the cylinder in a loop-scavenging configuration. NG operation at ignition timing set for maximum brake torque (MBT), was shown to have a lower in-cylinder peak pressure than gasoline operation due to the combination of low flame speed and high engine speed. This effect caused lower exhaust port temperatures and would inherently need a tuned exhaust designed separately from the OEM configuration [64].

Pradeep et al. conducted experiments on a 200 cc engine with air-injection into the transfer ports and induction of liquefied petroleum gas (LPG) into the intake manifold in the gas phase. The engine experienced a 40% reduction in HC emissions and an increase in power at 25% throttle. Low pressure direct injection (LPDI) within the boost port was also considered but only showed a

small reduction in HC emissions, while power density deteriorated at wide-open-throttle (WOT) [65]. Staged LPDI combined with high-pressure direct injection (HPDI) showed better combustion stability over HPDI alone [66]. In-cylinder LPDI reduced HC emissions by up to 93% at injection pressures of 4-5 bar for start-of-injection (SOI) ranging from 10-40 crank angle degrees (CAD) before bottom dead center (BDC). For WOT throttle conditions it was determined that injection at 30 CAD before BDC was the best balance between reduced HC emissions and maximum BTE. The combustion rate improved over the standard manifold PI operation, with higher CO and lower NO_x emissions due to a richer trapped mixture. Operation of the engine at different throttle positions did not require large variations in injection timing [22]. Tadesse and Aziz found that LPDI in the boost port, allowed for injection during intake opening, making the LPDI more effective because pressurized air kept fuel from flowing back out of the intake port [67].

Hu et al. examined LPDI of CNG for a four-stroke engine. They examined the optimal injection window for best fuel-air mixing. It was shown that compound direct injection with a primary injection pulse around 280 CAD before top dead center (BTDC) coupled with a secondary injection between 200-170 CAD BTDC was beneficial over a single injection period for improvements in mixing [68]. A 3 bar LPDI system was controlled by an overhead valve coupled to an air injection system and showed reduced emissions over carbureted models. The system also had excellent cold start and acceleration capabilities [69]. In residential NG applications where NG is available at low pressures, LPDI is beneficial over HPDI in terms of the required energy for gas compression. LPDI is better for operating in the homogenous charge region with a longer mixing duration as compared to HPDI being predominantly stratified. LPDI also had similar power output and torque when compared to HPDI [70].

While there have been a variety of research projects conducted around the direct injection of liquid or gaseous fuels for two-stroke engines, there have also been commercial interest in deploying direct injection fuel strategies. A novel approach was used by Mercury Marine in a variety of their outboard engines for small watercraft. They found that direct injection of gasoline lead to fuel stratification and therefore deployed a fuel and air direct injection system (based on the Orbital Technology) to ensure proper air fuel control and mixing [71, 72]. More recently, Husqvarna and KTM have begun to sell high-performance two-stroke dirt bikes equipped with LPDI, in the form of transfer port injection (TPI) of their 250 and 300 cc series engines [73–75]. While no technical

publications were found for their specific TPI applications, the companies claimed reductions in emissions of 40%.

2.5.2 Advanced Combustion

In addition, NG is widely used in advanced combustion systems such as HCCI, premixed charge compression ignition (PCCI), reactivity-controlled compression ignition (RCCI) and thermally stratified compression ignition (TSCI) systems along with other fuels [76–78]. HCCI, PCCI, and RCCI combustion modes showed improved thermal efficiency while simultaneously reducing both NO_x and particulate matter (PM) emissions [79, 80]. The deficiencies of HCCI and PCCI combustion were the high levels of CO and unburnt HC emissions in most cases. However, in recent years several researchers have demonstrated that boosted HCCI and PCCI combustion can exhibit nearly 100% combustion efficiency. Intake pressure was varied from 100 to 325 kPa absolute. For highest boost pressure combustion efficiency was 99% and brake thermal efficiency was around 47% [81].

Nieman et al. replaced the gasoline with NG to examine the sensitivity of RCCI combustion at high load to injection system parameters. Since NG had lower reactivity compared to gasoline, it was proposed as a better fuel for RCCI combustion to control the maximum pressure rise rate by using the large reactivity gradient that existed between these two fuels [81]. In addition, RCCI was shown to enable high load operation when compared to HCCI [82]. Literature has identified that RCCI can be controlled through the ratios of fuels, injection parameters (start-of-injection, SOI; number of pulses, etc.), level of exhaust gas recirculation (EGR), compression ratio and combustion chamber design [83]. Increasing the ratio of NG to fuels like dimethyl ether (DME) tended to improve efficiency with increase brake mean effective pressure and decrease HC and CO emissions [84].

HCCI was not implemented because of fuel composition variations throughout the US [85]. RCCI was not used because it required a secondary fuel – which is against the principle of using NG or LPG as the sole fuel source for CHP systems.

2.5.3 Exhaust Gas Recirculation

With new standards for emissions, especially NO_x, EGR implementation is widespread these days. While EGR helps to reduce the NO_x it can negatively impact combustion stability, especially at

low load operations [19]. Off-road engine emissions typically lag those of on-road engines in terms of lower emissions limits [86]. However, many off-road engines are implementing proven technologies such as EGR. Rates of EGR can be up to 30% of the total intake volume [87]. EGR is achieved both internally and externally [88]. Internal EGR is achieved on four-stroke engines through the use of variable valve actuation [89]. Alternatively, for two-stroke engines with fixed port geometries the exhaust design and exhaust throttling can serve as a method of inducing internal EGR. The lengths and angles of the convergent and divergent resonator sections directly impact the scavenging efficiency and thus level of internal EGR [10, 18, 42, 44, 46, 59].

For small, less sophisticated engines, external EGR can be achieved by passages between the intake and exhaust port manifolds. Such a method has been used to reduce emissions of small diesel fueled engines used for electrical generation [34]. Such a simplistic method was shown to decrease NO_x emissions by 2.7 to 25.6% depending on load, which was proportional to EGR rate. The rate of EGR and engine load also influenced combustion and electrical production stability.

However, the application of EGR onto two-stroke engines depends on the scavenging of the engine itself. EGR can be applied as external EGR as is common to four-stroke engines. Work performed by Johnson et al. on a large-bore, lean-burn, natural gas engine investigated the effects of EGR. The system used a low pressure external EGR loop and examined volumetric percentages of 0, 2.5 and 5%. Tests showed that indicated mean effective pressure (IMEP) was nearly constant over the span, while the coefficient of variation (COV) of IMEP decreased. A decrease in BSFC was reported for an external EGR rate of 2.5% and was attributed to the increased combustion stability. NO_x and formaldehyde emissions were noted to decrease while THC, CO, and volatile organic compounds (VOCs) increased at an EGR level of 2.5% [90].

Watson et al. simulated the performance of a small two-stroke engine with the application of exhaust pipe restrictions and validated the simulation results with experimental research. They showed THC emissions were reduced by 24% while the CO emissions were reduced by 25%. In addition, they presented simulated plots of trapping efficiency, delivery ratio, and scavenging efficiency for different exhaust throttling conditions [91].

A recent study by Hurakaldi et al. [92], explored the impact of EGR on a 100 cc, two-stroke, gasoline fueled engine and found that thermal efficiency improved while BSFC improved at higher speeds with EGR. Furthermore, they concluded that at lower EGR rates, NO_x emissions were

reduced without impact on performance and emissions while at higher rates, the performance and emissions were deteriorated along with the reduction of NO_x . A similar study examined EGR on a different 100 cc, two-stroke gasoline fueled engine [93]. They also showed reduced NO_x emissions with increased levels of EGR but reported increased CO and THC emissions. Note that in both cases the EGR was external.

In electrical generation systems, for the sake of the generator, the engine operates at a constant speed to keep the electricity frequency fixed. Those engines usually operate at WOT conditions to obtain peak efficiency. As a consequence of balancing the electrical supply and demand, it is necessary to vary the engine load. One method to achieve this without losing efficiency is through application of EGR. While in four-stroke engines, internal EGR can be achieved using variable valve timing, in two-stroke engines it can be achieved by exhaust throttling. As part of my research, I investigated the effect of exhaust throttling on an engine's performance and emissions, which could later be used as a load control method [60].

Note that with DI, internal EGR induced by exhaust throttling was redundant for mitigating short-circuiting since HC was already decreased by DI. On the other hand, given that external EGR deteriorates the combustion stability, one should consider internal EGR and keep in mind that it would most likely decrease the efficiency rather than decreasing emissions.

2.6 CHP Systems

A suite of research projects was focused on development of CHP systems that use NG as the fuel, as part of the ARPA-E GENSETS program [7, 94]. The program target was to generate 1 kW of electrical power at high efficiencies for in-home power generation. In addition, these power sources can be used to develop heat used for domestic hot water, home heating, or other uses. The Environmental Protection Agency's (EPA) current CHP partnership supports the increased use of CHP systems due to the cost-effective emissions reduction they may provide. CHP systems benefit from dual stage energy utilization, such as electrical generation with waste heat being used for residential heating and hot water needs. Traditional (large-scale) electrical generation technologies have average efficiencies in the upper 30%. The average coal power plant efficiency in US was around 33%, while natural gas was 43% [95].

CHP systems however, are capable of achieving utilization factors (UF) over 80% [96]. Where UF is a ratio of both useful heat and work to the total heat energy (typically chemical fuel energy) supplied to the system. With an aim of developing efficient CHP systems, proper sizing of the heat-exchanging device relies heavily upon knowledge of the energy availabilities and the combined optimization of mechanical work and heat pathways.

Ondeck et al. introduced a framework for simultaneous optimization of the design and operating strategy of residential CHP systems to satisfy future power needs. They noted that new developments in small power generation were required [97]. Bianchi et al. developed guidelines for residential micro-CHP system designs, stressing the importance of proper sizing as a key factor for profitability and single family houses could allow for use of CHP systems that produce <5 kW of electricity [98].

Gokul et al. showed that further understanding of the need for highly efficient NG engines was found in a techno-economic analysis of CHP systems. The research showed the benefits of local power production from energy savings and emissions viewpoints. It is expected that if the CHP systems meet the ARPA-E GENSET program targets, CO₂, VOCs, CO, and NO_x emissions would also be reduced relative to conventional power plants [99].

Research was conducted on a microgeneration unit that produced 10 kW of electrical power – well above the power required for most residential applications. It focused on converting a diesel engine to NG and deploying advanced engine concepts such as the Atkinson cycle. Even with a larger, four-stroke engine with Atkinson operation, the overall electrical generation efficiency ranged from 24-31.5% [100]. Alternatively, Mikalsen et al. compared the Miller and Otto cycle for small NG engines for use in small-scale CHP systems. They showed that while the Miller cycle improved efficiency, it was at the cost of power density [101]. Honda demonstrated a 1.5 kW CHP system with an over expanded Atkinson cycle for improved thermal efficiency. Yanmar on the other hand presented a high efficiency unit with 5 kW output [102].

2.6.1 Energy Balance

CHP systems are well-defined by their electric efficiency and UF. To fully understand how to improve the design to target the highest UF with maximized electric efficiency, quantifying all energies associated with the system was necessary. As such, 1st and 2nd law analyses were

performed by researchers for different engine applications for similar purposes [103]. Li et al. performed a thorough energy analysis on a four-stroke engine with three different combustion regimes, two of which used NG fuels. They found that HCCI and RCCI operation with NG, demonstrated lower exergy destruction than conventional diesel combustion [104]. An energy balance was performed by Ausserer et al. on a small two-stroke engine and showed that brake power accounted for 13% of the total incoming fuel energy, while short-circuiting losses were 40-60%, and incomplete combustion was approximately 20% making it the second largest loss pathway [105]. Trattner et al. studied small, SI, two- and four-stroke engines up to 150 cc and outlined further possible loss pathways. Imperfect combustion, wall heat transfer, gas exchange losses, and mechanical losses were monitored. The study showed that heat losses were higher at throttled, part load operation as opposed to WOT operation [106]. Piecha et al. completed a detailed wall heat transfer analysis in addition to energy balance methods on a 46 cc two-stroke engine. They showed that the energy was split into 27% thermal exhaust, 19% unburned fuel, 19% effective or useful, 18% scavenging losses, 14% wall heat transfer, and 3% friction [107]. In other research, Orbaiz showed peak thermal efficiency for NG SI engines occurred during lean operation when in-cylinder heat loss and incomplete combustion were at a minimum [108]. Exergy balance simulations on larger scale CHP systems showed annual average exergetic efficiencies up to 62.8%. The results showed higher exergy recovery during warmer parts of the year [109].

Other energy and exergy balance research highlighted possible energy savings from advanced heat transfer designs. It was found the thermal barrier coating (TBC) improved thermal efficiency [110]. An exergy analysis examined impact of AFR and showed peak 1st and 2nd law efficiencies while operating slightly below equivalence ratio of 0.9 [111]. Ebrahimi and Koch examined the differences in the energy and exergy flow paths of SI engines compared to HCCI engines while designing a micro-CHP system for residential use. The work showed SI energy distributions of work output, exhaust losses, and heat transfer losses were all similar and in the range of 25-30% while incomplete combustion was between 5-10% depending on ignition advance [112]. Other areas of CHP research included simulation of the energy flow in a community pool of micro-CHP systems and how ambient temperatures affected the systems. Since the load of an individual micro-CHP unit was so small, they studied pooling of a large number of devices. This was considered necessary to provide services to the grid or to actively participate in electricity markets [113]. Note that my research focused on a single system independent of other CHP systems and the grid.

2.6.2 Fuel Quality Effects

A significant improvement in efficiency was observed with LPDI operation of a small two-stroke engine when compared to PI [61]. However, the effects of fuel composition on the CHP system viability were not explored. A change in fuel quality, could change the performance of the LPDI engine significantly.

In real applications, NG composition could vary both temporally and spatially. Also, widely available in the US for home heating applications is LPG and propane could potentially be used interchangeably with a NG system. Development of gaseous fueled products for use in multiple areas requires knowledge of sensitivity to fuel variations. Standard pipeline natural gas requires a minimum methane mole fraction of 75% [114–116]. Some companies have their own standards such as Union Gas where their natural gas will only vary in mole fraction from 87 to 96 % of methane in their supply region [117].

Methane number (MN) is the gaseous fuel equivalent of octane number. MN is a measure of the fuel's knock resistance, where a MN of 70 would correspond to equivalent knock characteristics as a mixture of 70% methane and 30% H_2 . Higher alkanes affect the combustion characteristics when utilized in an internal combustion (IC) engine. In a study examining fuel composition, ethane, propane, and butane were added separately into a known baseline NG blend. For all three additives, an increase in fuel energy density was counteracted by worsened knock resistance, lower fuel efficiency, and higher CO_2 emissions. This penalty was caused by required ignition retard [118].

Research was conducted on 5 different heavy-duty natural gas engines fueled with 8 separate fuel blends. Engine power was shown to increase slightly with decreased MN and increased Wobbe Index. For fuels with higher Wobbe Index the brake specific fuel consumption decreased [119]. The Wobbe Index is a measure of the interchangeability of fuel gases and their relative ability to deliver energy in combustion process. Another study found engine power was proportional to the Wobbe Index at WOT conditions [120]. Experiments conducted on a single cylinder SI engine examined the addition of 10-40% propane balanced with pure methane. It was found that increased propane content also increased IMEP, while it decreased the COV of IMEP and duration of combustion [121]. Methane and hydrogen mixtures have also been tested for SI engine power characteristics [122].

A study by Keith Bullin et al. in 2008 showed gas qualities from different reservoirs or even different wells of a single reservoir were variable. They studied multiple wells for different reservoirs including, Barnett, New Albany, Antrim, and Fayetteville shale gas. They showed that methane composition was as low as 27% in some wells. In Barnett shale gas for example, measurements showed that methane could vary from around 80% up to around 94% [85]. A summary of their findings is presented in *Table 2*.

Table 2. Natural gas quality from different reservoirs.

Shale Gas Reservoir	Methane [%]	Ethane [%]	Propane [%]	CO ₂ [%]	N ₂ [%]
Marcellus	79 to 95.5	3 to 16.1	1 to 4	0.1 to 0.9	0.2 to 0.4
Barnett	80 to 94	2.6 to 8	0 to 2.3	0.3 to 2.7	1 to 7.9
New Albany	87.7 to 92.8	0.8 to 1.7	0.6 to 2.5	5.6 to 10.4	-
Antrim	27.5 to 85.6	3.5 to 4.9	0.4 to 1	0 to 9	0.7 to 65
Fayetteville (avg)	97.3	1	0	1	0.7

2.6.3 Current Commercial CHP Systems

Currently, there are limited choices for commercial CHP systems for deployment at the home level [123]. One of the first was the Honda ECOWILL. Round robin research conducted on this current state-of-the-art micro-CHP prototype system showed 27.2% BTE from the driving IC engine with a total system UF of 74.5%. The total electrical efficiency was 23.5%. Other case studies that focused on the Honda technology showed an electrical efficiency of 22% [124]. The Honda technology used a four-stroke, NG engine that operated on an over expanded Atkinson cycle for improved thermal efficiency. Other commercially available systems typically have larger electrical power output capacity – for example Yanmar offers a 5 kW system [102]. Independent research on this unit was not verified but Yanmar advertised an efficiency of 28.3% with a UF of 85%. While some research has been completed, it is acknowledged that there is a critical gap in the literature surrounding performance data of 1 kW micro-CHP systems [125].

2.7 Emissions

Current downfalls of two-stroke engines include low efficiency and high fuel slip rates, which raise THC emissions. Most EPA regulations focus on gasoline engines in this displacement range and are applicable to stationary and handheld engines. For non-handheld engines under 66 cc (class

I-A), the EPA regulation for HC+NO_x is 50 g/kWhr and less. The same regulation applies to class IV handheld engines [126]. Fuel slip in NG engines is doubly important. First, due to their significant effect on fuel efficiency and second because of their combined greenhouse gas (GHG) effect. Methane's (CH₄) GHG effect is almost 25 times of CO₂ [127]. Catalysts could be implemented to reduce CH₄ emissions, but their CH₄ reduction efficiency is low [128]. According to CFR section 90, handheld and non-handheld engines are classified based on their displacement and their class defines the regulations for them as shown in *Table 3* [129]. The regulations applicable to engines examined in this work are bold.

Table 3. Engine classifications and regulations.

