# The study of syngas through the Partial Oxidation of methane and its role as an energy source

by

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# Abstract

The goal of this thesis is to explore the methods for syngas production with a focus on the Partial Oxidation of methane (POX) and to study its role as a source of energy. In our experimentation we studied the potential of a batch detonation method in a constant volume chamber. From these experiments, we found that the detonation products followed our predictions based on the POX reaction. Following this we moved to test the possibility of repurposing a spark ignition internal combustion engine for a continuous flow of syngas. Through these experiments we found that FT-IR and GC shows that syngas is producible.

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# Acknowledgements

I would like to first express my full appreciation to Dr. Sorensen, for guiding me through to my MS. I would next like to thank Dr. Matt Berg and Dr. Jeremy Schmidt for being on my committee.

# Dedication

This is dedicated to my family.

# Chapter 1 - Introduction

As every facet of our world grows in every direction, so too should we diversify our energy sources. One way that this diversity can take its next step is by recognizing the limitations of current energy reservoirs. A study in fossil fuel reserves, suggests that by 2042 the world will be restricted to coal as its single available fossil fuel source [1]. That, and other research, shows the need to restructure some of the most basic energy assumptions the world relies upon. One of these prominent modern energy sources is synthesis gas, a combination of hydrogen and carbon monoxide. The reactants for syngas have been shown to stem from the byproducts of oil drilling [2] and bio-waste [3]. This thesis will show the ability to make use of methane, under the assumption we are using filtered natural gas, to produce synthesis gas. This will be done by making use of an internal, spark ignition, combustion engine along with an alternative method involving a gaseous detonation in a constant volume chamber. However, before the experimental explanation we will discuss the chemistry/physics behind the importance of synthesis gas; that will be followed up by a brief description of the necessary engineering background information. This will then end with a discussion of possible alternative for synthesis gas production and other environmentally friendly energy sources, that are still developing.

## Important Terminology

The purpose of this section is to introduce a selection of information that serves an index to the primary topics of the thesis. This will be split into two major parts; firstly, it will focus on introducing the chemistry and physics foundation that the later sections will stand on. Then it will provide an understanding of an engine and its cycle.

### Chemistry & Physics Supplementary Information

This section serves the purpose of introducing and discussing the idea of carbon neutral energy, in relation to the environmental impacts, it will also bring into focus and define synthesis gas. After these definitions, we will dive into a discussion of hydrogen production methods with a focus on several specific chemical reactions.

Today, the environmental impact of greenhouse gases and the future of renewable resources has a tight hold on the mindshare of the world's growing population. Due to this, some clarification of these terms, and their relation to this thesis, would only benefit the readers.

To begin with, carbon neutral energy, is any energy produced that does not add to the $CO_2$ levels in the atmosphere. To emphasis the importance of a carbon neutral energy, it is currently estimated that in 2018 the world emitted 46.94 billion tonnes of greenhouse gases (GHG), which includes 34.81 billion tonnes of $CO_2$

from fossil fuel use, making up 74.15% of GHG. That has led to an overwhelming $CO_2$ atmospheric concentration of 417.68 part per million (ppm) as of 2022 which has grown from 277.15 ppm, since the start of the industrial revolution. This has contributed to a global average temperature rise of 1.05 C [4]. Fig. 1.1 shows the average temperature anomaly rise. This shows the growing need for a carbon neutral energy source to curb the growing global temperature rise.

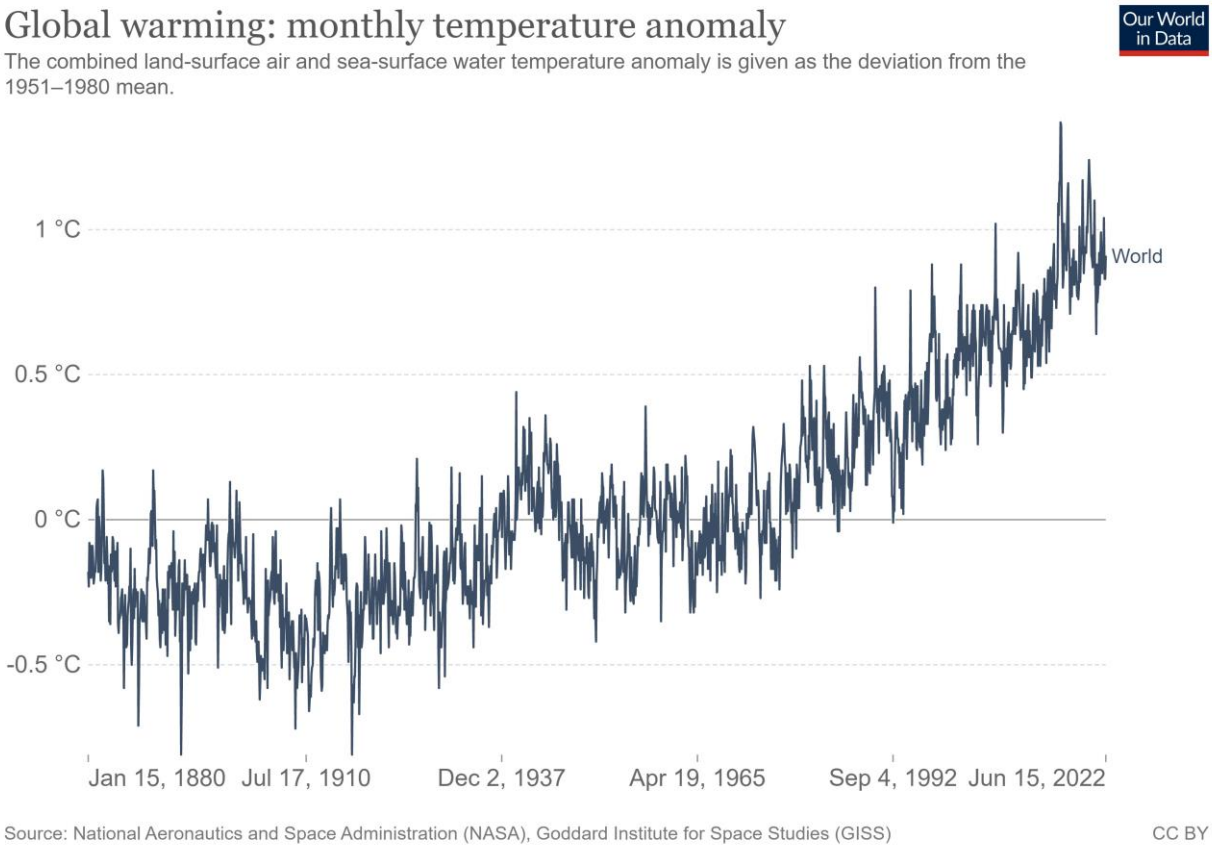


**Figure 1.1 The global temperature anomaly.**

Having glimpsed a facet that is the rising problem of carbon producing energy sources, it is prudent to introduce the goal of this thesis. That is the

production of synthesis gas, commonly referred to as syngas, from the reaction of air and a feedstock of methane, as a substitute for natural gas. Syngas is largely a gaseous mixture of hydrogen and carbon monoxide. As most of the natural gas is a byproduct of a nonrenewable resource, syngas production from this is not the total solution to the climate problem; however, as a carbon neutral energy source this is a next step that pivots energy production towards the use of more environmentally friendly energy sources.