Engine class	Type	Displacement [cc]	HC+NO _x [g/kWhr]	NMHC+ NO _x [g/kWhr]	CO [g/kWhr]
Class I-A	non-handheld equipment engine	V_d < 66	50	-	610
Class I-B	non-handheld equipment engine	66 ≤ V _d < 100	40	37	610
Class I	non-handheld equipment engine	100 ≤ V _d < 225	16.1	14.8	610
Class II	non-handheld equipment engine	225 ≤ V _d	12.1	11.3	610
Class III	handheld equipment engine	V _d < 20	50	-	805
Class IV	handheld equipment engine	20 ≤ V_d < 50	50	-	805
Class V	handheld equipment engine	66 ≤ V _d < 100	72	-	603

2.8 Simulation of Two-stroke Engines

Most two-stroke engine simulations focused on simulating 3D geometries with CFD modeling of the in-cylinder phenomena. Fuel injection and 1D simulations were found to be limited. A CFD model showed that 10 bar liquid fuel injection benefitted fuel jet penetration by induced fuel air mixing and reduced short-circuited fuel. It also allowed for shorter injection duration, and wider range of SOI as compared to 3 or 5 bar operation [130]. However, it was noted that these benefits were at the expense of the energy needed to compress the fuel, which is typically a few percent of the fuel energy delivered to the engine. Another CFD study showed that an LPDI system should be placed in the cylinder wall to decouple injection timing from port timing. It was found that for

a high power output speed of 7500 RPM the injectors would be best placed opposite to the exhaust port in order to harness the flow of the scavenging process for mixing. It was also found that mixing was promoted by placing the injector at an angle toward piston crown at BDC and opposed to the scavenging flow [131]. In a follow up study, it was shown that the LPDI setup had superior efficiency, and reduced brake specific fuel consumption over PI and carbureted fuel systems. HC emissions were also reduced by factors of 3-8 depending on throttle position [132].

Yang et al. presented research on premixed, lean-burn, NG engine operation studying the effects on combustion instabilities and injection timing. CFD modeling showed that for lean NG mixtures at low load, there was a band of injection timing that produced unreliable mixture concentrations and poor flame kernel formation. Injection was best performed early or late – avoiding the 30 to 90 crank angle degrees (CAD) after top dead center (ATDC) region [133]. A CFD model of NG direct injection by Fan et al. found that burn rate increased by nearly 30% under an optimized injection strategy versus premixed fueling via the intake [134].

2.9 Review Summary

Based on literature review and GENSETS project's targets, I identified a primary path to achieve the program targets. Although the literature provides energy audits of two-stroke engines, when it comes to small displacement LPDI NG engines, none exist that offer an attractive pathway for local CHP applications. In addition, fuel variation effects were not addressed by literature. To investigate it, I tested three different NG compositions and propane. A full energy distribution analysis was required at every step to determine the energy efficiency improvements. This research - by combining literature review, experiments, 1D and 3D simulations - led to a framework for energy optimization of micro-CHP systems operating on gaseous fuels. **Table 4** presents the summary of path to improve the system's energy efficiency.

Table 4. Summary of engine evolution for higher efficiency.

Action	Method to Implement	Outcome
Baseline Conversion to NG	Experimental	An energy optimization framework for micro-CHP application driven by small two-stroke engines from literature review, experiments, data analysis, 1D simulation, and 3D simulation.
Air Handling (Intake and Exhaust)	Literature Review, Helmholtz theory formula, Experimental	
Low Pressure Direct Injection	Literature Review, Experimental	
Final System Level Optimization	1D simulation interface with genetic algorithm optimization, Experiments	
In-cylinder Optimization	3D CFD simulation of engine, Experiments	
Fuel Quality and CHP	Literature Review, Experimental, Data Analyses	

3 Methodology

3.1 Experiments

3.1.1 Laboratory

I assisted Dr. Derek Johnson in the development of a micro-engine laboratory specifically for research and development of small displacement engines under 3 kW. **Figure 3** shows a schematic of the laboratory setup. **Table 5** presents a detailed description experimental apparatus. Quality assurance (QA) of apparatuses was performed and data were recorded at low-frequency of up to 10 Hz (averaged for 1 Hz analysis). The research laboratory system is shown in **Figure 4**.

Figure 3. Setup schematic [135].

Table 5. List of laboratory apparatuses and their purposes [135].

Purpose	Tools	Memo
Ignition and Injection Control	Hardware: Microsquirt Open ECU Software: Tuner Studio	
Engine Brake Torque Measurement	Hardware: Magtrol HD-715 hysteresis load absorber and a DSP6000 dynamometer controller Software: Inhouse	HD-715 Maximum Torque: 55 in-lb Max Speed: 25000 RPM Accuracy: $\pm 0.25\%$ (full scale)
Exhaust Gas Concentrations	Hardware: MKS 2030 FTIR continuous gas analyzer. Software: MultiGas 2030	Measuring frequency: 5 Hz
Exhaust Oxygen Concentration	Hardware: 755-R Rosemount Paramagnetic Oxygen Analyzer Software: In-house	Range: 0-25 % oxygen Repeatability: $\pm 1\%$ of full-scale Zero and Span Drift: $\pm 1\%$ fullscale per 24 hours
Intake Air Flow Measurement	Hardware: HEISE PTE1 Pressure Calibrator along with HSQ-2 module, HSQ-1 module, and an eight standard cubic feet per minute (SCFM) laminar flow element (LFE) Software: In-house	HSQ1 (Pressure Difference) Range: 0-25 inch of H ₂ O Sensitivity: $\pm 0.002\%$ of span Repeatability: $\pm 0.02\%$ of span HSQ-2 (Absolute Pressure) Range: 0-30 PSIA Sensitivity: $\pm 0.002\%$ of span Repeatability: $\pm 0.01\%$ of span
Test room Temperature, Relative Humidity (RH), and Barometric Pressure	Hardware: Omega I-server environmental instrument Software: In-house	RH Accuracy: $\pm 2\%$ RH Repeatability: $\pm 0.1\%$ Temp. Accuracy: $\pm 0.5^\circ\text{C}$ for 5 to 45°C Pressure Accuracy: ± 2 mbar for 10 to 1100 mbar
In-cylinder Pressure Measurements	Hardware: Kistler Kibox data logger along with a 6054A piezoelectric pressure transducer Software: Kibox Cockpit	Range: 0- 300 bar Sensitivity: 13.4 pC/bar Sensitivity change: $\pm 2\%$ for 23 to 200 C Frequency: 312.5 kHz
Fuel Flow Measurement	Hardware: MC-20 series Alicat Mass Flow Controller (MFC) Software: In-house	Maximum Flow: 20 SLPM Accuracy: $\pm (0.8\% \text{ of Reading} + 0.2\% \text{ of Full Scale})$ Repeatability: $\pm 0.2\%$ Full Scale Operating Range: 0.5% to 100% Full Scale
Engine/Exhaust Temperatures	Hardware: k-type thermocouples along with an ICP device Software: In-house

Figure 4. Research laboratory system [135].

3.1.2 Design of Experiments

Engine design space, project's objectives, and literature review were the basis of design of experiments. A high-level summary of designed experiments is shown in *Table 6*.

Table 6. High-level overview of designed experiments.

Steps	Action	Observations/Considerations	Memo
1	Engine selection for 1kW limited to 30 mm stroke.		Research on a 30 cc engine, with four transfer ports (baseline engine). The engine used piston-controlled port timing crankcase compression (not reed valves).
2	Baseline Conversion to NG Operation	% fuel efficiency $\approx$ 7, DR $\approx$ 0.28, Brake Power $\approx$ 230 W	
3	Intake Optimization	fuel efficiency $\approx$ 10%, DR $\approx$ 0.53, Brake Power $\approx$ 500 W	
4	Exhaust Optimization (Multi-cone and double-cone)	fuel efficiency $\approx$ 13%, DR $\approx$ 0.9, Brake Power $\approx$ 870W	
5	Selected a similar engine with slightly higher displacement and modified scavenging strategies	fuel efficiency $\approx$ 16%, DR $\approx$ 0.85, Brake Power $\approx$ 1400W	34 cc engine with a rear boost port. Transferred the intake and exhaust optimization to the new engine (boosted engine). The new engine used reed valve induction for crankcase compression.
6	Retune the intake and exhaust for the new engine		
7	Low-Pressure Direct Injection	fuel efficiency $\approx$ 24%, DR $\approx$ 0.9	
8	1D modeling and exhaust resonator optimization with genetic algorithm with fine control of injection and ignition timing	fuel efficiency $\approx$ 26%	
9	Stratification investigation and optimize the spark plug location	fuel efficiency $\approx$ 27%	
10	Operate different fuels and detailed analysis on their effect on CHP system		

3.1.3 Engines

As stated in *Table 6*, two engines were used in this research. **Figure 5** shows both engine design overviews. Note that the boosted engine (left) was used for direct injection through final optimization. *Table 7* shows both engines' specifications. Note that the boosted engine had higher bore size, modified transfer ports, and added rear boost port. These combined with a reed valve, resulted in higher brake power output on the boosted engine, while maintaining the maximum stroke of 30 mm. Note that stroke limitations were imposed at a maximum of 30 mm based on

linear system design constraints beyond the scope of this research. The crankcase used for both engines were similar.

Table 7. Second experiment engine specifications.

	Baseline	Boosted engine		Baseline	Boosted engine
Number of	1	1	Number of ports	5	6
Type	2-Stroke	2-Stroke	Boost Port	No	Yes
Bore	34 [mm]	38 [mm]	Reed Valve	No	Yes
Stroke	30 [mm]	30 [mm]	Compression Ratio (Geometric)	Variable	12.76 (measured)
Connecting Rod Length	52 [mm]	52 [mm]	Compression Ratio (Effective)	Variable	8.15 (measured)
Induction	Naturally	Naturally	Exhaust Port Open	96 CAD	92 CAD ATDC
Displaced	30 [cc]	34 [cc]	Transfer Port Open	120 CAD	120 CAD ATDC

Figure 5. Baseline engine (right) and second (boosted) engine design (left).

3.1.4 Air Handling

Intake Optimization

Intake optimization was easy and quick to implement for experimental validation. Engelman's electrical analogy (Equations 1-3) was used to convert intake system (**Figure 6**) equivalent to capacitances and inductances.

$$\text{Inductance } (I) = \left(\frac{L}{A}\right) \quad \text{Eq. (1)}$$

$$\text{Capacitance } (C) = V \quad \text{Eq. (2)}$$

$$\omega_n = \frac{1}{\sqrt{IC}} = \sqrt{\frac{k}{m}} \quad \text{Eq. (3)}$$

Figure 6. Helmholtz resonator [136].

The natural frequency of the such an intake was calculated by Equations 4-6.

$$f_H = \frac{c}{2\pi} \sqrt{\frac{A}{L \times V}} \quad \text{Eq. (4)}$$

$$L = l + .3d = \text{effective length} \quad \text{Eq. (5)}$$

$$V_{eff} = \frac{V_d}{2} + V_{cl} \quad \text{Eq. (6)}$$

Where, V_d is swept volume, V_{cl} is the clearance volume, V_{eff} is the effective volume based on effective length L , and c is the speed of sound. The peak delivery ratio was expected to occur when the natural frequency of intake resonator was about twice the piston frequency.

Exhaust Optimization

A general design of an exhaust resonator is shown **Figure 7**. At exhaust port opening (EPO), high pressure gases will form a wave front that moves down the pipe. The first expansion inverts the positive pressure wave into a negative wave (suction wave). This is the function of first expansion in the exhaust resonator design, to improve scavenging [33]. This suction wave helps to clear burnt gas from the cylinder and draw the fresh charge through the transfer ports [33].

Figure 7. Exhaust suction wave [33].

The suction wave reflects from the nozzle-shaped section (convergent cone) to recharge the cylinder as the port closed (**Figure 8**). This improves trapping efficiency.

Figure 8. Reflected positive pressure wave to recharge the cylinder [33].

Exhaust tapered sections can be single cone or multi cones. The multi cones have the ability to tune the engine over a wider range of engine speeds when compared to single cone [37]. Two exhaust resonators were designed and manufactured using Helmholtz theory to target operation at 5400 RPM [59]. The baseline engine came with an off the shelf (OTS) exhaust design. **Figure 9** shows a double cone design for the exhaust resonator.

Figure 9. Double cone exhaust design.

Double cone exhaust design recommendation by literature was calculated from Equation (7) to (18) [33]:

$$L_T[in] = \frac{E_0[degree] V_s[\frac{ft}{s}]}{N(RPM)} \quad \text{Eq. (7)}$$

$$L_1 = L_T - \frac{L^2}{2} \quad \text{Eq. (8)}$$

$$L_2 = \frac{D_2}{2} \cot(A_2) \quad \text{Eq. (9)}$$

$$L_3 = D_1 \times 6 \quad \text{Eq. (10)}$$

$$L_4 = \frac{D_2 - D_1}{2} \cot(A_1) \quad \text{Eq. (11)}$$

$$L_5 = L_1 - (L_3 + L_4) \quad \text{Eq. (12)}$$

$$L_6 = \frac{D_2 - D_3}{2} \cot(A_2) \quad \text{Eq. (13)}$$

$$L_7 = D_3 \times 12 \quad \text{Eq. (14)}$$

$$D_1 = (1.1 - 1.15) \sqrt{\frac{4 \times A_{exhport}}{\pi}} \quad \text{Eq. (15)}$$

$$D_2 = \sqrt{6.25 \times D^2} \quad \text{Eq. (16)}$$

$$D_3 = D_1 \times (0.57 - 0.62) \quad \text{Eq. (17)}$$

$$V_s = \sqrt{\gamma R_i T_{exh}} \times 3.28 \left[\frac{ft}{m} \right] \quad \text{Eq. (18)}$$

E_0 is the exhaust open duration. A_1 and A_2 are 10 and 4.5 degrees respectively as recommended by literature for maximum delivery ratio and power [33].

Multi-cone resonator's design parameters were calculated based on Equation (19) to (35) [33] [18]:

$$D_0 = \sqrt{\frac{4 \times A_{exhport}}{\pi}} \quad \text{Eq. (19)}$$

$$D_1 = a_1 \times D_0 \quad \text{Eq. (20)}$$

$$a_1 = (0.0083 \times BMEP^2) - 0.1917 \times BMEP + 1.7 = 1.125 \quad \text{Eq. (21)}$$

$$L_1 = L_T \quad \text{Eq. (22)}$$

$$L_2 = 0.275 \times L_T \quad \text{Eq. (23)}$$

$$L_3 = 0.183 \times L_T \quad \text{Eq. (24)}$$

$$L_4 = 0.092 \times L_T \quad \text{Eq. (25)}$$

$$L_5 = 0.11 \times L_T \quad \text{Eq. (26)}$$

$$L_6 = 0.24 \times L_T \quad \text{Eq. (27)}$$

$$L_7 = L_6 \quad \text{Eq. (28)}$$

$$D_4 = 3.25 \times D_0 \quad \text{Eq. (29)}$$

$$\chi_1 = \left(\frac{L_2}{L_2 + L_3 + L_4} \right)^{1.5 \times \ln(D_4/D_1)} \quad \text{Eq. (30)}$$

$$\chi_2 = \left(\frac{L_2 + L_3}{L_2 + L_3 + L_4} \right)^{1.5 \times \ln(D_4/D_1)} \quad \text{Eq. (31)}$$

$$D_2 = D_1 \times \exp(\chi_1) \quad \text{Eq. (32)}$$

$$D_3 = D_1 \times \exp(\chi_2) \quad \text{Eq. (33)}$$

$$D_5 = D_4 \quad \text{Eq. (34)}$$

$$D_7 = D_6 = D_1 \quad \text{Eq. (35)}$$

Where *BMEP* in Equation (21) was calculated based engine speed of 5400 RPM and 1 kW brake power.

Figure 10 shows the OTS exhaust design and **Table 8** shows its dimensions. **Figure 11** shows two exhaust designs. The alpha was a multi cone diffuser and the beta was single cone diffuser.

Table 9 and **Table 10** show the dimensions for the two designs based on 5400 RPM frequency, exhaust port timing, and exhaust temperature form experiments.

Figure 10. OTS exhaust design.

Alpha Design

Beta Design

Figure 11. Both exhaust resonator models [59].

Table 8. OTS exhaust design dimensions.

Diameter/ Angle	Value	Length	Value [mm]
D ₁	25.4[mm]	L ₁	250
D ₂	50 [mm]	L ₂	50
D ₃	15.8 [mm]	L ₃	125
A ₁	14 [degree]	L ₄	50
A ₂	14 [degree]	L ₅	120.6

Table 9. Alpha exhaust design dimensions.

Diameter	Value [in]	Length	Value [in]
D ₀	0.63	--	--
D ₁	0.71	L ₁	4.89
D ₂	1.04	L ₂	13.43
D ₃	1.60	L ₃	8.94
D ₄	2.06	L ₄	4.49
D ₅	2.06	L ₅	5.37
D ₆	0.71	L ₆	11.72
D ₇	0.71	L ₇	11.72

Table 10. Beta exhaust design dimensions.

Diameter/ Angle	Value	Length	Value [in]
D₁	0.71 [in]	L₁	4.26
D₂	1.775 [in]	L₂	6.76
D₃	0.426 [in]	L₃	35.4
A₁	4.5 [degree]	L₄	3.82
A₂	7.5 [degree]	L₅	5.11

3.1.5 Injection Strategies and Control

To improve engine breathing and power density, the baseline engine was replaced with the custom boosted engine. The experimental methods of intake and exhaust tuning were then employed on this engine but peak BTE still remained low at only around 16%. Nearly 40% of the fuel energy was lost as slipped fuel. Thus, there was a need for direct injection but due to limitations on available pressures; we focused on application of LPDI for residential applications.

For NG engines, LPDI offered benefits over the fumigated or PI methods because both the fuel and air were gaseous and competed for intake charge volume. Due to this, LPDI may raise trapped mixture mass and reduce slip in two-stroke engines. Both options used relatively low injection pressures (<5 bar). PI occurred in either the intake or crankcase. For these injection locations, the fuel air mix communicated with the exhaust port for the entire duration. This led to high CH₄ slip, which contributed to lower efficiency and high GHG emissions. LPDI decreased the exposure of the fuel air mix to the open exhaust port, which decreased CH₄ slip. HPDI might present a unique solution, since the fuel never communicates with the open exhaust port but HPDI requires excessive compression power to use low-pressure NG available at residential applications. To target reduced compression work, this research focused on a semi-novel method to deliver low pressure natural gas directly to the combustion cylinder through the use of an outwardly opening poppet style injector to achieve LPDI. **Figure 12** and **Figure 13** show the modifications applied for LPDI research on the boosted engine.

Figure 12. Direct injection setup, showing relocation of the spark plug for LPDI (left), Port injection (right) [135].

Figure 13. Full engine CAD model (a) and LPDI experiment setup (b).

For LPDI to work in harmony with a tuned exhaust resonator, injection timing control parameters must be adjusted to optimal values. Also, there was an expected change in optimal spark timing due to operation with a more stratified mixture when compared to operation as homogeneous in the case of fumigation or PI.

3.2 Data Collection and Analysis

Data collection frequency was explained in *Table 6*. A set of data analyses was performed on the recorded data to track the system's behavior and for decision making. *Table 11* shows types of data analyses performed on experimental data.

Table 11. Summary of major data analyses from measurements.