If the goal of the world is to reach a point of total carbon neutrality and reliance on renewable energy sources, then due to the lack of flexibility in the energy infrastructure, a total conversion will take many steps, as partially envisioned by the U.S Department of Energy [5]. It makes sense to use and improve the already existing natural gas infrastructure. Using the infrastructure has the potential to reduce the need for gas flaring. Gas flaring is a common method of burning up the gaseous byproducts from the oil drilling process [2].

Now that there has been sufficient evidence of environmental motivation and impacts of carbon neutral sources and syngas. We turn our attention to several specific chemical reactions, used throughout the industry, that use methane as a reactant to produce syngas. The following information has been mainly split between the endothermic and exothermic reactions. The endothermic reaction pathways are reaction types that absorb energy from the system. For this

thesis, it will discuss the Steam Reforming of methane (in tandem with the Water Gas Shifting reaction) and the Dry Reforming of methane. However, the reaction that is expected to be seen in the experiments conducted is the Partial Oxidation of methane.

**Steam Reforming of Methane (SRM)**

Steam Reforming of methane is the reaction process, shown by the following reaction equation, in which methane passes over steam forming the products of carbon monoxide and hydrogen gas.

$$CH_4 + H_2O \leftrightarrow CO + 3H_2.$$

This method of syngas production is the most widely used method, and as shown to produce about 48% of hydrogen (Ferreira-Aparicio et al., 2005, p. 11). A downside to this method is that it is common for this reaction to be followed up by the Water Gas Shift reaction, this results in the need of an external energy source. However, alone the enthalpy change of SRM is

$$\Delta H° = 206\ kJ/mol.$$

**Water Gas Shift Reaction (WGS)**

The Water Gas Shift reaction is common follow up reaction to the SRM reaction, to maximize the amount of hydrogen produced. In this reaction, the carbon monoxide formed in SRM reacts with the water/steam allowing the oxidation of carbon monoxide forming carbon dioxide and the formation of hydrogen gas. This is given by the following reaction equation,

$$CO + H_2O \leftrightarrow CO_2 + H_2.$$

With the change in enthalpy being,

$$\Delta H° = -41.2\ kJ/mol.$$

The SRM followed up by the WGS reaction is an intensive process that requires many steps to extract a useful hydrogen source, along with this these two reactions have many problems, such as significant coking and heat transfer loss. One method that for getting around these shortcomings is using a membrane reactor, that promotes hydrogen production and separation [7].

**Dry Reforming of Methane (DRM)**

DRM refers to the chemical reaction process in which methane is ran over carbon dioxide giving the products of carbon monoxide and hydrogen gas, this given by the following reaction equation,

$$CH_4 + CO_2 \leftrightarrow 2CO + 2H_2.$$

Like the SRM this reaction is an endothermic reaction with an enthalpy change of

$$\Delta H° \approx 260kJ/mol.$$

DRM is seen as a reaction technique that has a future in areas that have large carbon dioxide and methane, such as natural gas fields, landfills, or large agriculture hubs. However, like SRM, DRM suffers from large coke depositions on catalysts [7], [8].

Now that there has been an overview of endothermic syngas producing reactions, we move to examine the exothermic reaction, these release energy to the

system, that we expect to see in our experiments. Exothermic reactions are generally preferred for this experiment due to the energy released; however, as the goal of this thesis is to focus on the carbon neutral energies, it must also prioritize the products.

**Partial Oxidation of Methane (POX)**

The POX reaction pathway, out of the three discussed here, is the only reaction that occurs in sub stoichiometric amounts and follows the general reaction equation of

$$C_nH_m + \frac{n}{2}O_2 \leftrightarrow nCO + \frac{m}{2}H_2.$$

Due to the exothermic nature of POX, when run in tandem with the endothermic reactions mentioned above, it can reduce the activation energy required for those reactions.

Syngas has a high variety of uses even beyond hydrogen gas's ability to carry energy. Medrano-Garcia et al. (2018) provides a multitude of uses for differing ratios; this includes at ~2 $H_2$/CO syngas is largely used for the Fischer-Tropsch Synthesis and methanol production, at ~ 1 $H_2$/CO (or possibly lower), it is useful to synthesize ethanol, higher alcohols, and dimethyl ether. As shown in this section, the Partial Oxidation of methane, is the more ideal reaction to produce syngas, when compared to the SRM (with the WGS) and DRM, not only for its

exothermic properties and products, but for the fact that is a single step synthesis of syngas.

# Chapter 2 - Experimental Methods

The Experimental Methods section discusses the details of both experiments. Along with both experiment setups, it is important to include the procedure and safety measures that are needed to conduct the experiments in both a safe and repeatable manner.

## Detonation Chamber

### Setup

The experiments were performed in a 17.1 L aluminum cylinder, shown below. The chamber's dimensions are as follows, there is an internal diameter of 24 cm and height of 37 cm, with walls that are 2.54 cm thick. The chamber and the lid are sealed together via an O-ring and 12 bolts. Various gases are passed through into the chamber via a custom manifold connected to the lid, this custom manifold contains the sparking system that will provide the energy to jump start the reaction. Above the manifold is the circuitry that directs the flow of gases towards or out of the chamber. Along with the manifold, directly attached to the lid is the manual valve that allows us to easily collect the gaseous products.