Measured Parameters	Basic Calculations	Other Calculations
Fuel flow	BTE & Indicated thermal efficiency (ITE)	Energy Balance
Air flow	Delivery Ratio	Volumetric Efficiency
Temperatures	Exhaust Heat Energy	Energy Balance
Exhaust gas concentration	Exhaust Molar Flow Using Carbon Balance	Trapping Efficiency
In-cylinder Pressure	ITE, Combustion Phasing, IMEP	

3.2.1 Basic Analyses

Gas exchange parameters were used repetitively in my analyses. Three major gas exchange parameters in two-stroke engines are:

1. Delivery ratio (DR)
2. Trapping ratio (TR)
3. Volumetric efficiency (VE)

Delivery ratio was calculated by Equation 36:

$$DR = \frac{\text{intake airflow (SLPM)} + \text{Fuel flow (slpm)}}{V_d(L) \times N(rpm)} \quad \text{Eq. (36)}$$

V_d is the engine displacement. Note that since fuel was gaseous it was included in the delivery ratio calculations in this research both for PI and LPDI.

For PI, fuel trapping and air trapping ratios are equal. In LPDI however, these two are different:

$$TR_{air} = 1 - \frac{O_2 \text{ in the exhaust}}{O_2 \text{ in the intake}} \quad \text{Eq. (37)}$$

$$TR_{fuel} = 1 - \frac{HC \text{ in the exhaust}}{HC \text{ in the intake}} \quad \text{Eq. (38)}$$

Note that mass-based approach was used in this study for trapping ratio estimation.

VE is the amount of fresh charge trapped inside of the cylinder compared to maximum theoretical value based on V_d and with no boost pressure.

$$VE = TR \times DR \quad \text{Eq. (39)}$$

3.2.2 Detailed Energy Analysis for CHP Application

The first step for completing a detailed energy analysis was to calculate exhaust molar flow rate. This enabled for calculation of all energy pathways in addition to brake power.

The energy distribution was itemized as following:

1. Indicated Power ($\dot{W}_{indicated}$)
2. Exhaust Energy ($\dot{E}_{ex}$)
 - a. Exhaust thermal energy ($\dot{Q}_{ex}^{th}$)
 - b. Exhaust fuel energy ($\dot{E}_{ex}^{fuel}$) from slipped fuel
 - c. Exhaust unburnt content from CO and H₂ ($\dot{E}_{ex}^{ub}$)
3. Heat Loss and Blow-by ($\dot{Q}_l$)

Note that all HCs in the exhaust were considered as slipped fuel, because without a fast in-cylinder sampling system, it was impossible to distinguish slipped fuel from unburnt fuel. We did not have access to fast sampling instrument.

$$\dot{E}_{in}^{fuel} = \dot{Q}_l + \underbrace{\dot{Q}_{ex}^{th} + \dot{E}_{ex}^{HC} + \dot{E}_{ex}^{ub}}_{\dot{E}_{ex}} + \dot{W}_{indicated} \quad \text{Eq. (40)}$$

Indicated power was calculated by Equation (12):

$$\dot{W}_{indicated} = IMEP \times V_d \times N \quad \text{Eq. (41)}$$

where V_d is displacement volume, N is speed, and $IMEP$ is indicated mean effective pressure.

Exhaust thermal energy, $\dot{Q}_{ex}^{th}$, was determined by Equations (42-44) [137]:

$$\dot{Q}_{ex}^{th} = \dot{n}_{exh} \left[\frac{\bar{C}_{p,exh}(T_{exh}) + \bar{C}_{p,exh}(T_{in})}{2} \right] (T_{exh} - T_{in}) \quad \text{Eq. (42)}$$

$$\bar{C}_{p,i}(T) = a_{0,i} + a_{1,i}T + a_{2,i}T^2 + a_{3,i}T^3 \quad \text{Eq. (43)}$$

$$\bar{C}_{p,exh} = \sum v_i \bar{C}_{p,i} \left[\frac{kJ}{kmol K} \right] \quad \text{Eq. (44)}$$

The exhaust molar flow rate ($\dot{n}_{exh}$) was calculated by an iterative CFR carbon balance algorithm and molar fraction of components (v_i) were measured from the FTIR continuous gas analyzer and the oxygen analyzer. Note that maximum error in energy balance based on carbon balance results was 3%.

HC losses from the combination of fuel slip and unburnt HCs was determined by Equation (45-47):

$$HC \text{ Loss Rate} = \frac{\dot{E}_{ex}^{HC}}{\dot{E}_{in}^{fuel}} \quad \text{Eq. (45)}$$

$$\dot{E}_{ex}^{fuel} = \sum_{C_1}^{C_3} \dot{n}_{exh} v_{exh,i} LHV_i \quad \text{Eq. (46)}$$

$$\dot{E}_{in}^{fuel} = \dot{m}_{fuel} \times LHV_{fuel} \quad \text{Eq. (47)}$$

where $v_{exh,i}$, is the molar fraction of component ‘i’ in the exhaust. Note that for NG only components from C₁ to C₃ were considered. Combination of the fuel short-circuiting on LPDI and unburnt HCs, formed the total HC losses. $\dot{m}_{fuel}$, was known from measurements and LHV_{fuel} was calculated from fuel composition on molar basis.

The exhaust unburnt energy, $\dot{E}_{ex}^{ub}$, considered CO and H₂ from incomplete combustion and was derived from Equation (48):

$$\dot{E}_{ex}^{ub} = \dot{n}_{exh} \times (LHV_{CO} \times v_{CO} + LHV_{H_2} \times v_{H_2}) \quad \text{Eq. (48)}$$

where, v_{CO} is the molar fraction of CO in the exhaust. v_{H_2} was calculated based on following reaction:

Where,

$$K_{wg} = \frac{[CO][H_2O]}{[CO_2][H_2]} \quad \text{Eq. (50)}$$

With known molar fraction of CO, CO₂, and water (H₂O) from measurements, H₂ mole fraction was estimated assuming a constant K_{wg} value. The equilibrium constant depends on temperature. In most combustion analyses, a value of 3.5 is assumed for this constant, which was based on an average combustion temperature around 1750 °C from 1D simulation results [138]. This temperature was estimated using 1D engine simulations. The rate of reaction for this temperature was reported around 9×10^7 which meant the reaction was fast enough to consider it as equilibrium [139]. Even though the reaction in Equation (49) is similar to the water-gas shift

reaction equilibrium, the constant equilibrium 3.5 is not the accurate value of the K_{wg} at the measurement temperature. The value was selected from empirical data, which showed to have a reasonable correlation with actual data and combustion analyses. In most cases, low H_2 concentrations yielded minimal inaccuracies in this calculation [140].

The heat transfer and blow-by loss, $\dot{Q}_l$, was obtained by Equation (51).

$$\dot{Q}_l = \dot{W}_{indicated} + \sum \dot{H}_{products} - \sum \dot{H}_{reactants} \quad \text{Eq. (51)}$$

$$\dot{H}_i = \sum \dot{n}_i (\bar{h}_{f_i}^o + \bar{h}_i + \bar{h}_i^o) \quad \text{Eq. (52)}$$

Where $\dot{H}_i$ is the enthalpy rate, $\dot{n}_i$ is the molar flow rate, $\bar{h}_{f_i}^o$ is the enthalpy of formation, $\bar{h}_i$ is enthalpy at the experiment condition, $\bar{h}_i^o$ is the enthalpy at ambient condition for component i.

3.3 1D Simulations

1D models are very useful tools for design optimization due to their fast response and thus they are also good tools for system level optimization. For a 1D model to be more accurate, in addition to very accurate dimension inputs, many correlations must be deployed to make the model both simple and realistic. The core of my 1D model is as follows:

1. Appropriate geometry simplification.
2. Accurate dimension inputs.
3. Correlations to model a component in the model, e.g. reed valve.
4. Correlations to model a phenomenon, like combustion, heat transfer, and gas exchange.
5. Boundary conditions such as wall temperatures and environmental conditions.

Note that since 1D models solve the model iteratively, they are not sensitive to initial conditions as long as they are within a reasonable range. Implementing the right correlations requires

knowledge, experience, and engineering judgement in the specific application. In this research GT-Power™ was used as 1D simulation tool, allowing semi-dimensional system simulation. **Figure 14** shows the inputs to the model developed in this research.

Figure 14. Input variables to the 1D model from experimental data and system design.

3.3.1 Governing Equations

The flow model involved the solution of the Navier-Stokes equations, namely the conservation of continuity, momentum, and energy equations. These equations were solved in one dimension, meaning that all quantities were in the flow direction representing the cross section average values. There were two choices of time integration methods, which affected the solution variables and placed limitations on time steps. The time integration methods included an explicit and an implicit integrator. The primary solution variables in the explicit method were mass flow, density, and internal energy. The primary solution variables in the implicit method were mass flow, pressure, and total enthalpy.

The whole system was discretized into many volumes, where each flow split was represented by a single volume, and every pipe was divided into one or more volumes. These volumes were connected by boundaries. The scalar variables (pressure, temperature, density, internal energy,

enthalpy, species concentrations, etc.) were assumed to be uniform over each volume. The vector variables (mass flux, velocity, mass fraction fluxes, etc.) were calculated for each boundary. This type of discretization was referred to as a “staggered grid” (**Figure 15**).

Figure 15. Schematic of staggered grid approach: scalars calculated at centroid, vector quantities at boundaries [141].

The conservation equations solved include[141]:

Continuity:
$$\frac{dm}{dt} = \sum \dot{m}_{boundaries} \quad \text{Eq. (53)}$$

Momentum:
$$\frac{d\dot{m}}{dt} = \frac{dpA + \sum \left[(\dot{m}u) - 4C_f \frac{\rho u |u|}{2} \frac{dx A}{D} - K_p \left(\frac{1}{2} \rho u |u| \right) A \right]_{boundaries}}{dx} \quad \text{Eq. (54)}$$

Energy:
$$\frac{d(me)}{dt} = -p \frac{dV}{dt} + \sum \left[(\dot{m}H) - hA_s(T_{fluid} - T_{wall}) \right]_{boundaries} \quad \text{Eq. (55)}$$

(Explicit Solver)

Enthalpy:
$$\frac{d\rho HV}{dt} = \sum \left[(\dot{m}H) + V \frac{dp}{dt} - hA_s(T_{fluid} - T_{wall}) \right]_{boundaries} \quad \text{Eq. (56)}$$

(Implicit Solver)

Where:

$\dot{m}$	boundary mass flux into volume, $\dot{m} = \rho Au$
m	mass of the volume
V	volume
p	pressure
ρ	density
A	cross-sectional flow area
A_s	heat transfer surface area
e	total specific internal energy (internal energy plus kinetic energy per unit mass)
H	specific enthalpy, $H = e + \frac{p}{\rho}$

h	heat transfer coefficient
T_{fluid}	fluid temperature
T_{wall}	wall temperature
u	velocity at the boundary
C_f	Fanning friction factor
K_p	pressure loss coefficient (commonly due to bend, taper or restriction)
D	equivalent diameter
dx	length of mass element in the flow direction (discretization length)
dp	pressure differential acting across dx

A single pipe part can be discretized into multiple sub-volumes, which provided a calculation of pressure at multiple locations at each time step. This better resolved the pressure distribution along the length of the pipe. Note that for the explicit flow solver, the time step required by a pipe was proportional to the discretization length. Smaller discretization lengths may result in longer run times due to smaller time steps as well as the fact that the solver has to calculate the solution at more locations [141].

$$\Delta t \propto \frac{\Delta x}{c + |u|} \quad \text{Eq. (57)}$$

where Δt is the time step for the explicit flow solver only (implicit solver time step is user-imposed), Δx is the pipe discretization length, c is the fluid speed of sound, and u is the fluid velocity. In this research, the explicit solver was used and the time step was calculated for each iteration based on minimum Δx and previous step's values for c and u .

3.3.2 Reed Valve Model

Reed petals were the most critical variables that affected the inflow and their operation was a function based on stiffness, flow area, and engine frequency. They were modeled as single-side supported beams that opened based on pressure difference and exposed area on each side (**Figure 16**). The Young's Modulus of the reed petals was measured experimentally in one of WVU's Strength of Material Laboratories as shown in **Figure 17** using a 20KN SHIMADZU tensile test machine. Experiments were performed using a tensile test cell which measured the force versus petal deflection to export the Young's Modulus for simulations.

Figure 16. Single-side supported beam deflection.

$$\delta_{max} = \frac{Pl^3}{3EI} \quad \text{Eq. (58)}$$

With known values of length (l), force (P), and maximum deflection (δ_{max}) from experiments and known moment of inertia (I) from petal geometry, the Young's Modulus was determined experimentally and used as an input within the 1D simulations.

Figure 17. Young's Modulus measurement experiments (left) and experimental results (right).

The GEM3D tool within GT-Power™ was used to convert complicated internal volumes into equivalent 1D components. This was achieved since a 3D scan of the cylinder and all the internal volumes was available. These simplifications were performed for the boost port, transfer ports, exhaust manifold, and reed valve internal volumes. This conversion led to proper geometry, considering the proper volumes, surface areas, inlet and outlet areas, flow area changes from inlet to outlet, inlet and outlet angles, and discharge coefficients. **Figure 18** shows the simplification of

the reed valve body to a 1D component. Notice that the area and angle of boundaries are very critical to achieve a more accurate split model.

Figure 18. Reed valve body simplification to a flow split element.

The port windows' shapes and timings were also accurately extracted from the 3D cylinder scan and final experimental assembly by accurately measuring the clearance height. Exhaust geometry was accurately measured from the experimental setup and imported to the model.

3.3.3 Boundary Conditions

Most boundary conditions for this model were thermal boundaries from the intake through the exhaust. These were imported or estimated from experimental results. Two other boundaries were environmental boundaries of pressure and temperature, measured by an environmental sensor.

Figure 19 shows the complete system model including intake, reed valve, engine, and exhaust resonator sub models.

Figure 19. 1D model in GT-Power™.

Baseline Validations

Calibration of the engine model was divided in two major steps: combustion model calibration and full engine model calibration.

Combustion Model Calibration

To isolate combustion from other errors associated in the full engine model, removal of the intake and exhaust systems when intake, exhaust, and cylinder pressures were available is common. This was a twostep process. First, the model was evaluated in the three-pressure analysis mode to accurately estimate the volumetric efficiency and trapping efficiencies, which were later used for combustion calibration. Note that in this study, the trapping ratio was estimated by measuring oxygen content in the exhaust and following formula:

$$\eta_{tr} = 1 - \frac{O_{2_{exh}}}{O_{2_{intake}}} \quad \text{Eq. (59)}$$

However, there are uncertainties associated with measurements especially in lean operations. GT-Power™ offeres a solution for estimating trapping ratio initial conditions for combustion calibration models. It had the ability of operating the model in analysis mode where the combustion sub model was completely turned off. Instead, in cylinder, exhaust and intake pressure curves versus crank angle for one cycle were provided for the model. Such a model is called a three-pressure analysis (TPA) model. With intake and exhaust average temperature provided in analysis mode, GT-Power™ artificially imposed a heat release to match the simulated cylinder pressure curve with the experiment. This allowed the 1D model solution based on experimental pressure curves and enabled calculation of all gas exchange parameters, including trapping ratio. In addition, initial burnt mass fraction needed for combustion calibration was calculated with the TPA model. As shown in **Figure 20**, a modified model was developed, and three pressure curves were used as inputs from experiments. The model attempted to impose an artificial combustion object that simulated the combustion and finally estimated the performance based on experimental data and geometry setup in the model. These included gas exchange properties and compositions.

*** Each curve is average of 200 cycles recorded in the experiments**

Figure 20. Three pressure analysis (TPA) model.

A predictive combustion model was then used for combustion calibration. The model attempted to estimate turbulent flame speed and match the heat release curve and consequently the pressure curve. A different model was developed for combustion calibration and it included only the cylinder, injector, and crank-train as shown **Figure 21**. Running the model in calibration mode allowed for exclusion of the intake and exhaust systems. Alternatively, volumetric efficiency, trapping ratio, and burnt gas fraction at the start of the cycle, were calculated from the TPA model and input to this model. **Table 12** presents the major inputs to the combustion calibration model and their source. As shown in **Table 12**, there were four calibration parameters.

Figure 21. Model for combustion calibration.

Table 12. Combustion calibration model inputs and parameters.

Categories	Objects	Source of data
Initial State	Volumetric Efficiency	Three Pressure Analysis Model
	Trapping Ratio	
	Residual Gas Fraction	
	Fuel Composition	Experiments
Wall Temperatures	Liner	Estimate from Experiments
	Head	Estimate from Experiments
	Piston	Estimate from Estimation
Heat Transfer	Woschni	Heat transfer multiplier is calibrated before and after combustion calibration
Combustion	Dilution Effect Multiplier	Calibration Parameter
	Flame Kernel Growth Multiplier	Calibration Parameter
	Turbulent Flame Speed Multiplier	Calibration Parameter
	Taylor Length Scale Multiplier	Calibration Parameter
Flame Object	Spark plug location	Taken from geometry, it affects the flame speed and combustion duration
	Head and piston Geometry	Taken from geometry and used to estimate the gas motion inside of the cylinder

Calibration was performed by minimizing the root mean square error (RMSE) between measured and predicted pressure curves. **Figure 22** shows an example of the difference between simulated and measured curves before calibration. The target was set to minimize the RMSE between simulated and all measured curves provided for calibration.

Figure 22. Pressure curve of an uncalibrated combustion versus measured curve.

Calibration was achieved using a genetic algorithm (GA) setup, where the objective was to minimize the RMSE between measured and simulated results. Factors were calibration parameters, which were varied by the GA platform. Engine speed of 5400 RPM was selected for optimization to match with experiments. The minimization of RMSE between measured and predicted curves was performed for all the selected data points and the best set of parameter values were selected.

For the validation of the full engine model with the intake and exhaust, the validation of air flow and crankcase pressure was completed using motored data. This model included the full intake, reed valve, cylinder, and exhaust resonator geometries as shown in **Figure 19**. That led to matching the compression side of the in-cylinder pressure curve. Note that in the motoring model there was no combustion. Secondly, calibrated combustion parameters were applied to the full model to validate the combustion pressure curve.

3.3.4 Exhaust Resonator's Genetic Algorithm Optimization

The calibrated model was used to perform a GA optimization on the exhaust resonator design. The baseline exhaust design in the model was the beta design presented in **Figure 11**. The beta design was used for all the experiments before GA optimization. **Figure 23** shows the parametric schematic of the baseline exhaust design. The best results (given that L_3 was adjustable) were determined experimentally and were presented in *Table 13*.

Figure 23. Baseline exhaust with geometric parameters labeled.

To assign a reasonable objective for the optimization problem required definition of the main function of the exhaust resonator. Exhaust resonators have two functions, (1) controlling the delivery ratio as defined by the divergent cone and (2) controlling the trapping ratio as defined by the straight section length (L_3) and the convergent cone.

For the following reasons, maximization of the engine's indicated efficiency was selected as the optimization objective. In crankcase compression two-stroke engines, unlike four-stroke engines, cylinder indicated efficiency is not equal to engine indicated efficiency. This was due to additional pumping losses imposed by the crankcase compression. Engine indicated efficiency considered the pumping loss associated with crankcase compression as well as the increased volumetric efficiency.

Table 13 shows the range of variable parameters that defined the design space for the optimization problem. These values were selected based on experience with the exhaust resonator experimental results and good engineering judgement from rules of thumb presented in literature [12] [33] [10].