The laboratory setup for the detonation chamber in total takes up four rooms. The most outer room that is easily accessible is the computer that run LabView,

this is the software that allows us to control the chamber. This includes the fill rates that are controlled by electronic flowmeters, but also the evacuation of the chamber via vacuum pumps. The next two rooms are on opposite sides of each other contain the vacuum pumps and our gaseous reactants. In between the 1st room and the both the 2nd and 3rd rooms in the chamber room. It is in this room that the detonations, inside of the chamber, takes place.

**Detonation Lab Safety Procedure**

The Detonation Chamber room and the computer control room are separated by a 0.476 cm thick wall. This latter room is the room that is occupied by the various scientists involved. It should be noted that these rooms follow the standards set by OSHA and are routinely inspected.

Our detonation process can be divided into three phases. The first phase can be described as the evacuation phase. Upon initializing the detonation start up sequence, all occupants of the detonation chamber room have already evacuated the chamber room, and it is closed off until the detonation has run its course. For an extra safety measure there is a light tower with a speaker that rings during each reaction phase.

During the first phase the chamber is opened to the vacuum pump valve that evacuates it to a -29” Hg gauge vacuum, which is monitored on the computer via the LabView software. The second phase is the fill phase. During this phase

Labview fills the chamber with the gaseous reactants. This leads to the final phase, the detonation phase. Immediately after the chamber is filled, the valves close, isolating the manifold and chamber together. Then the sparking system detonates the gaseous mixture, and an audible ring is heard that is caused by the detonation. Once the chamber room is deemed safe to enter, the pressure is read on the chamber, and the products are sampled and pulled into a Tedlar bag for analysis. The chamber is then evacuated and, depending on the reaction, needs to be cleaned before another experiment is conducted.

## Engine Method

This subsection will focus on providing an adequate description of the chosen engine and the experiment's setup. The secondary and tertiary topics discussed are the procedure we have chosen to maximize the safety and controllability of the experimental engine.

### Engine Specifications & Setup

The experiments conducted for the construction of this paper used a Kholer Command Pro CH395TF commercial engine with the provided natural gas regulator not attached. Table 1 shows the engine's specifications, as reported by Kohler. This engine model was chosen for these experiments due its availability to the general population.

| | |
|---|---|
| Model | CH395TF |
| Hp (kW) | 9.5 (7.1) |
| Displacement in $cm^3$ | 277 |
| Bore (mm) | 78 |
| Compression Ratio | 8.8:1 |
| Dimensions LxWxH (mm) | 404x427x424 |
| Certified RPM | 4000 |

**Table 2.1 The specifications of the CH395TF as reported by Kohler.**

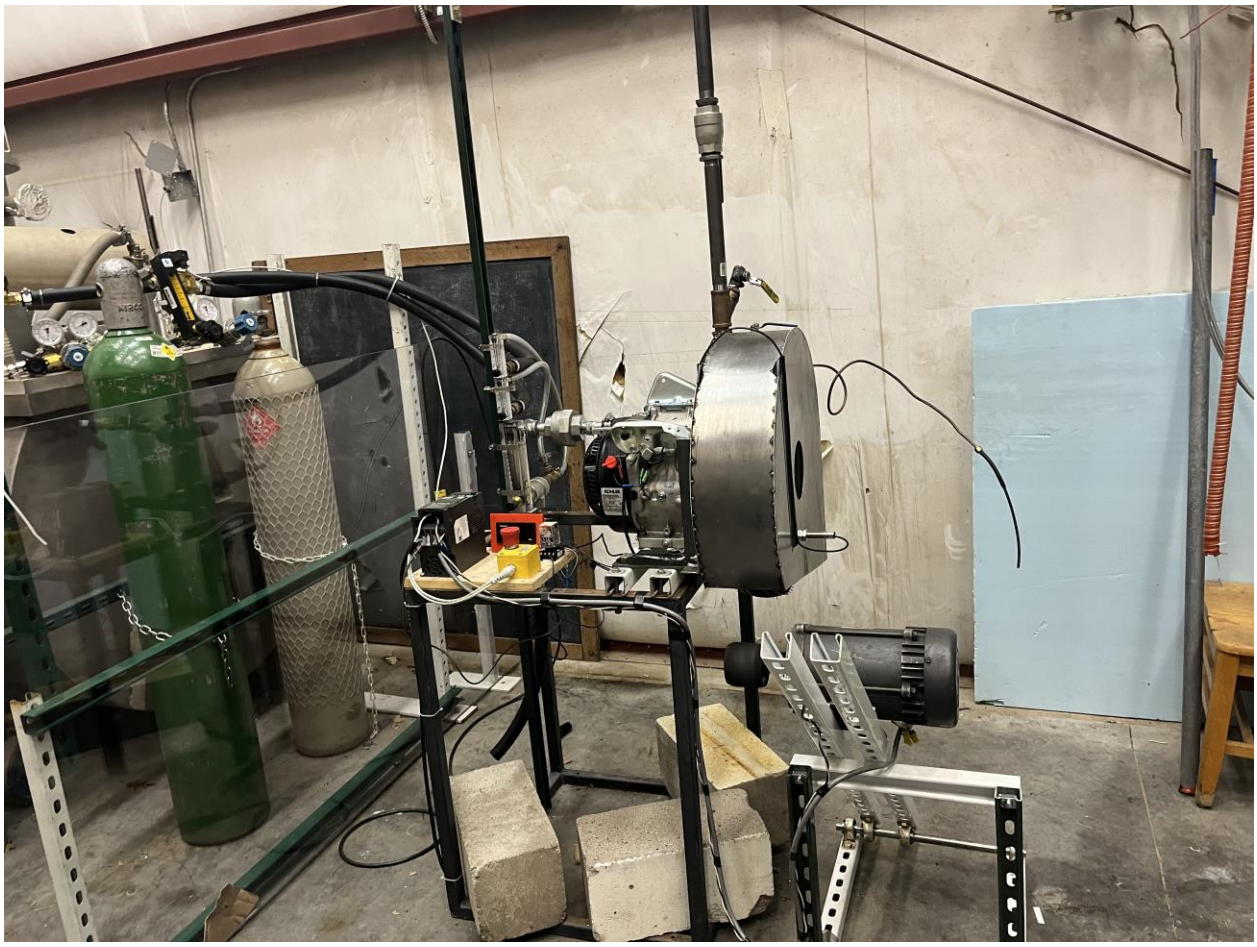

**Figure 2.1 The full engine setup. Left are the compressed gases; the middle has the engine and frame. Right is the electric start up motor.**

Figure 2.1 shows the set up for the spark ignition engine experiment. In this experiment, the engine has been attached to a frame and has been secured to the floor with cement bricks to reduce the vibrational motion caused by from operating the engine. The regulator, known as the *Tri-Fuel conversion kit*, was removed, and replaced with our own regulator set up. To overcome this issue, as shown in Figure 2.1, the mixed compressed gases (oxygen and methane) and air were controlled via

a fine-tuning manual mass flow regulator. Attached to the input orifice of the fine-tuning regulator is a T-valve, with two positive flow connections. The first of the two, is the source of the mixed compressed gases, as mentioned earlier, the other opening is the source of uncompressed air that is pulled in by the engine. To allow for the possibility of running the engine without the addition of air, there is a manual valve that shuts off the flow of air. In the setup, before the compressed gases are mixed, each gas has two regulators, one that allows for a large flow. Then, closer to the mixing point, on the engine's frame is a manual mass flow regular that allows for the gases' flow to be fined tuned.

Continuing with a description of the setup, attached to the rotating arm is a wheel that is used to turn over the engine. Turnover is done by connecting a 3-phase push-to-start electric motor that is only in physical contact with the engine for cold starting. Covering the wheel is a custom wheel well that has a tachometer, used to measure rpm, placed on the well.

A 4-way pipe connection that connects to the exhaust of the engine, has been attached for multitude of purposes. One orifice has a long vertical pipe to allow uncollected exhaust to flow out. The second hole has a manual valve that allows us to insert a thermometer into the exhaust piping. The last orifice, has another manual valve attached that connects to copper tubing, which is used to dissipate

the exhaust's heat to a temperature that allows us to collect an exhaust sample in a Tedlar bag.

**Operational Safety Measures**

This section will discuss the precautions taken and accessories added to the set up to ensure the safety of the people using the engine. To present the information in a meaningful way this section is split into three parts. The first part will focus on changes made directly to the engine and compressed gas tanks. The second, will focus on the electric motor used to turn over the engine. The last part will explain the steps taken to ensure the lab environment is safe.

The engine itself has had numerous changes made to it to ensure only purposeful use. Due to the addition of a custom gas regulation set up there has been a normally-open manual emergency shut off valve that will not only close the intake opening on directly on the engine, but will also cut off the flow of gases from the air-fuel mixing point. The compressed gas tanks and the engine have each been secured to their own metal frame that has been bolted to the ground, to prevent any unnecessary motion from the engine. On the engine’s crankshaft the wheel has been encased in a metal box, this to prevent any unnecessary contact with the wheel while the engine is being operated.

This takes us to the electric motor that will be used to turn over the engine during the start up. To prevent any unplanned contact between the engine’s wheel

and the motor, the motor attached to custom metal sled that must be raised to wheel. This allows us to take advantage of gravity as the force that actively wants to keep the motor and the wheel separated. The motor must be activated by inputting the correct sequence on a three-to-one phase power converter, which has been placed in a spot for a second person will do this. Even after the correct sequence is used, a push-to-start button, on the sled, must then be pressed by the person raising the motor to the engine's wheel. These safety measures ensure that the motor is only used as planned.

To ensure that the environment is safe for the experimenters the engine has been placed in a well-ventilated area. The room has a large raising metal door and a large exhaust fan placed in the wall; these prevent the buildup of harmful gases in the room. Along with these inherent environmental safety advantages, a pipe has been attached to the exhaust hole, so that the exhaust is expelled away from the experimenters. Ear plugs have been made available for noise reduction. The room has also been equipped with a fire extinguisher and marked emergency exits. These safety measures ensure that the room may be occupied and emptied safely throughout the experiment procedure, by the participants.

**Procedure for Manual Operation of Engine**

Before starting the engine, the most important task is to ensure the personnel safety equipment is distributed; this includes earplugs, and face/eye protection. The

next most important step is to allow a proper air flow throughout the room and to start up the exhaust fan. Moving to the engine, after confirming that the methane flow is minimized and oxygen content is high, the engine is ready for the startup procedure.

Engine startup is accomplished via the electric motor; to do this the correct start up code and desired rpm, for the electric, must be entered into the power converter. Then, the electric motor is brought into contact with the wheel, attached to the engine's crankshaft, while simultaneously pushing the startup button attached to the motors handle. After turning over the engine, the electric motor is returned to the lowered position.

During the operation of the engine, the oxygen/air content is slowly lower while simultaneously, and cautiously, raising the fuel (methane) flow into the intake valve. Once the engine is running "smoothly," achieving a semi-periodic pulse, at the desired $\frac{O}{C}$ ratio, a sample can be collected. Sampling of the engine's exhaust is done by connecting the sample bag to the copper pipe. To collect an exhaust sample using only compressed oxygen, the manual valve that allows for the intake of atmospheric air must be slowly closed during the previously mentioned step. To shut down the engine, the emergency shutoff valve may be activated, cutting off the flow of compressed gas to the engine. These operating

procedures discussed prioritize the safety of the experimenters and the surrounding environment.

## Predicted Results

A key part to scientific research is developing a theory then testing it, leading to reevaluating the theory repeatedly. Thus, it makes sense to start with this, which comes in the form of a general reaction equation,

$$xCH_4 + yO_2 \rightarrow \alpha CO + \beta H_2O + \gamma H_2 + \delta CO_2.$$

These products were chosen due to the expectations of seeing both an incomplete and complete combustion reaction of the fuel. The products for a typical combustion reaction are $CO_2$ and $H_2O$, while an incomplete combustion reaction generates CO and $H_2$.

Now that we have the general reaction equation, we want to predict the molar breakdown of our products, this means determining the values of $\alpha, \beta, \gamma,$ and $\delta$. We can do this by determining the limiting factors for the formation of each product. An example of this is that methane is the only carbon source thus limits the production of carbon monoxide and carbon dioxide, giving the equation,

$$x = \alpha + \delta.$$

Using this same reasoning, it leads to the development of two more equations:

$$2x = \gamma + \beta \ \& \ 2y = \alpha + 2\delta + \beta.$$

These are determined from the hydrogen and oxygen limiting factors. However we only have three equations, but we have four unknowns. This means we need to develope a fourth equation. This task is however easier than it seems, due to the closed nature of our system, we can easily apply the ideal and combined gas laws. Giving the equation,

$$n_f = \frac{p_f n_i}{p_i},$$

With $p_i$ and $n_i$ being the initial pressure and moles from our reactants, while $p_f$ and $n_f$ describing the final pressure and moles of our gaseous products, respectively. This leads to last equation needed to predict the outcome of the reaction,

$$n_f = \alpha + \gamma + \delta.$$

Giving the system of equations that's easily seen and solvable in the form of an augmented matrix.

$$\left[\begin{array}{cccc|c} \alpha & 0 & 0 & \delta & x \\ 0 & \beta & \gamma & 0 & 2x \\ 2\alpha & 2\beta & \gamma & 0 & 2y \\ \alpha & 0 & \gamma & \delta & n_f \end{array}\right]$$

This is the completed set of equations that will describe the reactions we expect to see from the detonation occuring with in our chamber, assuming that you know the molar values of each reactant and the combined molar value of the gaseous products. To solve this augmented matrix, one just needs to use Gaussian

Elimination [17]. To be able to repeatedly predict the products and the molar values of each product shows that the theory is sound and it is reproducible.