The number of designs in each generation was selected to be 20 and the maximum number of generations was 50, which yielded up to 1000 design points.

Table 13. Optimization target and design space.

Target	Maximum Engine Indicated Efficiency		
Variable	Baseline value [mm]	Lower Limit	Upper limit
D₁	15	13	21
D₂	45	35	65
D₃	10.5	8	15
L₁	41	20	80
L₂	167	100	250
L₃	818 (Adjustable in experiments)	650	1000
L₄	127	70	190

3.4 3D CFD Simulation

The core components of the CFD study used in this research are as follows:

1. Extracting and cleaning the geometry
2. Defining regions (Cylinder, Crankcase and exhaust)
3. Implement the proper equations to solve in the active domain
4. Grid control with fixed embedding and adaptive mesh refinement (AMR), where higher resolution was required such as around the spark plug at the experimental spark timing.
5. Proper initialization
6. Boundary conditions.

3.4.1 Engine Geometry

In two-stroke engine modeling, to consider the most realistic scavenging, in addition to the cylinder, the engine crankcase was also included into the simulations. This enabled consideration of the cylinder's upstream pressure caused by crankcase compression. **Figure 24** (a) shows the main geometry regions of the CFD model while **Figure 24** (b) shows the transparent fluid domain.

Figure 24. (a) Main geometry regions (b) transparent fluid domain showing piston, connecting rod and crank and reed petal locations.

3.4.2 CFD Model Boundaries

Intake Boundary

To reduce simulation time, instead of modeling the physical reed petals, a reed valve flow rate was assigned to the boundaries. This flow rate was obtained from the verified 1D model of the system. Any error from 1D simulation was removed by integrating the mass flow curve and scaling it to match the experimental manifold air mass flow measurements. Note that a constant flow rate would not be an appropriate approach, because it affected the crankcase pressure. **Figure 25** shows the mass flow rate through the reed valve over the course of a single cycle which was an output of a calibrated 1D model.

Figure 25. Reed valve flow rate profile from verified 1D simulation results.

Exhaust Boundary

Due to presence of the exhaust resonator on the engine setup, a traveling wave caused pressure fluctuations at the exhaust port. These fluctuations were important because they affected the scavenging process and the final trapped mass inside of the cylinder. A high frequency piezo-resistive pressure sensor measured the exhaust pressure and that was assigned as the exhaust boundary conditions in the CFD simulation. Note that the exhaust pressure sensor location in experiments and exhaust boundary location in the CFD model were matched. **Figure 26** shows exhaust pressure near the exhaust port.

Figure 26. Exhaust boundary conditions from experimental measurements, an average of 200 recorded cycles.

Moving Boundaries

The piston had three moving boundaries interacting with different regions. The piston top interacted with the in-cylinder region. The piston skirt interacted with the cylinder wall and ports. The piston bottom interacted with the crankcase regions. The connecting rod and crankshaft were included in the crankcase region and defined the piston motion.

Thermal Boundaries

All walls in the system were considered to have a fixed temperature and it was estimated from the experimental results. **Table 14** presents the thermal boundary conditions.

Table 14. Thermal boundaries estimated from experimental results.

Wall Type	Temperature [K]
Cylinder Wall	450
Cylinder Head	550
Piston Top	550
Piston Skirt	450
Piston Bottom	400
Exhaust manifold	650
Crankcase, connecting rod and crank	400

3.4.3 CFD Model Initialization

Since the model solved only one cycle, a proper initialization was needed for accurate results. A pressure and temperature initialization were needed for each region, see **Table 15**. The model had three defined regions: cylinder, crankcase, and exhaust. For initialization, a combination of experimental and numerical data were provided. Temperature initialization was completed mostly with 1D modeling results while pressure initialization was from experiments.

Table 15. Initialization table for combusting engine.

Region	Parameter	Value at Simulation Start (EPO) [Unit]	Source
Cylinder	Pressure	458 [kPa]	Experiments
	Temperature	1250 [K]	1D modeling
Crankcase	Pressure	130 [kPa]	Experiments
	Temperature	360 [K]	1D modeling
Exhaust Manifold	Pressure	94 [kPa]	Experiments
	Temperature	648 [K]	1D modeling

3.4.4 Governing Equations

The dynamics of fluid flow were governed by equations that described the conservation of mass, momentum, and energy. Additional equations described turbulence and the transport of passive scalars and species. **Table 16** shows summary of the proper solver options for different equations.

Table 16. Solver options.

Equation	Description	Solved Variables
Mass	Conservation of Mass	Total mass in regions
Momentum	Conservation of Momentum	Pressure and velocity
Energy	Conservation of Energy	Pressure and temperature
Species	Species mass fraction in each region (Stratification)	Mass fraction
Passives	Monitor the flow motion and scavenging	Not affecting the solution
Turbulence	Monitor Mixing	TKE, Dissipated energy

Mass and Momentum Transport

The compressible equations for mass transport and momentum transport are given by Eq. (60-62):

$$\text{Mass} \quad \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = S \quad \text{Eq. (60)}$$

$$\text{Momentum} \quad \frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} + S_i \quad \text{Eq. (61)}$$

$$\text{Viscous stress tensor} \quad \sigma_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \left(\mu' - \frac{2}{3} \mu \right) \left(\frac{\partial u_k}{\partial x_k} \delta_{ij} \right) \quad \text{Eq. (62)}$$

In the above equations, u is velocity, ρ is density, S is the source term, P is pressure, μ is viscosity, μ' is the dilatational viscosity (set to zero), and δ_{ij} is the Kronecker Delta. Note that if a turbulence model (e.g., k-e) was activated, the viscosity was replaced by the total viscosity, which is given by Equation (63):

$$\mu_{tot} = \mu_{mol} + C_\mu \rho \frac{k^2}{\varepsilon} \quad \text{Eq. (63)}$$

where μ_{mol} is the molecular viscosity, C_μ is a turbulence model constant, k is the TKE, and ε is the turbulent dissipation.

Equations (60 and (61) both allowed for source terms. For the momentum equation, the source terms can arise from, for example, gravitational acceleration, spray coupling, or mass sources. For the mass conservation equation, the source term may arise from evaporation or other sub models. The momentum equation was solved in finite volume form. When solving the momentum equation, conserved values at the face were expressed in terms of primitive values at the cell center.

The pressure-velocity coupling was achieved using a modified Pressure Implicit with Splitting of Operators (PISO) method of Issa (1986) [142]. The PISO algorithm was implemented with a predictor step where the momentum equation was solved. After the predictor, a pressure equation was derived and solved, which led to a correction, this was then applied to the momentum equation. The process of correcting the momentum equation and re-solving can be repeated as many times as necessary to achieve the desired accuracy which was set to 0.001 in this study. This was equivalent of 0.1% variation between iterations. After the momentum predictor and first corrector step were completed, the other transport equations were solved in series. Momentum and mass transport can be solved for compressible or incompressible flows. For compressible flows, an equation of state was required to couple density, pressure, and temperature. CONVERGE contains several equation of state options: ideal gas, Redlich-Kwong, Redlich-Kwong-Soave, and Peng-Robinson. In this research, gas was solved as compressible and the Redlich-Kwong equation of state was used which is formulated as Equation (64) [143]:

$$p = \frac{RT}{V_m - b} - \frac{a}{\sqrt{T}V_m(V_m + b)} \quad \text{Eq. (64)}$$

where p is the gas pressure, R is the gas constant, T is temperature, V_m is the molar volume (V/n), a is a constant that corrects for attractive potential of molecules, and b is a constant that corrects for volume. The constants are different depending on which gas is being analyzed. The constants can be calculated from the critical point data of the gas by Equation (65-66).

$$a = 0.42748 \frac{R^2 T_c^{2.5}}{P_c} \quad \text{Eq. (65)}$$

$$b = 0.08664 \frac{RT_c}{P_c} \quad \text{Eq. (66)}$$

where, T_c is the temperature at the critical point, and P_c is the pressure at the critical point and they were 133 K and 3.77 MPa, respectively.

Passive and Scalar Transport

Scalar quantities may be passive or non-passive. This differentiation was drawn due to the form of the convergence criterion for the PISO algorithm. A passive scalar was a calculated quantity that did not directly affect the calculation of the temperature or the gas constant.

The compressible form of the passive scalar transport equation is given by

$$\frac{\partial \rho \phi}{\partial t} + \frac{\partial \rho u_j \phi}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\rho D \frac{\partial \phi}{\partial x_j} \right) + S \quad \text{Eq. (67)}$$

where u is velocity, ρ is density, D is the diffusion coefficient, S is the source term, and ϕ is a passive scalar. The diffusion coefficient is given by

$$D = \frac{\nu}{Sc} \quad \text{Eq. (68)}$$

where Sc is the Schmidt number, which can be defined for each passive individually.

3.4.5 Grid Control

The grid started with a base value. The two type of mesh refinements have been added to the simulation: fixed embedding and adaptive mesh refinement (AMR). Fixed embedding are those types that refine the mesh in the simulation regardless, while with AMR, depend on the gradient the parameter defines in AMR, it may or may not refine the mesh during the simulation. The simulation was run on WVU's Spruce Knob supercomputer network.

3.4.6 CFD Study Objectives

The objective of the CFD analysis was to examine charge stratification, especially around ignition timing, to determine the optimal location for the spark plug to enable lean combustion for improved efficiency. In addition, CFD results were qualitatively compared to experimental data.

4 Results and Discussions

4.1 Empirical Optimization on PI

4.1.1 Intake Optimization

Delivery ratio and power density

Intake length, diameter, and crankcase volume were translated into the frequency of the installed Helmholtz resonator. On the peak of tuning, the resonator's frequency was calculated as 185 Hz, which was almost twice the piston frequency (5400 RPM or 90 Hz). **Figure 27** shows that delivery ratio increased from 0.28 to about 0.52. This led to a change brake power from 0.22 to 0.5 kW – an increase by a factor of 2.27 as shown in the left of **Figure 27**.

Figure 27. Delivery ratio and power increased as length decreased to the target length, which yielded a tuned frequency of 185 Hz.

Combustion Stability

Higher fresh charge trapped inside the cylinder from intake tuning led to higher heat release per cycle and improved combustion stability. In addition, with higher trapped mass, stronger turbulences were created at smaller scales, which likely helped to create a faster flame front, thus causing combustion to be more stable. In general, turbulences tend to make the flame front more corrugated which inhibited growth of instabilities [144]. **Figure 28** shows the COV of IMEP for different intake lengths.

Figure 28. Combustion stability as defined by the coefficient of variation (COV) of IMEP for varied intake lengths.

4.1.2 Exhaust Optimization

Delivery Ratio and Power

Figure 29 shows further increases in delivery ratio for the alpha and beta exhausts as compared to the OTS exhaust. While the engine with the OTS exhaust showed delivery ratio of around 60%, the alpha and beta exhausts on average had delivery ratios of 95% and 85%, respectively. The alpha design used a longer multi-cone design for the diffuser (divergent cone) when compared to the beta. It created a stronger suction wave that pulled more gas out of the cylinder and resulted into a higher delivery ratio – but not necessarily a higher trapping efficiency.

Figure 29. Delivery versus AFR for all exhausts with a tuned intake.

Power density, which is directly related to the delivery ratio, was mostly affected by the divergent section as shown in **Table 17**. The divergent section of the OTS exhaust was the shortest which did not create a strong suction wave and led to the lowest delivery ratio. In addition, the lead pipe cross section area was larger than the exhaust port area, causing thermodynamic irreversibility from the sudden expansion. This was eliminated as much as possible (machining and component limitations) for the alpha and beta designs. The beta design showed the highest power output around a lambda of 1 - 55% higher than OTS exhaust. The alpha exhaust showed slightly lower power than the beta exhaust, but still 50% higher than OTS exhaust. Each case of **Table 17** corresponds to the AFR in figures and they follow the left to right trends.

Table 17. Maximum brake power output in kW for all exhaust configurations with a tuned intake.

Case	1	2	3	4	5	6	7
Beta	0.95	0.96	0.96	0.91	0.85	0.76	0.71
Alpha	0.85	0.92	0.93	0.91	0.87	0.81	0.74
OTS	0.35	0.54	0.60	0.62	0.62	0.59	0.51

Efficiency

Figure 30 presents the BTE for the different exhaust configurations with the tuned intake. The beta design showed the highest efficiency over a broad range of AFR. Around stoichiometric

operation, the OTS design showed higher efficiency compared to the alpha, but in rich and lean zones the alpha design showed better efficiencies. The alpha design yielded lower efficiency than the beta exhaust because of its longer diffuser section and lower trapping efficiency.

Figure 30. Efficiency as a function of air-fuel ratio.

4.1.3 Combustion Chamber

The combustion dome was modified to reduce sharp edges and squish volume. *Table 18* presents the results from the OTS and redesigned combustion chamber. The chamber geometry did not affect the delivery ratio; however, it improved the power output and efficiency by 10.4% and 8.8%, respectively. These data were collected with stoichiometric AFR, MBT timing, tuned intake, and the beta exhaust design.

Table 18. Results of combustion dome design change with optimized intake and exhaust.

	Lambda [-]	Power [kW]	BTE [%]	IMEP [bar]	Delivery ratio [%]
New Head	0.97	1.06	13	4.6	89
OTS Head	0.99	0.96	11.95	4.3	85

The power was not high enough to compensate the generator and friction losses and provide at least 1 kW of power. In addition, BTE was quite low with this engine, so a new engine was

selected. The new engine retained the same stroke but had a larger bore, included custom porting, added boost port, and used reed valve in hopes to further increase delivery and trapping efficiency.

4.2 LPDI

From this point forward, all the experimental results are from the second generation engine, identified as the boosted engine. Note that all of the intake and exhaust optimization work was transferred from baseline engine to the boosted engine using the same proven approaches. Also, when selecting the boosted engine, it was confirmed that the combustion chamber had a proper dome shape as this was previously showed to further increase efficiency in the baseline engine. The custom engines were provided by O'Neill Brother's Racing located in California.

Table 19 shows the summary of experimental conditions for migrating from PI to LPDI. After the LPDI was enabled to work with proper injection timing, it was observed that exhaust resonator's length needed to be readjusted. While injection pressure in PI operation was around 0.5 bar, on LPDI it was around 2 bar. The initial experimental study examined the effect of injection timing on engine performance. Then the effect of engine speed on LPDI operation was investigated. Engine performance parameters were compared for all cases. Note that for MBT ignition timing, a spark sweep test was performed for each case to find the MBT timing.

Table 19. PI and LPDI test conditions summary.

Variable	Setting		
Ignition	MBT		
AFR	12 -18		
Engine Speed on PI (N)	5400 RPM		
Engine Speed on LPDI (N)	4200, 4800, 5400, 6000 RPM		
Exhaust Resonator Length on PI	81.3 [cm]		
Exhaust Resonator Length on LPDI	69.9 [cm]		
Cylinder Head Temperature	130 °C		
Fuel	Natural Gas		
	C ₁ = 90.5 %	C ₂ =5 %	C ₃ =2.6 %
SOI of the PI test	90 CAD ATDC		
SOI on preliminary LPDI test	180,190,200,210 CAD BTDC		
SOI on engine LPDI engine speed	180 CAD BTDC		
Injection Pressure on LPDI	3 [bar]		
Injection Pressure on PI	<0.5 [bar]		

4.2.1 LPDI Operation and SOI effect

Moving to LPDI operation required less fuel and resulted in higher air mass flow when compared to PI. Higher fuel trapping ratio compared to air trapping ratio, made the AFR calculated from intake air mass flow appear higher than trapped AFR. For this reason, I chose to create a modified AFR parameter called λ^* . It is defined as follows:

$$\lambda^* = \frac{\dot{m}_{air}/\dot{m}_{fuel}}{AFR_{stoich}} \quad \text{Eq. (69)}$$

Note that λ^* was calculated based on total intake air flow and total injected fuel. For PI this value was equal to trapped lambda whereas in LPDI this value is higher than trapped lambda. Note that due to air short circuiting and contamination of two-stroke lubricating oil, a typical lambda sensor was not a reliable device to monitor in-cylinder lambda. One accurate way to measure the in-cylinder lambda could be using a fast sampling instrument which was not available in our experimental setup.

We used an alternative approach to sweep the rich to lean operating range in our experiments. Exhaust CO and COV of IMEP were monitored in all LPDI tests, where high CO content in the exhaust was an indicator of in-cylinder rich operation and increasing COV of IMEP at the lean limit was an indicator of passing the stoichiometric zone as shown in **Figure 31**. The bottom of the valley was assumed the stoichiometric region while the left side was considered rich and right side was lean operation. So, λ^* for LPDI is not the in-cylinder λ , but this approach was taken to cover the rich to lean operation range.

Figure 31. CO and COV of IMEP valley.

Figure 32 shows the delivery ratio for PI and LPDI with varied SOI. During PI operation, fuel displaced around 10% of the intake charge volume which was then available to air during LPDI and promoted an increased delivery ratio. Hence LPDI had higher trapped mass and higher in-cylinder peak pressures. As shown in **Figure 33**, conversion to LPDI increased maximum peak pressure from about 28 bar to 36 bar – or by 28.6%. This was important since it enabled the exhaust resonator to draw in more charge through the cylinder and additionally increase the delivery ratio. The SOI of 180 CAD BTDC showed the highest peak pressure in general which translated to the highest trapped fuel compared to other injection timings. This is doubly confirmed from efficiency results later in this section. Heat release curves in **Figure 34** show that the SOI of CAD 180 BTDC had the highest heat release rate in a cycle.

Figure 32. Delivery ratio on PI and LPDI running on different SOI, each point is averaged value for 90 seconds of steady state operation.

Figure 33. Peak pressure for PI and LPDI by varying the SOI, each point is averaged over 200 cycles on PI and LPDI operations.

Figure 34. Rate of heat release for PI and LPDI by varying SOI, each curve was averaged over 200 recorded cycles at steady state operation.

Figure 35 presents the average IMEP for PI and LPDI with varied SOI. LPDI yielded higher trapped fuel and thus showed higher power density. The peak IMEP was 4.7 bar, for LPDI at a SOI of 180 CAD BTDC. This was 23.7% higher than the peak value for PI. As shown in **Figure 35**, in all but three cases which were lean, LPDI operations showed higher IMEP when compared to PI. Lower IMEP in those cases was due to combustion instability caused by charge stratification.

Figure 35. IMEP averaged over 200 cycles on PI and preliminary LPDI operations vs λ^* .

Charge stratification was of the biggest concerns when operating on LPDI. It caused unstable combustion near lean limits as shown **Figure 36**. To understand mixture stratification for the LPDI case, a CFD study was required and performed later in this research. For LPDI operation with SOI of 180 CAD BTDC, a COV of less than 10% was achieved for λ^* less than 1.7. Some literature recommends an acceptable threshold of 10% for the COV of IMEP [19], while recently this criteria has been reduced to 5% by industry [61].

Figure 36. COV of IMEP averaged over 200 cycles on PI and initial LPDI operations vs λ^* .