# Chapter 3 - Experimental Results

This section will discuss the results from the experiments involving the detonation chamber. The detonations were conducted in 2 series of experiments. The first was conducted with compressed oxygen, the second used compressed air (composed of ~78% $N_2$, ~22% $O_2$). This will then lead into a presentation of the commercially available IC engine's ability to produce syngas.

## Detonation Chamber

### Oxygen & Methane Detonation

The product samples were collected immediately after each detonation along with the corresponding pressure. The O/C ratios detonated are greater than 1, this is due to the lower flammability limit. The LFL is lowest concentration in which a gas will ignite air [18]. The table below shows the various reactant ratios that were conducted with the compressed oxygen.

| O/C | $CH_4$ (Moles) | $O_2$ (Moles) | Initial Pressure (atm) | Final Pressure (atm) |
|---|---|---|---|---|
| 1.6 | 0.39 | 0.31 | 1.06 | 1.39 |
| 1.8 | 0.37 | 0.33 | 1.05 | 1.23 |
| 2.0 | 0.35 | 0.35 | 1.05 | 1.03 |
| 2.2 | 0.33 | 0.37 | 1.05 | 0.93 |

**Table 3.1 Ratios of O/C that successfully detonated**

It should be noted that an O/C ratio of 1.4 was attempted several times, however we were not able to achieve a detonation.

**Air & Methane Detonation**

Compressed air was chosen to be used for these experiments to determine the degree to which it was possible to use atmospheric air, instead of oxygen. Table 3 shows the reactants that were used for the portion of the detonation experiments, where in compressed air was used instead of compressed oxygen. The purpose for the distinction between atmospheric air and compressed oxygen, is due to the nitrogen gas that is present in earth's atmosphere, studies have shown that the POX reaction can produce NOx molecules that are harmful to the environment and for the purposes of this thesis we look to avoid this.

| O/C | $CH_4$ (Moles) | $O_2$ (Moles) | Initial Pressure(atm) | Final Pressure (atm) |
|---|---|---|---|---|
| 2.45 | 0.196 | 0.251 | 2.0 | 1.84 |
| 2.45 | 0.196 | 0.251 | 2.0 | 1.99 |
| 4.00 | 0.128 | 0.254 | 2.0 | 1.7 |
| 3.97 | 0.191 | 0.95 | 1.5 | 1.33 |

**Table 3.2 The reactants and both the initial and final pressures**

Transitioning to the post detonation analysis, sample of the products were collected immediately post detonation and sent off for analysis in groups. Fig. 3.1 shows the plot of the Gas Chromatography analysis for the oxygen detonations.

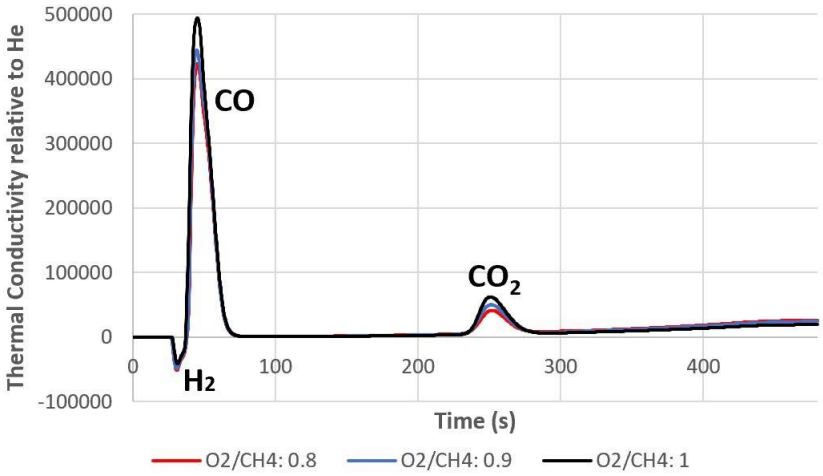


**Figure 3.1 The Gas Chromatography analysis for the O/C ratios: 1.6,1.8, 2.0. There were difficulties in collecting a sample of the 2.2 ratio detonation. All GC analysis was completed by Dr. Covarrubias**

From figure 2 it is clearly seen that there is noticeable a presence of hydrogen, carbon monoxide, and carbon dioxide in each of the detonations. This shows that syngas, is clearly producible in the oxygen detonations. Looking further into the GC analysis, fig. 3.2 show a close-up of the 3 regions belonging to fig 3.1 that show the detonation chamber is producing hydrogen, carbon monoxide, and carbon dioxide.