In line with combustion instability, combustion duration increased for unstable combustion cases as shown in **Figure 37**. Combustion duration was defined by the CAD from 10% mass fraction burned (MFB) to 90% MFB. The earliest SOI showed decreased combustion duration likely due to lower fuel trapping and power density. For the best case of SOI of 180 CAD BTDC, and with λ^* ranging from 1.4-1.5 similar combustion durations were observed for both PI and LPDI.

Figure 37. Combustion Duration averaged over 200 cycles on PI and initial LPDI operations vs λ^* .

Indicated efficiency is shown in **Figure 38** for PI and LPDI with varied SOI. The higher fuel trapping ratio was the major reason for the significant increase in efficiency between fueling configurations. It was found that a SOI of 180 CAD BTDC provided peak efficiency. Earlier SOI led to increased fuel slip in the scavenging flow before exhaust port closing (EPC).

Figure 38. Indicated thermal efficiency on PI and LPDI, averaged over 90 seconds steady state operation for each point vs λ^* .

To investigate the difference in slipped HC in the exhaust, **Figure 39** shows the brake-specific THC emissions for PI and LPDI with varied SOI. THC was defined as the sum of C1-C3 exhaust components and it was dominated by CH₄ as expected. For the best LPDI case, THC emissions were reduced by 73% when compared to PI.

As stated above, for this engine size and application, the EPA regulation for HC+NO_x is <50 g/kWhr [86]. The LPDI with SOI of 180 CAD BTDC met current regulations (**Figure 39** and **Figure 40**). Though CH₄ is not currently regulated for these engine families.

Figure 39. THC emissions on PI and preliminary LPDI vs λ^* , averaged over 90 seconds of steady state operation. These emissions arise both from the scavenging process and from incomplete combustion.

Figure 40. NMHC plus NO_x on PI and preliminary LPDI vs λ^* , averaged over 90 seconds of steady state operation.

The detailed energy break-down comparison for PI and LPDI is presented as part of the speed effect study in the next section.

4.2.2 Effect of Engine Speed on LPDI Operation

After determining the optimal injection strategy for an engine speed of 5400 RPM, the engine was operated at different speeds to examine any potential benefits from different speed operation.

Figure 41 shows the delivery ratios for varied engine speed while the SOI was held optimal. Delivery ratio increased at LPDI operation with two mechanisms: absence of gaseous fuel in the intake and higher in-cylinder pressure at EPO. Higher pressure at EPO created a stronger suction wave causing more flow through the engine. Because of highly unstable combustion at 4800 RPM, peak pressures were very low, which in turn yielded weaker suction waves. This caused lower delivery ratio at this speed.

To examine one variable at a time, the exhaust resonator geometry was kept fixed for all cases at the previously optimized length for 5400 RPM. Other than exhaust resonators effect, at 4200 and 4800 RPM, lower piston speed naturally led to a weaker suction within the crankcase and less flow

through the engine. The exhaust resonator had a strong effect on in-cylinder charge, and poor tuning led to unstable combustion. This effect led to higher THC emissions at 4800 RPM.

Figure 41. Delivery ratio vs λ^* for PI and LPDI, each point is averaged over 90 seconds of steady state operation.

As explained in section 3.2.2, five major energy pathways were identified for this engine. While 6000 RPM LPDI showed the best overall performance, PI showed the worst performance. A full energy balance analysis for these two extreme cases is presented in **Figure 42**.

Fuel loss (slipped and unburnt) ranged from 38% to 41% of total fuel energy in PI operation. This was comparable with previous research [105]. On LPDI operation, fuel slip ranged from 9% to 15% of total fuel energy.

Heat loss was second in PI ranging from 29% to 33%. In LPDI heat loss was the highest loss ranging from 29 to 36% of the total fuel energy. This size of engine showed higher heat losses compared to those reported for larger engines [51]. The main reason was the considerably larger area to volume ratio compared to larger engines.

Exhaust thermal energy ranged from 16% to 18% for PI while it ranged from 25 to 28% for LPDI. This higher percentage was due to lower total fuel injected in LPDI and almost the same amount of exhaust thermal energy.

Indicated efficiency was only 14.5 to 16.8% in PI operation and it ranged 26% to 29% with LPDI operation. Reducing the slipped fuel was the main reason for increased energy efficiency.

Due to well-mixed charge in PI operation, combustion inefficiency was as low as 3.4% during richer combustion. This was where the LPDI had higher incomplete combustion energy content.

Figure 42. Energy balance of LPDI at 6000 RPM and PI at 5400 RPM as percentage of total injected fuel energy, data was averaged over 90 of seconds steady state operation.

For LPDI, heat losses were less than PI. However, given the engine's small size, its area to volume ratio was considerably large at EPC (200 [m⁻¹]), a higher portion of released heat was lost by convective and radiative heat transfer. For perspective, the same bore and stroke ratio in a 500 cc engine yielded an area to volume ratio of around 80 [1/m]. Since fuel slip was reduced by conversion to LPDI, the largest loss pathway was heat loss, which ranged from 29 to 36% of the total fuel energy. Combustion inefficiency increased, due in part to increased cyclic variability as shown in the COV of IMEP – likely caused by mixture stratification. Average indicated efficiency for LPDI was 29% as compared to 15% for PI. To investigate each energy pathway in more detail, they are presented here separately.

Heat Loss

Figure 43 shows the heat losses for PI and LPDI with varied speed. As percentage of total fuel energy, LPDI showed an increase compared to PI. This was mainly due to lower total fuel required per cycle in LPDI.

For a better comparison on a trapped energy basis, in-cylinder heat release was used to compare heat transfer as shown in **Table 20**. To compare all cases, PI operation at 5400 RPM was used as the baseline. For the comparison, a parameter was calculated dividing heat loss by in-cylinder heat release for each case. Then a relative change of that parameter is presented in **Table 20**, considering the PI 5400 RPM as baseline. For all LPDI cases, heat losses decreased, and the amount of reduction was higher with increased speed. For the same engine speed as the baseline (5400 RPM), LPDI operation decreased cylinder heat loss by about 31 to 39% when compare to PI as the baseline.

Figure 43. Heat transfer rate as a percentage of total injected fuel energy vs λ^* for PI and LPDI, each point was averaged over 90 seconds of steady state operation.

Table 20. Heat transfer change on LPDI relative to PI based on in-cylinder heat released, heat loss was averaged over 90 seconds steady state operation and heat release was average over 200 cycle recorded.

Case no.	1	2	3	4	5	6
LPDI 6000 RPM	-31.52	-31.89	-34.78	-33.41	-34.76	-36.04
LPDI 5400 RPM	-30.71	-30.66	-32.12	-32.32	-38.61	-36.11
LPDI 4800 RPM	-17.60	-30.05	-30.41	-21.65	-16.12	-14.14
LPDI 4200 RPM	-14.22	-12.25	-14.82	-6.92	-2.29	-1.79
PI 5400 RPM	baseline	baseline	baseline	baseline	baseline	baseline

Figure 44 shows the impact of different speeds on the rate of heat release (ROHR) at a given λ^* . For each point the integral of this curve showed the heat release energy per cycle. LPDI at 6000 RPM, had the highest trapping efficiency and a higher ROHR. This resulted into a higher in-cylinder pressure (**Figure 45**).

Figure 44. Rate of heat released averaged on 200 cycles for different speeds on LPDI near stoichiometric operation.

Figure 45. In-cylinder pressure averaged on 200 cycles for different speeds on LPDI near stoichiometric operation.

Figure 46 shows the peak pressure results for all operating points averaged over 200 cycles. Higher peak pressure served as a mechanism to increase the delivery ratio from a stronger suction wave at the divergent section of exhaust resonator. Note that when examining the ROHR curve (**Figure 44**), higher peak pressure was expected at 6000 RPM as ignition timing was set to MBT in all cases.

Figure 46. Peak pressure averaged on 200 cycles for different speeds on LPDI and 5400RPM on PI.

Indicated Efficiency

Figure 47 presents the indicated efficiency for all PI and LPDI cases. Since this research was geared toward free piston engine development, indicated efficiency was examined to remove any effect in friction changes within the driveline system (i.e. clutch and bearing wear). LPDI operation, showed higher indicated efficiency throughout the entire engine operation range compared to PI. This was mainly due to improved volumetric efficiency and reduced fuel slip. **Table 21** shows the tabular results for each case compared to PI as baseline. The peak increase in indicated efficiency for the same engine speed as PI, was about 76%. This further increased by up to around 90% at 6000 RPM.

Figure 47. Indicated efficiency for PI and LPDI vs λ^* , averaged over 90 seconds steady state operation for each point.

Table 21. Indicated efficiency change on LPDI operation relative to PI, exhaust sensible was averaged over 90 seconds steady state operation and heat release was average over 200 cycle recorded.

Case no.	1	2	3	4	5	6
LPDI 6000 RPM	+81.46	+89.65	+88.34	+87.27	+83.16	+75.49
LPDI 5400 RPM	+68.55	+75.75	+72.43	+69.08	+72.82	+56.05
LPDI 4800 RPM	+34.13	+65.89	+63.62	+62.00	+55.00	+53.85
LPDI 4200 RPM	+45.84	+47.68	+45.03	+41.56	+39.80	+37.83
PI 5400 RPM	baseline	baseline	baseline	baseline	baseline	baseline

Exhaust Thermal Energy

Figure 48 shows the results of exhaust thermal energy as fraction of total fuel input energy. The increase in LPDI was due to the dramatic reduction in fuel slip and the redistribution of the relative contribution for each energy pathway. Similar to heat transfer results in *Table 20*, the exhaust sensible energy was compared to in-cylinder heat released and presented in *Table 22*. Data showed very little change for the same engine speed as PI.

Figure 48. Exhaust thermal energy as a fraction to total fuel input energy vs λ^* for PI and LPDI, averaged over 90 seconds steady state operation for each point.

Table 22. Exhaust thermal energy change on LPDI operation relative to PI based on in-cylinder heat released.

Case no.	1	2	3	4	5	6
LPDI 6000 RPM	-4.72	-5.28	-3.95	-2.67	-1.58	-3.53
LPDI 5400 RPM	1.44	0.39	0.31	0.30	1.06	0.36
LPDI 4800 RPM	-10.93	-17.82	-16.20	-13.89	-10.88	-11.40
LPDI 4200 RPM	-5.49	-11.16	-11.15	-9.30	-6.96	-9.38
PI 5400 RPM	baseline	baseline	baseline	baseline	baseline	baseline

Exhaust Chemical Energy (HC, CO)

Chemical energy was divided in to two types: THC (unburnt and slipped), and CO as a result of incomplete combustion. **Table 23** shows the fuel slip rate as a percentage of total injected fuel for all the cases. PI showed the highest fuel slip rate around 38% of total fuel injected. **Figure 49** shows that LPDI operation at 6000 RPM had the lowest fuel slip rate with best case of 5.78% fuel slip.

Table 23. Fuel slip rate on LPDI and PI operation as a percentage of total injected fuel.

Case no.	1	2	3	4	5	6
LPDI 6000 RPM	9.52	6.78	5.78	6.02	7.91	10.81
LPDI 5400 RPM	13.94	12.68	11.83	12.12	12.89	16.23
LPDI 4800 RPM	21.16	14.54	11.52	11.22	12.04	12.04
LPDI 4200 RPM	16.44	15.02	14.56	13.32	12.12	15.29
PI 5400 RPM	37.61	37.45	36.41	36.03	36.02	36.11

Figure 49. Fuel slip rate as a percentage of total injected fuel.

Fuel slip rate changes are presented in **Table 24** considering PI at 5400 RPM as the baseline. All LPDI operations showed more than 60% reduction in fuel slip peaking at 6000 RPM for an intake lambda of 1.55 - an 87% reduction in exhaust THC energy when compared to PI.

Table 24. Fuel slip rate on LPDI operation relative to PI.

Case no.	1	2	3	4	5	6
LPDI 6000 RPM	-80.10	-86.22	-87.28	-86.50	-81.79	-75.07
LPDI 5400 RPM	-70.50	-74.25	-75.08	-73.49	-72.96	-69.37
LPDI 4800 RPM	-61.35	-78.40	-81.82	-81.48	-80.40	-79.98
LPDI 4200 RPM	-74.61	-77.34	-76.98	-78.87	-80.62	-76.07
PI 5400 RPM	baseline	baseline	baseline	baseline	baseline	baseline

Figure 50 presents the exhaust chemical energy from CO. We recognized two major stratification mechanisms for LPDI and PI operations:

1. Strong stratification originating from limited mixing times for LPDI given high engine speeds in general.
2. Added stratification originating from lower turbulent intensity at reduced speeds regardless of PI or LPDI.

Strong stratification of the gaseous fuel in LPDI operation, increased the CO contribution in the exhaust chemical energy. Lower speeds likely had lower tumble strength and mixing which increased stratification and CO emissions. **Table 25** shows the exhaust CO energy for LPDI and PI operation. LPDI at 4200 RPM, yielded 28 times higher exhaust CO energy when compared to PI.

Figure 50. Exhaust CO energy as a percentage of total injected fuel energy for PI and LPDI, each point was averaged over 90 seconds of steady state operation.

Table 25. ECE (CO) on LPDI operation relative to PI.

Case no.	1	2	3	4	5	6
LPDI 6000 RPM	2.35	2.12	6.29	11.53	11.32	13.35
LPDI 5400 RPM	1.88	1.37	3.84	11.84	8.27	4.49
LPDI 4800 RPM	3.08	2.99	11.07	24.95	18.87	17.98
LPDI 4200 RPM	2.91	3.19	12.57	28.83	24.72	21.07
PI 5400 RPM	baseline	baseline	baseline	baseline	baseline	baseline

Combustion Phasing

Figure 51 presents the 50% MFB. Since engine geometry and fuel type were held constant, the ignition timing was always set to MBT. MFB 50% was around 12 CAD ATDC for most stable operation. During leaner operation, combustion was stretched and had higher durations likely due to instabilities.

Figure 51. 50% MFB averaged on 200 cycles for different speeds on LPDI and 5400 RPM on PI.

Combustion Stability

As shown in **Figure 52**, due to stratification along with turbulence and flow momentum at lower speeds, the COV of IMEP increased as speed decreased. At 4800 RPM the combustion was very unstable likely because of the exhaust resonator effects on the trapped mixture. More stable

combustion at higher speeds allowed for a wider range of AFR adjustments not afforded at lower speeds.

Figure 52. COV of IMEP averaged on 200 cycles for different speeds on LPDI and 5400 RPM on PI.

Emissions

The current research engine falls in the class I-A according to CFR classifications presented in **Table 3**. Class I-A non-handheld equipment is described by displacement in the range of less than 66 cc and their CO is regulated at 610 g/kWhr as presented in **Table 3**. HC+NO_x is regulated at 50 g/kWhr. This is where NMHC+ NO_x is not currently regulated for this size engine. The closest regulated class for NMHC+ NO_x is class I-B with 37 g/kWhr limit. The class I-B are non-handheld engines with displaced volume between 66 and 100 cc.

Figure 53 shows the CO emissions for LPDI and PI. The root cause of higher CO in LPDI was discussed above. CO regulations for I-A and IV engines were 610 and 805 g/kWhr, respectively. Even with the increased CO emissions from LPDI, levels for all speeds were well below the regulation limits.

Figure 53. CO emissions on PI and different speeds on LPDI, averaged over 90 seconds of steady state operation for each point.

HC emissions in NG engines had two major parts, NMHC and CH_4 . Both emissions were important from an efficiency standpoint, however NMHCs affect the local air quality and are most frequently regulated along with NO_x . **Figure 54** shows the CH_4 emissions for all the cases. LPDI operation at 6000 RPM showed an 85% reduction in CH_4 emissions. Total HC plus NO_x emissions for the highest efficiency case was 27.3 g/kWhr – which was lower than the standard threshold of 50.

Figure 54. Methane emissions on PI and different speeds on LPDI, averaged over 90 seconds of steady state operation for each point.

NMHC+NO_x emissions are shown in **Figure 55**. Operation at 6000 RPM showed the highest reduction due to lower fuel slip.

Figure 55. NMHC emissions on PI and different speeds on LPDI.

4.3 1D Simulation

A 1D simulation was performed to first understand the system's behavior. Then it was used for GA optimization of the exhaust resonator as well as to provide initial and boundary conditions for my CFD study.

4.3.1 Baseline Model Verification

The first step in 1D model validation was to ensure flow was estimated accurately. This was verified with measured crankcase pressure and intake air flow as compared to modeled results. **Figure 56** shows crankcase pressure from experiments and simulation. The maximum pressure difference between experiments and simulation occurred during scavenging and it was +0.08 bar (+7%) error. Part of this error could have been attributed to the location at which sensor was installed and delay time of response whereas for 1D simulation, volumes had no dimension and respond immediately. The sensor was installed at the bottom of the crankcase. Low speed operation made this deviation more prominent. Maximum negative error was at peak pressure and it was -0.04 bar (-2.6%). The engine motoring pressure curve was captured as hot motoring at 3600

RPM. Hence, the model was run at this speed for this validation. Reed valve petal areas, Young's Modulus, and port discharge coefficients were the most impactful parameters in this validation. The exhaust resonator's dimensions showed to be very impactful on the crankcase pressure, so caution was taken to avoid any dimensional measurement errors. Note that intake air mass flow from simulations was within $\pm 3\%$ of its value in the experiment's dependent on the engine settings (*Table 26*).

Figure 56. Motoring crankcase pressure at 3600 RPM for engine operating with beta design, experiment curve was averaged over 200 cycles.

Gas exchange parameter calibration included port discharge coefficients and was performed first using the motoring pressure curves and they were held constant afterward. However, one must know that other parameters such as exhaust dimensions will affect the gas exchange significantly. As presented later, the model showed to have reasonable fidelity for gas exchange parameters such as delivery ratio. **Figure 57** shows the crankcase pressure where the model was operated on a different engine speed and in the firing condition. The maximum pressure difference between experiments and simulation occurred during scavenging and it was +0.06 bar (+6.5%) error. Maximum negative error was at peak pressure and it was -0.02 bar (-1.3%)

Table 26. Summary of intake air flow results at two conditions.

Condition	Intake Air Flow		
	Experiments	Simulation	Relative Error
3600 RPM Motoring	105	108	+2.8%
5400 RPM Combustion	175	178	+1.7%

Figure 57. Combusting crankcase pressure curves at 5400 RPM engine speed operating on beta exhaust, experiment curve was averaged over 200 cycles.

Figure 58 shows the in-cylinder combustion pressure curves. For accurate trapped mass verification, the compression portion of in-cylinder pressure before spark timing was considered. Matching the compression curves before the start of the combustion confirmed that the trapped mass in the simulation matched with experiments. The RMSE error before starting the combustion calibration was 0.009 and at the end of combustion calibration it was 0.002 leading to the following simulation curve.

Figure 58. In-cylinder combustng pressure at 5400 RMP engine speed operating with beta exhaust design, experiment curve was averaged over 200 cycles.