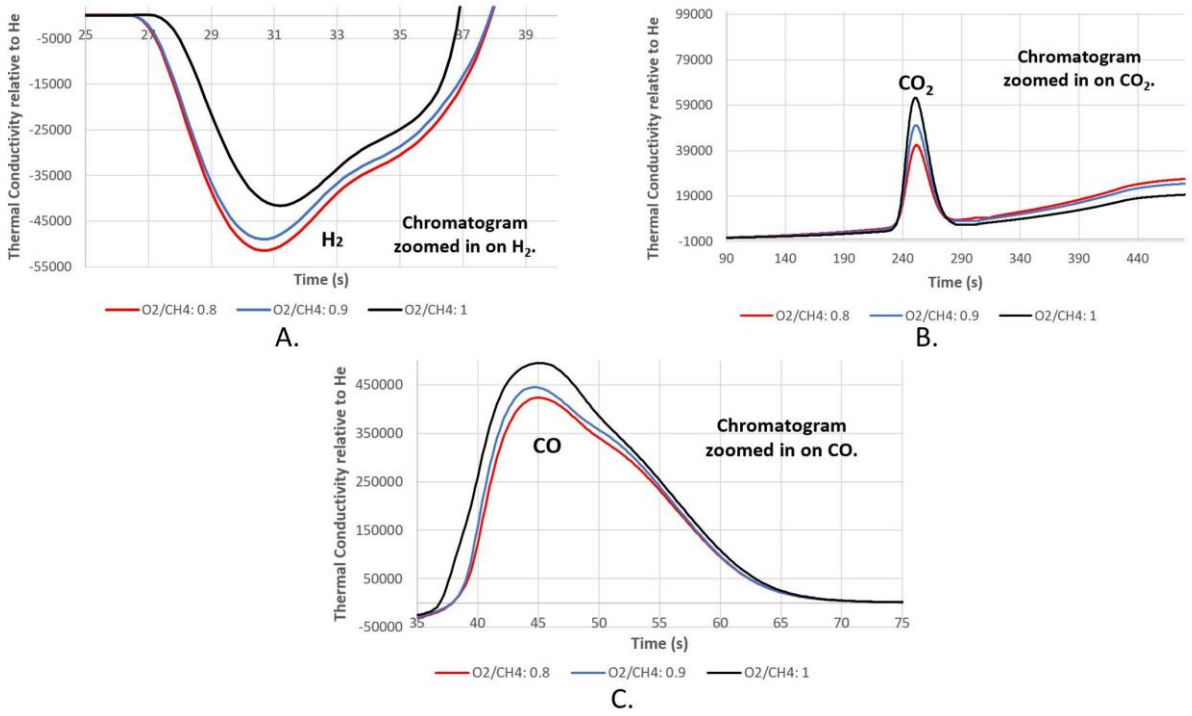


**Figure 3.2 The zoomed in region corresponding to $H_2$ gas, $CO_2$, and CO of Figure 1 respectively.**

The analysis was performed by Dr. Jose Covarrubias. The key take aways from the GC plots, after being compared to a standardized curve, is that the area under and the intensity of the curves gives the concentrations of the gases present.

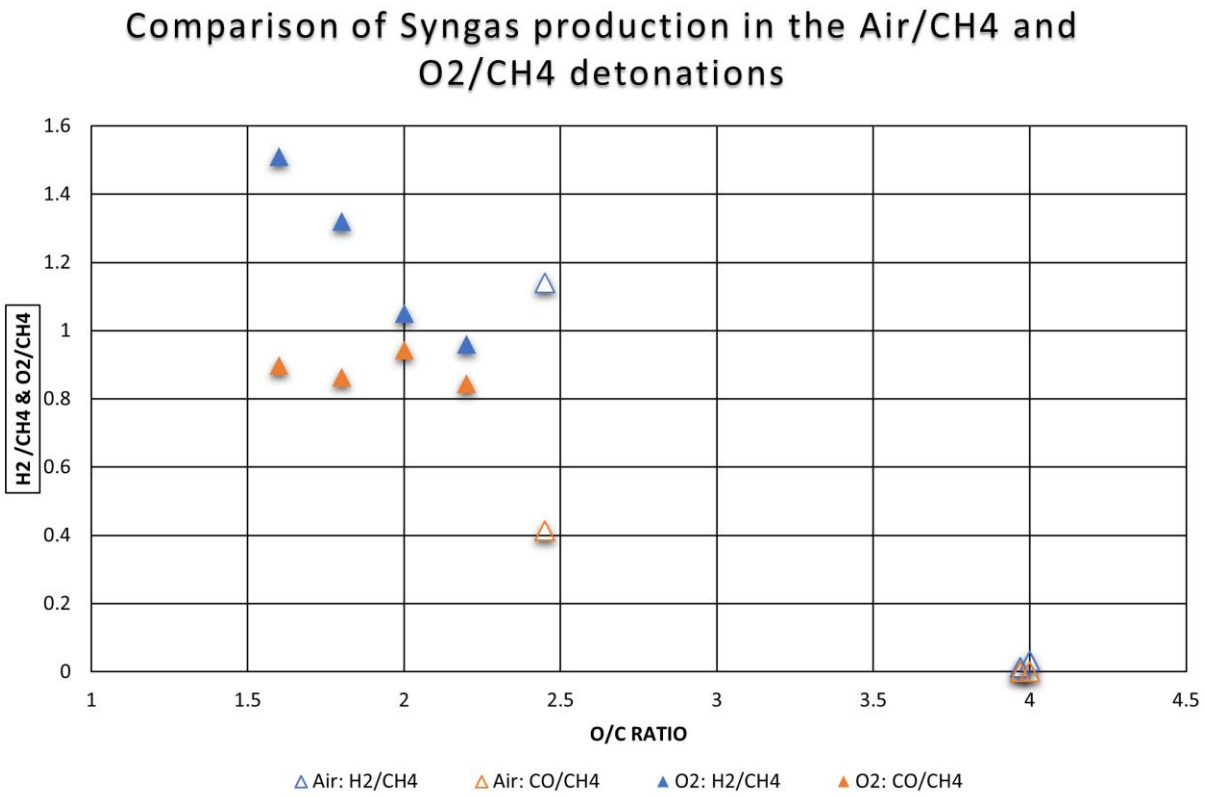


**Figure 3.3 A comparison between the air and oxygen detonations**

Using the Tables 3.1 and 3.2, fig. 3.3 was created, from this there a couple of trends. There is a notable trend that shows as $O/C$ increases, there is a downward trend in $H_2/CH_4$ & $CO/CH_4$. This first trend is an expected result to see, as when we compare it to the reaction equation for the POX, this reaction occurs at sub-stoichiometric quantities thus as we deviate from this by increasing the oxygen content in the reactants, we expect to see less of the products from the POX of methane. However, the reverse is true, extrapolating from this upward trend in syngas production as $O/C$ ratios decrease, $H_2/CH_4$ & $CO/CH_4$ both increases.

Looking specifically at the experiments that used compressed air as the oxidizer, rather than compressed oxygen, we see, from fig. 3.3 that for an $O/C$ ratio of ~2.5 we produce $H_2/CH_4$ at 1.12 and $CO/CH_4$ at 0.413; and this means that we produce syngas at a ratio of 2.71 $H_2$/CO. From the oxygen experiment extrapolation and the air experiments it shows the versatility of the detonation chamber in syngas production. This uniqueness of the detonation chamber allows for multiple use case scenarios, one being the end goal of fuel cells that according to (Liu et al., 2010) utilizes syngas at a ratio of ~2 $H_2$/CO. and as mentioned previously, ethanol and dimethyl ether primarily is produced using ~ 1 $H_2$/CO and methanol is synthesized from ~2 $H_2$/CO [9].