Lastly, exhaust pressure waves, which affected the in-cylinder gas dynamics, were validated for 5400 RPM as shown in **Figure 59**. Exhaust geometry and thermal boundaries were the most sensitive parameters. Notice that at EPO a pressure wave started down the resonator and right before EPC the reflected wave pushed some slipped charge back in to the cylinder which improved the trapping efficiency. These two areas were of highest important whereas the area in between will not significantly affect the cylinder gas dynamics. Maximum positive error between simulation and experiment was +.05 bar (3.35%) at the EPO pressure pulse.

Figure 59. Exhaust pressure wave validation at 5400 RPM engine speed operating on beta exhaust design; experiment curve was averaged over 200 cycles.

Note that since engine operation was designed to be at 90 Hz for this study, the model calibration and validation were performed at this speed and full load. The same model served as the baseline model for GA optimization of exhaust resonator.

4.3.2 GA Evolution Curve and Sensitivity Curves

For the GA used to optimize the exhaust, seven parameters were considered as factors. A total of 20 designs were set for each of the 50 generations. The full engine simulation started with the beta design values as the initial case. Exhaust dimensions as explained in section 3.3.4, were set to randomly be selected toward an optimal solution by the GA platform. **Figure 60** shows the 1D model's indicated efficiency results for the different iterations as a function of design points. Over 600 design points were examined in this study but due to marginal improvements after around 150th design, the plot was truncated at the 400th design point. Notice the asymptotic behavior of

the plot after 150th design. It showed that on the beta exhaust, efficiency was around 25%, while the optimized design showed up to around 28%. This difference was later investigated with experiments. Note that LPDI engine with the beta exhaust and tuned intake was the most efficient configuration achieved before implementing the GA.

Figure 60. Indicated efficiency evolution versus design iteration.

Figure 61 shows the 1D model engine efficiency sensitivity to different dimensions of the exhaust resonator design. A copy of the exhaust resonator parametric figure is shown to quickly cross reference dimension locations. The length of the divergent cone (L2) and length of the straight section (L3) of the resonator were the most important parameters in the exhaust design. This was understandable because the function of the divergent cone was to create a suction wave, which directly affected the delivery ratio. On the other hand, the straight section of the resonator timed the reflected wave and affected the trapped mass inside of the cylinder. The length of the converged cone showed to be the third most important parameter. It controlled the intensity of the reflected wave (amplitude) and more sensitivity of the response to L3 showed that reflected wave timing was more impactful than reflected wave amplitude. According to this discussion, the most impactful parameters were divergent cone's angle, straight section length, and convergent cone's angle.

Figure 61. Engine response sensitivity to the exhaust design parameters.

Table 27 shows the dimension comparison between beta design and optimized designs. For A_1 , literature recommends a range of 3 to 4.5 degrees. It was reported that lower values resulted in weaker reflected pressure waves, with longer durations. In experiments for the beta design, 5.13° was used for A_1 because of commercial availability of conical sections in the market. Another parameter affecting the wave strength was L_2 , which was related to A_2 . For A_2 , literature recommended an upper limit of 10° for peak power and with a lower acceptable value of 7° [33]. Based on high costs associated with rolling thin cones of such size, we used a commercially available cone with an angle of 7.7° .

After optimization, A_1 and A_2 were shown to be in the range which was recommended by literature. A_2 was closer to lower limit of the recommended range, while A_1 was closer to the higher limit. The most significant difference between rules of thumb presented in literature and this 1D simulation optimization was the length, L_2 , which was 31% greater from 1D simulation results

when compared to the beta design. Given the sensitivity of the system response to this parameter as shown in **Figure 61**, it was expected to change results as presented later in this section.

Table 27. Comparing the beta design and 1D simulation optimized design, 1D simulation started with beta design dimensions as baseline values of the exhaust resonator.

Variable	Beta Design [mm] (literature)	Optimized design [mm] (1D)	Percent difference
D₁	15	17	+13.3
D₂	45	50	+11.1
D₃	10.5	12.9	+22.9
L₁	41	64	+56.1
L₂	167	219	+31.1
L₃	818	738	-9.8
L₄	127	134	+5.5
A₁	5.13 [°]	4.3 [°]	-16.2
A₂	7.73 [°]	7.88 [°]	1.9

Optimized design validation

As **Figure 61** shows, system response had a high sensitivity to the straight section of the exhaust resonator. In addition, for LPDI experiments it was realized that engine stability was also sensitive to the length of the straight section. So, it was expected that an adjustment in the experiment was required for the best results. While the first result of the GA showed 738 mm for the straight section of the optimized design, in experiments, the most stable results were obtained for a length of 788 mm. The idea was that in the GA optimization, an increased delivery ratio was proportional to flow momentum during scavenging and a stronger reflected pressure wave for trapping purposes. This function combined with LPDI operation, which takes place while exhaust port is still open, was expected to help with mixing and providing higher fuel trapping and consequently an increased efficiency.

Figure 62 shows the optimized exhaust resonators pressure curves from experiments and simulation. This is to make sure gas dynamics of the model were working as expected without further calibrations. Maximum positive error between simulation and experiment was +.05 bar (4.1%) at EPC pressure pulse.

Figure 62. Exhaust pressure waves validation for the engine operating with optimized exhaust at 5400 RPM and full load; experiment curve was averaged over 200 cycles.

Figure 63 shows the combusting in-cylinder pressure of the engine operating with the optimized exhaust at 5400 RPM and full load. The RMSE error between simulation and experimental pressure curve was 0.0025.

Figure 63. In-cylinder pressure validation of the engine with optimized exhaust at 5400 RPM full load operation; experiment curve was averaged over 200 cycles.

4.3.3 Experimental Comparison of Optimized Exhaust with the Beta

Note that 1D optimization was completed at a single operating point (5400 RPM and full load). This allowed faster modeling and comparisons. We extrapolated the AFR change behavior by

means of an experimental study. In addition, in this program, it was never intended to operate on part-load for power generation. Notice that simulation started with the point near to beta design and reached near to optimized line after GA optimization.

Figure 64 shows delivery ratio results for the two exhausts designs obtained in the experiments. Notice that lambda was calculated based on total air versus total injected fuel and that is why it was higher than usual. In addition, due to the optimized design's higher delivery ratio and lower air trapping in general compared to fuel, the optimized design showed higher λ^* values. Notice that stars show the results from 1D simulation. The error on the plot represents absolute error compared to corresponding experimental points.

Figure 64. Delivery ratio for beta design and optimized design. Stars are showing results from 1D simulation.

Note that according to the literature, it is quite possible to have delivery ratios above 1 for tuned engines. Heywood showed that crankcase compression, two-stroke engines that include tuned intake and exhausts can exhibit delivery ratios greater than unity [10].

Figure 65 shows the engine brake efficiency as measured in the experiments. Note that in experiments we compared the engine brake efficiency while for simulations I used engine indicated efficiency including crankcase pumping losses. Note that the friction, combustion, and heat transfer sub models were associated with the error in brake thermal efficiency. By minimizing the RMSE between experiments and simulation pressure curves, this approach yielded the best results. The other theory was that because of the non-standard combustion hardware configuration it was in general more difficult to achieve a good calibration across a wide range of operation. This non-standard configuration included non-central spark plug location and stratified charge with LPDI.

Figure 65. Engine BTE for exhaust optimization.

Figure 66 shows the total HC energy content for engine operation with both exhaust resonators. Note that this parameter was not investigated in simulations. Instead with a pressure analysis model and experiment results, fuel fraction burnt was adjusted to account for incomplete combustion and escaped fuel. This ensured efficiency values were realistic.

Figure 66. Exhaust HC content.

4.4 3D CFD Simulation

The objectives of the CFD simulation were to investigate two phenomena:

1. To understand of the exhaust resonator's effect on cylinder gas dynamics
2. To investigate the mixture stratification before the start of combustion.

The 3D model included the full engine geometry including crankcase, piston, crankshaft, and connecting rod as shown in **Figure 67**. Intake mass flow boundary conditions were provided by 1D simulations. However, the intake air flow from 1D simulation had around 2% relative error when compared to experiments. So, the mass profile was scaled such that the total air flow into the crankcase matched with experiments. The exhaust boundary was directly defined by experimental data. Experimental exhaust pressure was averaged over 200 recorded cycles.

Figure 67. Full engine geometry modeled in CONVERGE™.

Figure 68 shows the crankcase pressure for both 1D and 3D simulations along with experimental data for comparison. The results showed a good consistency between simulations and experiments. This was completed to ensure gas dynamics during scavenging were not affected by an incorrect pressure from the crankcase.

Figure 68. Crankcase pressure, 1D (GT-Power™) simulation, 3D (CONVERGE™) simulation, and experimental data, experiment curve was averaged over 200 recorded cycles.

The in-cylinder trapped mass was accurate and equal to 22 milligrams (mg), which matched the results from TPA. It was also confirmed with compression side of the in-cylinder pressure curve matched with experiments. Then we examined in-cylinder gas dynamics. **Figure 69** shows gas dynamics affected by the exhaust resonator. The red zone shows the fuel and a color bar is provided on the plot. The spectrum shows the stratification and blue represent anything other than fuel injected in that cycle.

The intent of the figure was to focus on how the reflected pressure wave helped with charge trapping. From 142 to 116 CAD BTDC, it showed that the tumble motion created by the boost port dominated the dynamics but enabled some fuel to escape from the cylinder. Injection timing was optimized for highest fuel trapping during the experiments prior to the 3D simulation. As the piston approached EPC timing and around 106 CAD BTDC, the reflected pressure wave started to affect the in-cylinder charge by pushing some escaped charge back into the cylinder. This continued until 98 CAD BTDC where it pushed nearly all the escaped fuel back into the cylinder. In addition, the strong tumble motion helped to keep most of the fuel mass from short circuiting.

Figure 69. Exhaust resonators effect on in-cylinder gas dynamics and fuel trapping efficiency.

Figure 70 shows in-cylinder stratification evolution before spark timing. Note that color bar is shows the methane mass fraction from 0 to 10%. The red zone shows area with 10% methane mass fraction and blue shows 0% methane mass fraction. After EPC, the combination of tumble and swirl motion changed the stratification paradigm inside of the cylinder. Simulations showed that

the fuel air charge was not fully mixed by the point of ignition, meaning that there were some richer zones. Spark plug location initially was selected for ease of installation and convenient machining. According to the simulation, this location of the spark plug was outside of the bulk rich zone. While most literature recommend to keep the spark plug on the exhaust side of the combustion chamber [10], in this particular study, simulation showed that the intake side was more desirable based on the in-cylinder stratification from LPDI.

Figure 70. In-cylinder stratification evolution at different cranks angle degrees before TDC, spark timing was at 26 BTDC, color bar is showing methane mass fraction, red is showing 10% and blue 0% methane mass fraction.

4.4.1 Experimental Validation for Spark Plug Location Optimization

The theory behind spark plug location was that since most of the fuel was shown to be trapped in the CFD study, it was likely that most of HC emissions in the exhaust were due to charge stratification and that the spark plug location was outside of the majority rich zone. To determine the impact of spark plug location, engine modifications were completed, and new engine configuration was tested.

Figure 71 shows the delivery ratio for the engine operating with the two different spark plug locations. The new optimal location yielded a higher delivery ratio. This was due in part to higher peak cylinder pressures resulting into higher pressure at EPC. This impacted the performance of the exhaust resonator diffuser, which enabled a stronger suction wave through the cylinder. It is also noted that relocation enabled slightly leaner operation. As shown in **Figure 71**, achieving delivery ratio higher than unity is possible [10].

Figure 71. Delivery ratio comparison for base location and optimized location of spark plug, each datapoint is averaged over 90 seconds of continuous data measurement.

Figure 72 shows the BTE for engine operation on two spark plug locations. Optimized spark location showed a peak BTE of 27.5% where the original spark location peak BTE was around 26%. As discussed later, the major differences were increased combustion efficiency and lower unburnt fuels.

Figure 72. BTE comparison for base location and optimized location of spark plug, each datapoint is averaged over 90 seconds of continuous data measurement.

Figure 73 and **Figure 74** show total HC and incomplete combustion (CO) energy losses for the two spark locations. THC decreased with the optimized spark location over the entire λ^* range. While the best result for baseline spark location was 7%, THC loss with the optimized spark location showed a minimum of 4.5%, a 32% relative reduction. In addition, THC losses were less dependent on AFR with optimized spark location. This was due to the new location within the rich zone and that burn duration, as shown later, was shorter.

Figure 73. Exhaust total HC comparison for base location and optimized location of spark plug, each datapoint is averaged over 90 seconds of continuous data measurement.

CO energy content also decreased with the optimized spark location. Another factor which helped to reduce both CO and HC, was that at the start of combustion the spark plug region was less stratified. This required lower fuel mass and decreased the likelihood of incomplete combustion.

Figure 74. Exhaust Co and H₂ energy for base location and optimized location of spark plug, each datapoint is averaged over 90 seconds of continuous data measurement.

Figure 75 shows the sum of THC and incomplete combustion energy losses for two spark locations. Base location of spark showed a minimum combustible loss of around 10% where the optimized location showed a minimum value of 6%, a 40% relative reduction. When comparing the total combustible losses averaged over the λ^* range, the reduction was even higher, at around 50%, due to higher losses in richer operations.

Figure 75. Total combustible content of exhaust for base location and optimized location of spark plug, each datapoint is averaged over 90 seconds of continuous data measurement.

Due to the reasons discussed above and as shown in **Figure 76**, the indicated efficiency for the new optimized spark location was higher. Spark base location yielded a maximum indicated efficiency of 30.4% where with optimized spark location showed a maximum value of 31.4%.

Figure 76. Indicated efficiency for base location and optimized location of spark plug, fuel flow was averaged over 90 seconds of continuous data measurement and IMEP averaged over 200 cycles.

Figure 77 supports the claim of shorter combustion duration with optimized spark location. Combustion duration in experiments was defined as the time for 10-90% MFB in units of CAD. While the original location showed an average combustion duration around 50 CAD, the optimized spark location showed an average around 40 CAD. This shorter combustion duration ensured a lower COV of IMEP in most of the engine operation conditions as shown in **Figure 78**. Note that even with imperfect mixing on LPDI, the combustion stability approached the range for PI operation with perfect mixing. This shows the effectiveness of all the improvements including the exhaust and spark location optimization. Referring to **Figure 52**, for 5400 RPM with the beta design and original spark location, only 3 points were below 5% COV and those points were near rich limits. Whereas with optimized exhaust (base location line in **Figure 78**) combustion stability was acceptable over a wider range of operation. Combustion stability showed even further improvement with spark location optimization.

Figure 77. Combustion duration comparison for base location and optimized location of spark plug, each datapoint is averaged over 200 engine cycles.

Figure 78. COV of IMEP for base location and optimized location of spark plug, each datapoint is averaged over 200 cycles.

4.5 Fuel Quality Effect on the Performance

After finalizing all optimizations on engine design, a fuel study was performed. The objective was to investigate the effect of fuel quality on system performance. Additionally, by adding an oxidation catalyst a detailed energy analysis was performed to identify the maximum potential of the system for micro-CHP systems operating on different fuels.

Table 28 shows the selected fuels properties. CNG1 had a higher methane and lower ethane content when compared to CNG2. Methane and propane represented the ends of the spectrum for current fuels used in residential applications. MN was calculated from Cummins Inc. proprietary methane number calculator [145].

Table 28. Tested fuel properties.

Specifications	CNG1	CNG2	Methane	Propane
C1 mol percent	90.5	86	100	0
C2 mol percent	5	12	0	0
C3 mol percent	1	1	0	100
C4 mol percent	0	0	0	0
N2 mol percent	2.5	0.5	0	0
CO ₂ mol	1	0.5	0	0
LHV [kJ/kg]	46,480	48,482	50,000	46,350
AFR stoich	15.87	16.51	17.12	15.57
M (kg/kmol)	17.60	18.20	16.04	44.10
MN	82.8	75.3	100	34.2

Initially combustion stability was investigated as shown in **Figure 79** to compare different fuels operation from leaner to richer regimes. Our focus was on the stable operating points and extra lean and rich conditions were examined to determine the maximum operation spectrum. It was found that combustion stability strongly affected the performance as presented in **Figure 80** to **Figure 83**. Note that in **Figure 78**, all the experiments were performed using CNG1.

Figure 79. Combustion stability for different fuels, each point was averaged over 90 seconds of steady state operation.

Figure 80 shows the BTE and brake power for different fuels. CNG2 and propane showed the highest efficiency while methane and CNG1 showed lower values. Propane and CNG2 had heavier

hydrocarbon content. In the context of LPDI, they seemed to operate better than lighter gaseous fuels. A more detailed energy analysis is presented next.

Figure 80. BTE and brake power for different fuels, each point was averaged over 90 second of steady state operation.

Figure 81 shows the heat transfer for different fuels. Methane showed the highest heat transfer rates for the NG fuels while propane heat loss varied across its narrower AFR region. CNG2 having heavier hydrocarbons, showed better performance in terms of lowered heat losses and due to faster combustion as shown in **Figure 82**. Propane had the highest power density and trapped energy per cycle, which showed the highest heat transfer of any operating points. Heat transfer was directly affected by peak pressure and combustion duration which varied with each fuel.

Figure 81. Cylinder heat transfer for different fuel operations, each point was averaged over 90 second of steady state operation.

The reason that methane showed a higher heat loss was in part due to higher ignition delay and longer combustion duration as shown in **Figure 82**. Longer ignition delay forced the experiments for methane toward more advanced ignition timing to keep the combustion stable and achieve MBT timing. This earlier ignition timing led to higher peak pressures for methane. Having higher peak pressures and longer combustion duration allowed for additional heat transfer losses for methane. Ignition timing was around 18 CAD BTDC for propane and varied from 21 to 23.5 CAD BTDC for the different NG compositions.

Figure 82. Ignition delay and combustion duration for different fuels, each point was averaged over 200 recorded cycles.

Figure 83 shows the exhaust chemical energy from incomplete combustion (dominated by CO) and slipped fuel (C1-C3). Note that we could not experimentally, distinguish unburnt HC from slipped HC. However, the CFD study showed 98-99% of the fuel was trapped, so that ratio could be used as an offset.

Propane, the heaviest/densest fuel, showed the lowest HC in the exhaust. This was mainly due to its longer hydrocarbon chain which was easier to engage in combustion (requiring lower activation energy). The faster combustion as shown in **Figure 82** confirms this explanation. However, a higher charge stratification expected from denser gaseous fuel, did not allow for complete combustion and propane showed the highest unburnt energy. Pure methane was on the other side of the spectrum compared to propane and CNG1 and CNG2 were in between. CNG1 being the lighter CNG showed a behavior more similar to pure methane.

Figure 83. Unburnt (CO and H₂) energy and total HC energy in exhaust, each point was averaged over 90 second of steady state operation.

4.5.1 CHP Potential Analysis

Previously all the energy pathways were quantified in detail. However, for a more realistic estimation, the heat potential of unburnt products in the exhaust must be considered. While hydrocarbons in NG and propane are difficult to catalyze, the CO can be easily oxidized which would improve the exhaust heat content for recovery in a CHP system.

Platinum based oxidation catalysts have low performance in catalyzing HCs, especially lower alkanes at low temperatures[146], [147], [148]. However, oxidation of CO is well established [149] and literature has shown high conversion efficiencies (>90%) at temperatures of 200 °C and lower. CO oxidation is exothermic, and its heat release can be calculated from Equation (70):

$$\Delta_r H = \Delta_f H\{CO_{2(g)}\} - \Delta_f H\{CO_{(g)}\} - \Delta H\{O_{(Pt)}\} \quad \text{Eq. (70)}$$

Where, $\Delta_f H$ is the enthalpy of formation and $\Delta H\{O_{(Pt)}\}$ is the heat required to release O radicals from the platinum sites. $\Delta_r H$ was reported to be about 173 kJ/mol [150]. Using this heat release rate and a 99.3% oxidation efficiency, the theoretical added heat from CO oxidation was calculated. The total available heat from CO oxidation is presented in **Table 29** which shows the averaged added heat energy from oxidation. The values were calculated as a percentage of the total fuel energy injected and the total CO energy. All fuels showed about 40% recovery of total CO

energy and propane with the highest CO output, showed the highest values. Note that because of the catalyst and resonator sensitivity to heat, precautions must be taken to ensure that minimum light-off temperatures are obtained, and that placement does not negatively impact resonator performance.

Table 29. CO oxidation added heat averaged over the range of AFR, numbers are calculated based on experimental CO concentration from Equation (70).

Energy Fraction	$\dot{E}_{CO}^{Oxidation} / \dot{E}_{Fuel}^{in}$	$\dot{E}_{CO}^{Oxidation} / \dot{E}_{CO}^{exh}$	Relative increase in exhaust sensible heat
Unit	%	%	%
CNG1	2.23	39.7	10.0
CNG2	2.05	39.1	9.0
Methane	2.36	38.7	10.2
Propane	3.37	44.6	15.1

4.5.2 Heat Recovery Analysis

Table 30 shows a detailed breakdown of all energy categories, which could be considered in estimating the peak utilization of micro-CHP system operating on each fuel. Note that for each fuel, data was averaged over the range of operating AFR. Peak utilization values were calculated based on full heat recovery of both cylinder and exhaust heat. Exhaust gas temperature and cylinder head temperature were included as they would be the inlet/boundary temperatures for the design of the heat exchangers. The cylinder heat has a lower quality compared to the exhaust heat since its heat transfer would occur at a lower temperature. The Consumer Product Safety Commission recommends a domestic hot water upper temperature limit of 49 °C. Therefore, both heat sources could serve as heat inputs to domestic hot water [151]. In deploying a heat exchanger for the exhaust, caution should be taken to not affect the resonator and catalyst performance.

Table 30. Cylinder and exhaust heat for different fuels and their occurring temperatures for best BTE points, peak UF is based on 100% heat recovery.

	$W_{indicated}$		$\dot{Q}_l$		T_{cyl}	$\dot{E}_{ex}^{th}$		$T_{exh-out}$	CO Oxidation Heat		Peak CHP Energy	Peak UF
	[kW]	[%]	[kW]	[%]	[C]	[kW]	[%]	[C]	[kW]	[%]	[kW]	[%]
CNG1	1.71	30.51	1.99	35.46	122.51	1.25	22.26	338.91	0.23	4.00	5.04	89.83
CNG2	1.79	32.08	1.91	34.29	116.44	1.28	22.93	352.17	0.24	4.09	5.08	90.90
Methane	1.78	29.61	2.17	36.07	124.33	1.38	23.05	364.15	0.27	4.30	5.43	90.40
Propane	1.82	31.35	2.08	35.83	121.87	1.30	22.29	352.83	0.37	6.21	5.36	92.22

To estimate the system's UF with varied heat exchanger effectiveness from 50% to 100% as presented in **Table 31** and shown in **Figure 84**. Peak utilization factor was obtained based on full heat recovery of exhaust and cylinder heat. Note that propane, as the most power dense fuel, showed the highest peak UF of 92.2%, while methane showed the lowest peak UF of 89.8%. Lower fuel slip combined with higher heat transfer made propane the best performing fuel from a UF standpoint. As heat exchanger effectiveness increased, those fuels showing highest heat content (propane and methane) started drifting upward showing a better UF.

Table 31. System's UF calculated for incremental heat exchanger effectiveness values, cylinder heat transfer plus exhaust heat accounted for total available heat in heat exchanger.

Heat Exchanger Effectiveness	UF										
	0.50	0.55	0.60	0.65	0.70	0.75	0.80	0.85	0.90	0.95	1.00
CNG1	60.1	63.1	66.0	69.0	72.0	74.9	77.9	80.9	83.8	86.8	89.7
CNG2	61.4	64.3	67.3	70.2	73.1	76.1	79.0	82.0	84.9	87.8	90.8
Methane	59.9	63.0	66.0	69.1	72.1	75.1	78.2	81.2	84.2	87.3	90.3
Propane	61.7	64.8	67.8	70.9	73.9	76.9	80.0	83.0	86.1	89.1	92.1

As tested in multiple national laboratories, a current state-of-the-art micro-CHP prototype system produced 27.2% connecting rod thermal efficiency, 23.5% fuel to electrical efficiency with a total system UF of 74.5% [125]. Connecting rod thermal efficiency was calculated by deducting any losses in the crank and clutch system. This could be equivalent to rod efficiency in a linear engine setup. It was found that heat transfer plus exhaust sensible heat accounted for around 3.4 kW, 65% of total fuel energy - to produce around 1.38 kW brake power and 1.17 kW electricity. The system

was able to recover around 2.5 kW out of 3.4 kW total heat, yielding a heat exchanger effectiveness of around 75%.

If the same effectiveness is applied to the current research system, referring to **Table 31**, the UF ranges from 74.9% for CNG1 and 76.9% for propane. Higher total heat plus lower fuel loss caused propane and CNG2 to show a better UF.

Figure 84. Overall utilization factor versus the required heat exchanger effectiveness for the CHP system.

4.6 Oxidation Catalyst Experiments

An oxidation catalyst was tested on the two ends of the fuel spectrum. Propane was tested since it was the highest alkane and assumed to be catalyzed easier than methane. Pure methane was tested since methane is the most difficult fuel to be catalyzed. The objective was to investigate the catalysts effect on the system performance parameters. Of the biggest concern were efficiency, added heat (CO oxidation) for recovery, exhaust methane, and NMHC oxidation.

A platinum only catalyst was tested. These catalysts have showed CO oxidation efficiencies up to 99.3%. **Figure 85** shows an example of continuous data from a cold start test that included an oxidation catalyst. At around the catalyst inlet temperature of 250 °C there is an inflection point

in the temperature versus time curve, which corresponded to a dramatic decrease in post catalyst CO concentration. The average resonator outlet temperatures for all fuels was greater than 250 °C.

Figure 85. CO oxidation plot from cold-start to light-off temperature of the catalyst.

The catalyst was a flow through design, but the addition of any catalyst and exhaust piping could add backpressure on the exhaust which could negatively impact performance of the resonator and engine. **Figure 86** presents the changes in delivery ratio for methane and propane. Note that the added backpressure did decrease delivery ratio, but in both cases the tuned system was capable of achieving delivery ratios at or above 1.0.

Figure 86. Delivery ratio before and after catalyst installation for methane and propane operation, each point was averaged over 90 seconds of steady state operation.

Figure 87 shows the effect of the added catalyst on indicated efficiency. While methane showed less than a 1% reduction in absolute value of the efficiency, propane had about a 1% reduction in indicated efficiency. While a decrease in efficiency is proportional to a decrease in UF, it could be offset if the additional exhaust heat was recovered. This reduction was compensated with an increase in total heat available in both fuels operations as shown in **Figure 88**. Methane showed a 2-4% increase in total heat dependent on the AFR and propane showed a 3-6% increase. This additional heat originating from the catalyst could then be used in CHP system. Note that the additional heat was calculated after the catalyst, so harvesting it would not affect the catalyst's performance. For both methane and propane, adding the catalyst reduced the peak BTE between 0.5 and 1% in absolute value. However, the available heat increased more than 2% for methane and more than 3% for propane. Even with lowest heat exchanger effectiveness (50%), the system's UF would improve for both fuels.

Figure 87. Indicated efficiency before and after catalyst installation for methane and propane operation, each point was averaged over 90 seconds of steady state operation.

Figure 88. Total available heat before and after catalyst installation for methane and propane operation, each point was averaged over 90 seconds of steady state operation.

The source of additional heat was mainly from the oxidation of CO in both cases. A higher increase in propane heat was due to additional NMHC oxidation in catalyst as shown in **Figure 88**. For propane, while nearly all CO was oxidized, only some of the fuel was oxidized as shown in **Figure 89**. Fuel oxidation was higher during richer operation since the catalyst temperature was higher at those points. As the engine moved toward leaner operation, exhaust HC energy started converging to the case of no catalyst operation. That meant at those points, the catalyst did not oxidize the HC in the exhaust. In methane operation however, the catalyst did not affect the HC, which was all methane. Engine operation was pushed toward a richer regime to examine if it could trigger methane oxidation, but it only added the unburnt fuel as additional HC energy as shown in **Figure 90**. Note that unburnt is referred to CO plus H_2 energy content.

Figure 89. Propane operation chemical energy losses before and after catalyst, each point was averaged over 90 seconds of steady state operation.

Figure 90. Methane operation chemical energy losses before and after catalyst, each point was averaged over 90 seconds of steady state operation.

4.7 Energy, Emissions, and Cost Analysis

Figure 91 through **Figure 94** show the energy distribution of each fuel at the operating point with peak BTE and COV of IMEP less than 5%.

Figure 91. Energy distribution of peak BTE point with COV of IMEP less than 5% for CNG1, results are averaged for 90 second steady state operating condition.

Figure 92. Energy distribution of peak BTE point with COV of IMEP less than 5% for CNG2, results are averaged for 90 second steady state operating condition.

Figure 93. Energy distribution of peak BTE point with COV of IMEP less than 5% for pure methane, results are averaged for 90 second steady state operating condition.

Figure 94. Energy distribution of peak BTE point with COV of IMEP less than 5% for pure propane, results are averaged for 90 second steady state operating condition.

Table 32 shows the summary of UF calculations for the peak BTE operating point of each fuel. Even though CNG2 had the highest BTE, propane operation showed the highest UF due to added exhaust heat.

Table 32. System UF at peak BTE point for each fuel in [%] of total fuel injected, 75% effectiveness was assumed to waste heat recovery.

	Brake Power [kW]	Brake Efficiency [%]	Heat recovery based on 75% effectiveness [%]	Calculated CO Oxidation heat (40% of CO energy) [%]	Systems UF [%]
CNG1	1.47	27.4	44	1	72.4
CNG2	1.55	29.6	43.6	1	74.2
Methane	1.55	27.8	44.9	1	73.7
Propane	1.69	29.2	45.5	1.4	76.1

Table 33 shows the emissions for peak BTE operation for the various fuels. The GWP values of methane, ethane, and propane for 100 year time horizon used in this investigation were 25, 5.5 and 3.3, respectively [152]. Note that CO₂ equivalent emissions were the sum of CO₂, and the CO₂ equivalents from use of GWPs of methane, ethane, and propane.

Table 33. Specific emissions in g/kWhr for two ends of the fuel spectrum, values represent raw emissions for peak BTE points with COV of IMEP less than 5%.

	CNG1	CNG2	Methane	Propane
Methane (GHG)	11.03	8.94	12.10	0.29
NMHC	0.48	0.55	0.30	5.63
NO_x	7.83	8.58	10.19	10.2
NMHC+NO_x	8.31	9.13	10.48	15.83
CO	21.25	18.91	20.74	30.98
CO₂	673	632	644	739
Equivalent CO₂	950	857	944	765

The engine energy distribution of a small, state-of-the-art micro-CHP system from Honda, tested in multiple national laboratories, is presented in **Figure 95** and **Table 34** [125]. The engine was four-stroke and utilized an advanced Atkinson cycle to improve the efficiency.

Table 34. Energy distribution for Honda micro-CHP system.

Energy Group	Value	
	[kW]	[%]
Total fuel	5.05	100
Work (electric)	1.2	23.7
Cylinder Heat Transfer	1.9	37.6
Exhaust heat	1.4	27.7
Exhaust Chemical Energy	0.16	3.12
Friction + Pumping Loss	0.19	3.76
Generator Loss	0.20	3.96

Figure 95. State-of-the-art micro-CHP system's engine energy distribution.

To compare the potential of the optimized system with an oxidation catalyst, the energy distributions are presented in **Figure 96** and **Figure 97** for peak BTE points of methane and propane, respectively.

Figure 96. Engine energy distribution operating on methane with oxidation catalyst installed after exhaust resonator, the operating point was the peak BTE with COV of IMEP less than 5%.

Figure 97. Engine energy distribution operating on propane with oxidation catalyst installed after exhaust resonator, the operating point was the peak BTE with COV of IMEP less than 5%.

Table 35 provides a comparison of the two fuel extremes with catalysts as compared to Honda commercial system. When comparing the Honda system with methane operation, the data shows that the optimized system, with simple two-stroke technology, was comparable in terms of BTE and overall UF. The two-stroke showed an impressive power density when compared to Honda

system. Note that the Honda engine was PI, so that part of power density was sacrificed the lower cost PI injector.

Table 35. Engine and system comparison for Honda state-of-the-art CHP system and engine used in this research, methane and propane were run on the two-stroke engine.

	Engine Performance and Specifications						CHP System
Cases	Brake Power [kW]	Displacement [cm ³]	Engine Type	Power density [W/cm ³]	Brake Efficiency [%]	Heat recovery based on 75% effectiveness [%]	Systems UF [%]
Methane	1.53	38	Two-stroke	40.3	26.5	46.4	72.9
Propane	1.66	38	Two-stroke	43.7	27.7	48.4	76.1
Honda Engine tested on methane	1.38	163	Four-Stroke	8.5	27.7	46.8	74.5

Table 36 shows the specific emissions for methane and propane operation for the engine with oxidation catalysts installed. For each case, the peak BTE point with COV of IMEP less than 5% was selected. Note that non-handled equipment with $V_d < 66$ were in the class I-A engine family and regulated emissions are presented in the last column. Based on these regulations, the current application research engine will pass the regulation. However, given that the engine application would be for power generation, comparing the emissions with power plant data would give a more realistic estimate of the system's impacts. This analysis is presented later in this section.

Table 36. Specific Emissions in g/kWhr for all fuels, values represent measurements after DOC catalyst for peak BTE points with COV of IMEP less than 5%.

	Methane	Propane	Non-handheld equipment regulations (Class I-A)
Methane (GHG)	16.61	0.30	-
NMHC	3.31	5.48	-
NO _x	12.29	9.54	-
NMHC+NO _x	15.59	15.02	50
CO	0.16	0.38	610
CO ₂	696	832	-
Equivalent CO ₂	1122	858	-

Figure 98 shows the waterfall chart including all the experimental modifications that were validated. The original engine was converted to operate on fumigated NG and yielded an 8% BTE. Applying intake and exhaust optimization each added around 2% (absolute, each), making the engine about 12% efficient. On the original engine, we performed a study on combustion chamber shape and there were improvements in both power density and efficiency [59]. However, the engine brake power was still below 1 kW even with those improvements. Therefore, we revisited the options for improved engine designs, specifically the cylinder bore, porting, and intake method. Finally, an engine was selected which had the desired combustion chamber shape, modified transfer ports, added boost port, and reed valve on the crankcase. This is shown as cylinder optimization in the waterfall chart and was obtained by the boosted engine operation that included optimized intake and exhausts, which improved BTE to 15%. All of the additional modifications were then applied on the boosted engine. Direct injection was expected to improve efficiency dramatically since it was shown that around 38% of the fuel was slipping with PI operation. LPDI added 9% to BTE, which improved BTE to 24%. A 1D simulation and optimization was then performed that targeted an improved multi-variable exhaust design. This 1D optimization yielded an additional increase of about 2% to the BTE. A 3D simulation was performed to investigate in-cylinder stratification. It was found that the spark location could be optimized, and that such modifications added another 1.5% BTE making the engine operate at around 27.4% BTE. Note that fuel variation was not included in this waterfall chart and BTE could be higher based on the fuel variation study presented before. Peak BTE occurred for CNG2 with 29.6% brake power from total fuel injected.

Note that some modifications were dual objectives. For example, intake and exhaust optimizations were important for both for efficiency and power density. However, their effect on power density was so high that they could not be eliminated even if they had only marginally improved the efficiency. This is important when a cost analysis discussion is presented.

Figure 98. Final waterfall chart showing the evolution of system BTE when each modification was applied. Note – results presented for CNG1.

Figure 99 shows the price stepping chart starting from the baseline up to the most efficient design. A baseline price included \$299 for the baseline engine and the costs associated with conversion to natural gas - this included the ECU which was \$360 plus ignition coil setting the baseline price at \$760. The intake optimization excluded the stock intake and carburetor (-\$45 for carb, -\$6 for air filter housing while it added \$60 for the new intake. Exhaust optimization excluded the stock exhaust for \$9.99 where it added \$250 for the new design. For cylinder optimization the difference was between the costs of the stock engine which was \$299 and the full custom engine - \$695. LPDI added \$500 and spark rotation added \$150. The final price for a single unit development was \$2055. The estimation of mass production costs of course could be reduced based on economies of scale. **Table 37** shows the net cost of each hardware optimization.

Figure 99. Stepping chart for price evolution for single engine modifications to achieve highest BTE as presented in Figure 98.

Table 37. Net cost of hardware optimization for engine optimization.

	Net added Cost [\$]	Engine Cost [\$]
Baseline		760
Intake Optimization	10	770
Exhaust Optimization	240	1010
Cylinder Optimization	395	1405
LPDI	500	1905
1D Optimization	0	1905
Spark Location	150	2055

Due to similar nature of optimization for the same color highlighted rows in *Table 37*, they were merged together and used in *Table 38* for a cost analysis. This meant that spark location optimization was merged into cylinder optimization and 1D optimization was merged with exhaust optimization.

According to US Energy Information Administration (EIA), the annual average price of natural gas delivered to residential customers was between 10 to 11 US dollars per 1000 cubic feet (\$/MCF) over the past 5 years [153] [154]. A median value of \$10.50 was used for this cost analysis. EIA performed a residential energy consumption in 2015, including 118.2 million homes in US. Average annual electricity usage was 10,720 kW-hr or equivalent to 1.24 kW constant usage throughout the year [155]. This average power value was used for calculating the fuel cost necessary to produce it.

Intake optimization, exhaust optimization, and LPDI needed additional hardware installation on the final engine design. Therefore, each of these changes were separately applied to the baseline to isolate each change. Each of these modifications were applied separately to the baseline and savings and return of investment (ROI) were calculated. Note that results from 1D optimization of exhaust was merged with empirical exhaust optimization and result for spark plug location optimization was merged with cylinder optimization for a simpler comparison. Results showed that LPDI had the highest potential in savings. Intake optimization had the quickest return on investment (ROI), while exhaust optimization and LPDI showed similar ROI values.

Table 38. Cost analysis of three major modifications on the engine, based on 1.24 kW output for one year 24/7 operation.