## Engine Results

This section will present the results and observations that stem from the operation of a commercially available Spark Ignition IC engine. These results

come from the analysis using the FTIR and GC instruments. Fig. 3.1, 3.2, 3.4, and 3.6 show the results of FT-IR & GC, performed by Dr. Jose Covarrubias.

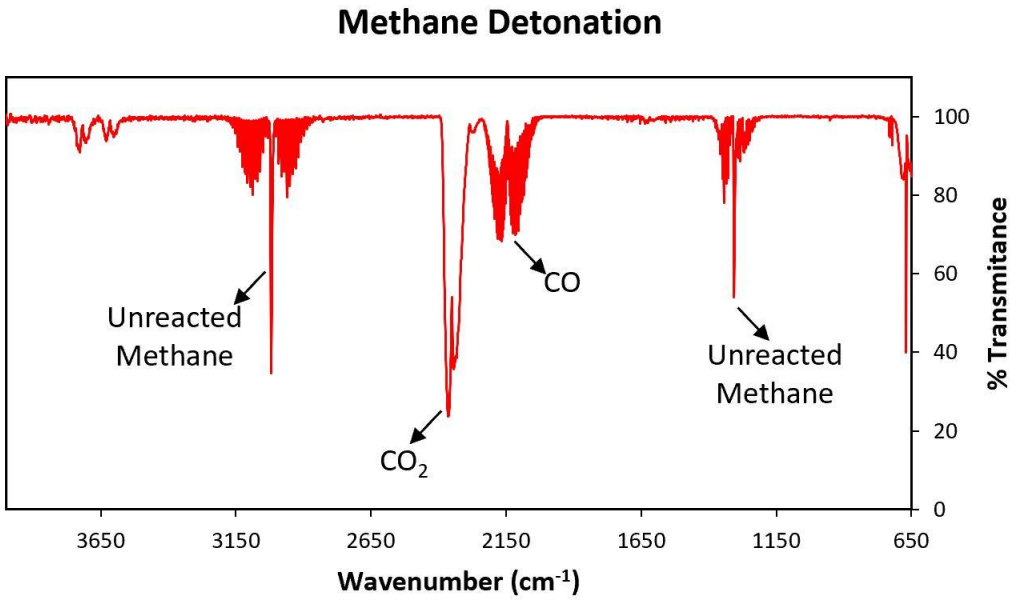


**Figure 3.4 The FT-IR analysis of exhaust produced by the engine**

Fig. 3.4 shows the FT-IR analysis of the engine exhaust gas. Ideally the plot would show the spectral read out for CO and $CO_2$. CO is seen in range of 2000-2500 $cm^{-1}$, while $CO_2$ is seen in the ranges of 500-750 $cm^{-1}$, 2250-2500 $cm^{-1}$, and 3500-4000 $cm^{-1}$ [21]. However, there is also a noticeable drop in transmittance in the ranges of 1150-1400 & 2800-3150 $cm^{-1}$ when comparing this to the NIST online database, this lines up with unreacted methane as seen in fig. 3.5. The presence of methane in the exhaust gas is not surprising as there many factors that

can result in hydrocarbon emissions, such as air-fuel leanness and in chamber turbulence [22].