	BTE [%]	Fuel needed for 10,720 kWh engine output [ft³]	Annual fuel cost [\$]	Saving/ year [\$]	ROI [years]
Baseline	8.00	526,597	5529		-
Only Intake Optimization Applied to Baseline	10.00	421,277	4423	1106	0.01
Only Exhaust Optimization Applied to Baseline	11.20	376,140	3949	1580	0.16
Cylinder Optimization Applied to Baseline	10.57	398,506	4184	1345	0.29
LPDI Applied to Baseline	11.89	354,256	3720	1810	0.28
All together Applied to Baseline	27.50	153,192	1609	3921	0.19

To analyze how the optimized engine performed in terms of cost and emissions, when compared to current energy providers a large-scale comparison was performed. To form proper combinations

of energy sources used in residential applications, a simplified matrix based on possible combinations in **Table 39**. This formed the way following analysis plots were generated. Note that with GENSETS it was considered that both electric and heat for a home would be provided by the micro-CHP system.

Table 39. Simplified energy source combination of residential applications for cost and emission analysis.

All Energy		Electricity Source		
		Average electric (From NG and coal power plants)	GENSETS Operating on NG engine	GENSETS operating on Propane engine
Heat Source	Average electric (From NG and coal power plants)	State1: Electric+ Electric Heat		
	Pipeline NG	State 2: Electric+ NG Heat		
	Propane	State 3: Electric+ Propane Heat		

To simplify the matrix, cost and emissions for coal and NG power plants were averaged in most plots. In addition, to obtain electricity and emissions output from the current optimized system, a generator and transmission efficiency of 86% and 94% were applied to engine power output respectively as performed in literature [125]. Note that the data for NG and propane operation were obtained from after catalyst installation experiments operating on methane and propane, respectively.

Figure 100 shows the cost analysis for electricity generation from the current system operating on NG and propane when compared to average energy from the electric grid. The cost of electricity generation was \$1125 for grid electric where it was \$1826 and \$4991 for NG and propane, respectively. For electricity use only, the current grid price showed an advantage.

Figure 100. Electric generation cost from grid, NG engine and propane engine, engine is referred to the current research engine.

When including the heat energy in the analysis, the current system showed improved potential with NG operation as shown in **Figure 101**. Note that electric was referred to as the average value from coal and natural gas power plants. Analyses showed that using grid electric plus NG heat would result in a cost of \$1723 for annual energy consumption of 10,720 kW-hr. Based on 75% waste heat recovery (WHR) assumptions from literature, 94% transmission efficiency, and 86% generator efficiency the current engine operating on NG could result into \$1826 annual cost, yielding lower annual energy costs than two conventional cases shown in **Figure 101**.

Figure 101. Total energy cost form different source of heat for homes.

As for emissions, CO₂ equivalent and NO_x in metric tons were calculated for power plants, NG, and propane operation on the current engine. **Figure 102** shows the CO₂ equivalent results from different sources of energy for total energy consumption per year. In all bars the assumption was that the electric was provided from average value of the grid reported by coal and NG power plants. The difference of bars in each case was the energy source used for heat. If electric was used as the heat source, it showed that it would increase the CO₂ emissions. Using NG as the heat source proved to be the best option when using grid electricity. Methane and propane lines show the carbon footprint lines if the current engine drives a CHP system to provide the total energy of the home. The ‘Coal and Coal’ line was worst case scenario when the conventional electric and electric for winter heating were both provided by a coal power plant. Note that government data did include powerplants that were combined cycle.

Figure 102. CO₂ equivalent results for different sources of total energy.

Figure 103 shows the NO_x emissions in metric tonnes per year, for different energy sources. The current grid average showed an average value of 0.018 tonnes per year to produce 10,720 kWh. Note that government power plant data included sites where aftertreatment systems were deployed [156]. So, the lower NO_x included sites that deployed SCR and our engine can achieve lower NO_x with a similar NO_x reduction strategy. The current engine showed 0.152 and 0.118 metric tonnes for methane and propane operations, respectively. This means that for this engine to meet the current power plant NO_x emissions levels, an SCR system with conversion efficiency of above 88% would be required. Achieving this range of conversion efficiency is possible with the right combination of exhaust temperatures and SCR material. Copper based SCRs have shown above 90% conversion efficiency at inlet temperatures of 200 to 330 °C, while iron SCRs have shown above 90% conversion efficiency at temperatures of 330 to 530 °C [157]. Note that due to presence of excessive oxygen in the exhaust flow in two-stroke engines, the implementation of three-way catalysts would not be effective.

Figure 103. NO_x emissions from different sources of energy providing total energy of a home in a year.

5 Conclusions and Framework

5.1 Summary

The objective of this research was to use literature, experiments, and 1D and 3D models to optimize the energy efficiency of a NG two-stroke engine for CHP applications. Based on the results of these efforts a general framework was developed which can serve as a tool for other researchers and industry. The goal was to use the optimized engine design in the GENSETS application.

An experimental laboratory was developed to measure system performance and emissions. In-cylinder, crankcase, and exhaust pressures were recorded in crank angle resolution by Kistler™ Kibox. Low frequency (1-10 Hz) data including mass flows, temperatures, dynamometer, and emission analyzers outputs were measured using an in-house software. The engine was controlled by an open source ECU and its software. Most of the slider crank engine experiments were performed at 5400 RPM. A data analysis platform was developed to combine both high and low frequency data for analysis. This included basic calculations, carbon balance, energy distribution and more. Experiments started with gasoline engine that was converted to operate electronically with an ECU on and using NG. Optimization initially started with intake, exhaust, and cylinder designs mostly from literature recommendations. Then a thorough experimental investigation was performed for LPDI operation. After implementing LPDI, a proper baseline was identified for 1D system simulations and used for exhaust resonator optimization using a genetic algorithm in GT-Power™. These new data served as a baseline for subsequent CFD simulations. In 3D simulations, gas dynamic effects on fuel trapping and charge stratification within the cylinder were investigated and spark plug location was optimized. This step closed the optimization efforts and direction moved toward assessment of gaseous fuel composition impacts on the system performance considering the engine as an energy source for a micro-CHP system. Two natural gas blends, pure methane, and pure propane were tested and analyzed. An oxidation catalyst was then added, and pure methane and propane were tested representing both ends of the gaseous fuel spectrum. Finally, a techno-economic analysis was performed to determine the potential of the system in energy markets and to highlight the cost benefits of major framework steps.

5.2 Major Conclusions

- A framework for energy optimization of small two-stroke engines for micro-CHP application was developed. Following this framework, a relatively simple LPDI two-stroke engine can achieve similar performance as an advanced over expanded four-stroke engine at much smaller size. The framework may more than triple the BTE compared to conventional two-stroke designs.
- The best case BTE was achieved by CNG2 showing 29.6% This was lower than ARPA-E target. However, looking at the state-of-the-art micro-CHP system's engine, it was at 27% BTE. This is the common issue in this size engines that they suffer from high heat transfer in the order of 35% of total fuel energy [135]. This is where bigger size engines with around 500 cc displacement per cylinder, see below 20% of total fuel energy lost as heat transfer [51].
- NG port fuel operation with no intake and exhaust optimization was only at 8% BTE.
- Intake optimization increased the power by a factor of 2.17, delivery ratio by 80% and BTE by 25%, relatively.
- Exhaust optimization from literature recommendations and commercially available components improved the BTE 20% relative to non-optimized stock exhaust operating on PI. It showed 40-65% relative improvements in delivery ratio dependent upon design and adjustments for peak power. It was observed that if the design target is maximizing trapping ratio, one must sacrifice some delivery ratio gains.
- With new cylinder including the head optimization, added boost port, enlarged bore, and modified transfer ports, BTE by 25% relative to baseline engine. It was observed that delivery ratio increased relatively 20% and power density increased by 25%.
- LPDI increased the BTE by 60% relative to PI, recovering most of the slipped fuel, owing to a higher efficiency and balanced energy distribution which improved UF.

- A 1D simulation optimization showed another relative increase in BTE of 8.3% compared to literature recommended exhaust designs. When combining effects of 1D simulation optimization with recommended literature designs, BTE increased by 40% non-optimized stock exhaust operating on PI.
- While literature's rule of thumb was mostly focused on one factor (independent variable) and objective at a time, 1D simulation was able to combine all factors and find the best combination within the design space for variety of objectives which in this case was thermal efficiency.
- A 3D CFD model helped with spark plug location optimization based on charge stratification at spark timing, yielded an additional relative increase of 5.7% for BTE when compared to non-optimized location. This impact was attributed in the form of chemical energy recovery and more complete combustion. It decreased the combustion duration by more than 20% when compared to non-optimized location. In optimizing spark location, engine speed impacts the charge stratification in the cylinder and spark timing determines at what crank angle degree one must examine the charge distribution for spark plug placement. The benefits shown here were for engine speeds of 5400 RPM and spark timing at 26 CAD BTDC.
- In fuel variation tests, denser NGs with higher alkanes showed higher BTE mostly due to lower incomplete combustion and unburnt products. Propane showed the highest power density and higher heat available for CHP systems. This made its UF to be the highest among fuels tested.
- In oxidation catalyst tests, it was shown that except for rich cases of propane operation, a platinum only oxidation catalyst did not have any major effect on HC oxidation. However, the catalyst added heat from 2 to 6% for methane and propane, which would translate to an improved UF which more than offsets slight reductions in brake thermal efficiency.
- With 75% heat exchanger effectiveness and available heat from experiments, this size engine can supply up to 24,000 kWh heat for a year while generating 10,720 kWh of electricity. Six month average US winter heat energy was reported around 14,000 kWh.

This shows that this system may be capable of meeting the required heat for home while supplying the needed electric power.

- With optimal spark location, even with a stratified mixture, a highly stable combustion (COV of IMEP less than 5%) with at least 20% faster combustion was achieved.
- Applying LPDI resulted in the largest reduction in fuel costs to produce 10,720 kWh (US annual average electricity). It would have saved \$1810 on NG price when compared to PI operation. Exhaust optimization (including 1D simulations), cylinder optimization (including spark location), and intake were next in the line for savings. Total savings on fuel cost with all optimization applied was estimated as \$3910 annually.
- If class I-A emissions regulations for non-handheld devices was a compliance metric, the optimized engine was compliant with regulations. However, one should note for this category only HC+ NO_x and CO are regulated whereas in power generation all data including CO₂ equivalents and NO_x were important.
- When comparing CO₂ equivalent to data from coal and NG power plants, depending on different combinations of heat source for the home, this optimized engine could serve as the prime mover for a micro-CHP system with better performance. With coal power plant electric and any other source for heat, the optimized engine had lower CO₂ emissions for both methane and propane. If all heat was provided by the average value for coal or NG power plants, the system would still emit less CO₂ equivalent emissions.
- When comparing the NO_x emissions with power plant data, the conclusion was that the engine operating on NG would require an SCR with 84% or more NO_x conversion efficiency to perform equally or better than current power plants (many of which employ similar SCR technologies). This value was 88% for propane operation. Copper SCR systems have their peak conversion efficiency at lower temperature when compared to iron SCR and would likely perform well given the ranges of experimental exhaust temperatures.
- As for the cost of energy per year based on 10,720 kWh annual consumption, the optimized engine would operate very close to the current cheapest energy source combination, which was using average electric from the grid and NG for heating purposes. This would cost \$1753 while the optimized micro-CHP system providing the total energy of the house with

NG, would cost \$1826 on fuel standing lower than any other common combinations. Propane operation could cost up to \$4992 so, it did not seem like a viable option for large scale deployment except to serve remote, off-the-grid locations where it was the only available energy source.

5.3 Framework

Using a combination of experimental and modeling research combined with literature, I have developed a framework for optimization of micro-CHP applications that use gaseous fuels and two-stroke combustion cylinders. This general framework can be used by researchers and industry as a set of “rules of thumb or guidelines” for the design or modification of small engines that could serve as the prime movers of micro-CHP systems. Following these guidelines will significantly improve the utilization factor and performance of a micro-CHP system by improving efficiency, reducing emissions, maximizing useable heat, and improving combustion stability.

Note that this optimization focused on an application where power, stroke, and frequency were defined as fixed targets. Stroke and frequency limitations were imposed by nature of future application to oscillating linear alternators whereby frequency and stroke are limiting design factors. Included in this framework are empirical elements from literature that should be included when a set of initial design variables may be more flexible.

1). General Engine Design or Selection

- It was shown that increased speed enabled improved efficiency mainly from a reduction in heat loss. Reciprocating speed impacts on wear/durability and electrical generation speed and efficiency must be investigated.
- Power density – engine design should include a boost port and reed valves, as they are often excluded for small engines which would serve micro-CHP systems.

2). Operation requirements

- This framework requires electronic control of the engines, which is typically neglected for engines of this displacement range. This requires proper hardware and calibrations for robustness. A trigger wheel with ability to discretize each revolution to at least 10 CAD intervals and an ECU. The ECU can achieve higher resolutions by interpolating and be used for high resolution control of ignition and injection (0.1 of CAD).

3). Intake Optimization for Improved Breathing

- Literature estimates that intake resonators with frequency about 2 times the piston frequency should yield the highest improvement in delivery ratio and power. This was confirmed in this work with laboratory experiments as well as improvement in BTE.

4). Exhaust Optimization for Further Improvements in Breathing

- Literature suggested methods for designing exhaust resonators with the aim of improved power density, however, exhaust tuning was also demonstrated as important for efficiency optimization.
- Rules of thumb in literature can be used with commercially available components following Helmholtz theory to improve delivery ratio and trapping efficiency.
- More improvements can be made with slight geometric adjustments. A 1D simulation can be used to determine a design that provides further improvements. This served as a cost-effective method (even though it required experimental efforts) because the final optimized design would be used for mass production of system components.

5). Cylinder Design Optimization

- Head design is recommended such that it is dome shape and dome's area is 50% of the bore area. The idea is to minimize the squish band volume and improve the combustion efficiency (reducing flame quenching). In the experiments it was observed that it could increase BTE by 10% relative improvements in the BTE and power density.
- A boost port is recommended by literature to increase the scavenging efficiency and tumble motion for a better mixing and this was confirmed here for small displacement two stroke engines.
- Transfer port area and angle are considered as impactful parameters for delivery ratio and mixing by literature and were validated with a custom design.
- Exhaust port timing and area is identified by literature as impactful for both delivery ratio and trapping ratio due to its direct interaction with exhaust resonator.

6). Low-Pressure Direct Injection

- Outwardly opening poppet style air injectors can serve as the basis for delivery of gaseous fuels onto small-displacement two-stroke engines as a method to simultaneously reduce emissions and improve efficiency. Such a physical design enables the use of low gas pressures which are more likely available and would negate additional compression work.
- Due to overlap of scavenging and injection event in LPDI operation, controlling SOI was of high importance for highest trapping ratio.
- DOI affects the injected plume penetration, charge stratification, and injector's ability to inject fast enough with engine's high speed. For engines of this size and speed with current commercial injectors, a fine balance must be selected. Note that an engine speed 5400 RPM combined with a short stroke (30 mm) there were only 11 milli seconds in an engine revolution. Total injection durations for this work were on the order of 1 milli second.
- Subtle ignition timing control is needed for maximum power output and best efficiency.

7). Optimal Spark Plug Placement

- CFD simulation showed that with LPDI, charge stratification investigations with crank angle resolution were necessary to find the optimal location for spark plug based on MBT timing and operating speed. Engine speed and fuel composition are two important parameters affecting the details of stratification in this study. Note that in addition to speed and timing, fuel characteristics should be examined to ensure accurate modeling of stratification.
- In experiments spark plug modification improved brake power, delivery ratio, combustion efficiency, and BTE.

8). CHP Analysis

- An oxidation catalyst added to the total recoverable heat from engine operation - 2-6% of total fuel energy for methane and propane. With 75% heat exchanger effectiveness this additional recovered heat would be added to CHP system's UF.

Note that the order in this framework matters. Engine selection effects all optimizations that follow. Intake optimization should take place first since it does not interact with the cylinder directly unlike exhaust resonator (especially where reed valves are implemented). Exhaust resonator optimization is recommended second to provide the best wave resonance for improving the cylinder trapping ratio. Cylinder optimization and LPDI can be completed together to optimize mixing. Cylinder optimization would help the power density, combustion efficiency and lower heat transfer. The LPDI strategy must be selected based on engine size and its scavenging paradigm. Completing these steps, a reasonable baseline would be formed for system simulation and optimization. Following the system optimization, CFD investigations for further optimization should be performed.

5.4 Recommendations

Initially, the outcomes of this research were to be transferred to an oscillating linear engine alternator. By the end of this dissertation the transition to linear engine has not happened. There are few recommendations when transferring this framework to the linear engine:

- Linear engine scavenging must be revisited with CFD and compared to slider crank engine. This is simply because linear engine piston velocity profiles are different than slider crank engines. This can be addressed with confidence, with additional CFD modeling.
- Linear engines have the ability to obtain variable compression ratios and its control in terms of combustion stability is more challenging. MBT timing and injection timing control should be revisited after transferring to the linear engine.
- If the linear engine operates at a different frequency compared the slider crank, the framework should be followed to achieve peak efficiency at the desired frequency. Note that for small variations in frequency, efficiency would not change dramatically but speed does impact multiple operating parameters.

As for slider crank research, a wide range of technology and hardware screening was performed to improve the BTE of a small displacement two-stroke engine to 27.5%. However, there are still some areas that could receive more attention for further improvements in the future.

- Note that this research effort was not completely exhaustive and further improvements could likely be made using subtle port and timing modifications by additional 1D and 3D simulations.
- Currently, due to central injection, the spark had to be mounted at an angle. However, combustion chamber shape was designed for a centrally installed spark plug. A comprehensive cylinder head optimization by CFD study should be performed to optimize the shape of the combustion chamber as well as spark plug and injector locations.

- For steady state operation and a given speed, further CFD modeling would help in further optimizing the port timing. For exhaust port timing optimization, a co-simulation of 1D and 3D CFD is recommended.
- An investigation on how much additional EGR can help to reduce the NO_x seems to be very crucial given the high NO_x level of the engine. If found effective, a new round of optimization can be performed to optimize the EGR level for minimizing the NO_x . Alternatively, an SCR system with conversion efficiency above 88% will allow the micro-CHP system to provide annual total energy of a home with equal or better NO_x than current power plants. This engine did not show any NH_3 in the exhaust so passive SCR would likely not be an option for NO_x reduction.
- Given that copper SCRs have their peak conversion efficiency at lower temperatures when compared to iron SCRs, a study of after-treatment configuration would help to find the correct placement for SCR and oxidation catalyst to ensure proper light-off, proper resonator temperature, and heat recovery.
- With the high amount of heat transfer for all fuels, applying a thermal barrier coating to cylinder head and piston crown, should be investigated in the future. This will likely enhance the heat content in the exhaust for waste heat recovery and may improve catalyst oxidation of HCs.
- Research should examine implementing a knock sensor or other novel approach to find the MBT ignition timing based on fuel quality variation. In this case, the knock sensor response should be used to determine the best combustion phasing which can represent a few percent change in BTE.

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