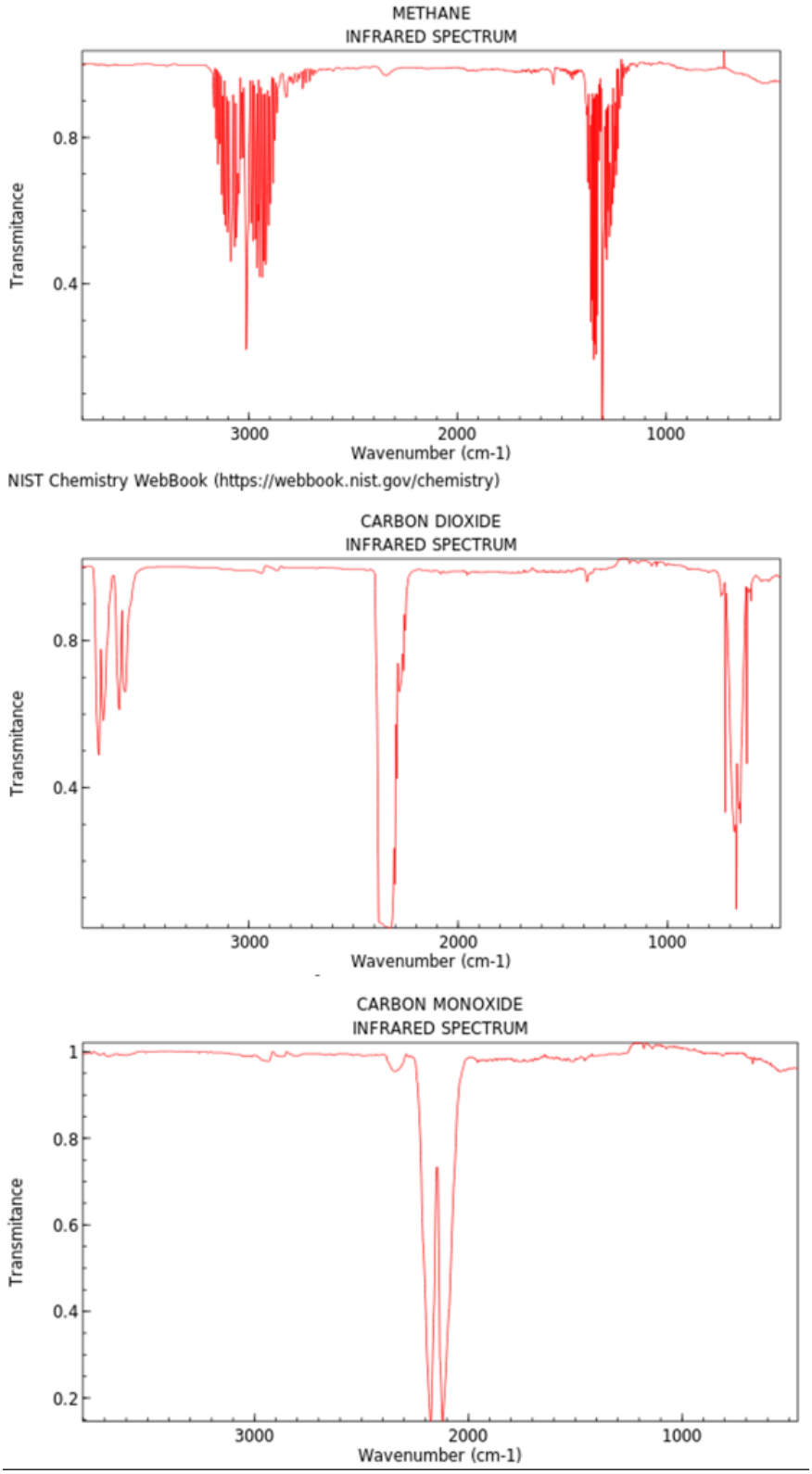


**Figure 3.5 The FT-IR analysis for methane, carbon dioxide, and carbon monoxide. FTIR plots come from NIST, William E. Wallace [21]**

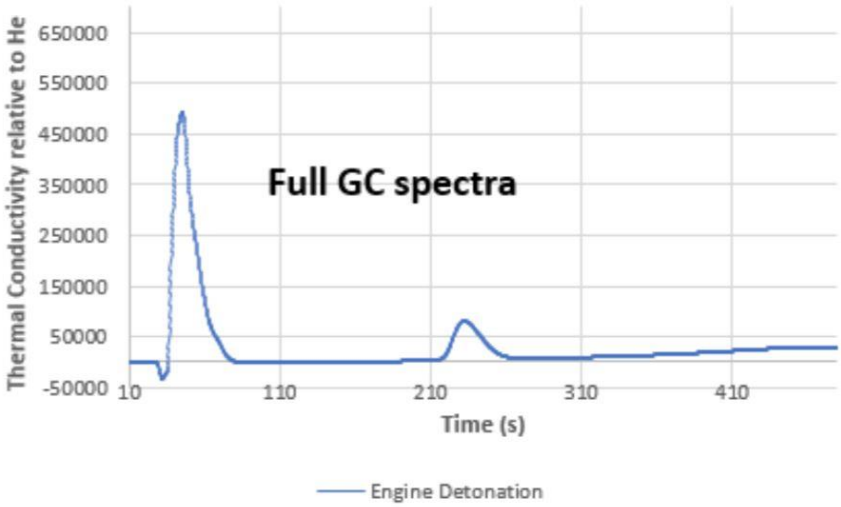


**Figure 3.6 The full GC analysis for the engine, running at O/C of 2.14**

Using the same data from fig. 3.6 we have calculated that the exhaust gas composition for an $O_2/CH_4$ of 1.07 is ~38% $H_2$, ~10% $H_2O$, ~44% CO & $CH_4$, and ~8% $CO_2$.

# Chapter 4 - Discussion

This section will build upon the syngas production results, to this end it will discuss the drawbacks to both methods, in terms of up scalability and distance from a carbon neutral energy source. After this we will look at the future of syngas production and other renewable energy sources.

## Engine vs. Detonation chamber

The set up for both experiments have advantages and drawbacks, making them difficult to compare. They both have different environments that suits their purpose. Starting with the engine, this thesis has shown that it is possible to use a

commercially available engine to produce syngas, allowing for the possibility for high adoption rate by the general population. Unlike the engine, the detonation chamber requires several specialized pieces of equipment, making this more difficult for the general population to attach to.

However, the detonation chamber, unlike the engine, has been shown to be highly variable in the reactions that can be performed. This can be seen by the pressures that it can be filled to, and the reactants that can be used. As noted earlier the engine, does not fully use the reactants, as seen in the engine's FT-IR exhaust analysis (fig. 3.4) that shows the possible presence of unreacted methane. Looking at the possibility of using each as a source of carbon neutral energy, it has been observed that the engine produces a soot, thus the formation of carbon. While the detonation chamber's reaction is highly predictable, this allows the user to reproduce any results multiple times and avoid carbon formation.

Since the goal of this thesis is to explore methods of syngas producibility and its role as a carbon neutral energy source, this being defined as an energy source that does not add to the carbon dioxide levels with in the atmosphere. Then it makes sense to discuss the hydrogen/carbon monoxide trends seen for both the detonation chamber and engine methods. This is done by considering the GC analysis seen in fig. 3.5, that as oxygen content increases in the reactants, so does the concentration of carbon monoxide and carbon dioxide, but conversely the

hydrogen content increases in the products. This trend shows that it is possible to minimize carbon dioxide while maximizing the hydrogen content, by lowering the $O_2/CH_4$ ratio. Resulting in a promising future for syngas produced in the Detonation Chamber, in a purely chemistry & physics sense.

## Future of Syngas Production and Carbon Neutral Energies

Looking at the future of syngas, a large concern is the reliance of methane as a reactant. Methane is largely a non-renewable resource stemming from fossil fuels that along with the purity requirements for methane makes it an impermanent option. With that concern in mind, it leads to the introduction of Biogas; this is a renewable source of energy that comes from the breakdown of organic waste via microorganisms in the absence of oxygen [23]. Biogas is largely a combination of methane and carbon dioxide [24]. However, even biogas has its own hurdles to overcome, such as, chemical contaminants that reduce the purity that depends on the source of biogas (Rafiee et al., 2021, p. 22). Though, biogas is not a carbon neutral energy source, due to the presence of carbon dioxide. Research has led to the development of carbon capturing and storage (CCS) technologies to assist in minimizing the impact of carbon producing energy sources [25].

Renewable energies span far past syngas. To name a few there is electricity that stems from solar power, hydro power, and wind power. In fact, in 2021 the world produced a combined total 7042.94 terawatt-hours from solar, hydropower

and wind power alone [4]. However, renewable energy is dominated by the fossil fuel energy having produced 16,992.07 terawatt-hours, showing that as the fossil fuel usage decreases limiting our low-carbon energy sources might not be an immediate option for majority of the world. These facts show that there is large need for diverse low-carbon energy sources as we live in a diverse world.

# Chapter 5 - Conclusion

In this thesis it has been shown through two different methods that syngas, a combination of hydrogen and carbon monoxide gas, can be produced in a manner that makes syngas close to a carbon neutral energy source and as an alternative to current, but less desirable, sources of energy. With the first method, the detonation chamber, it showed that syngas is producible in batches and can be precisely configured for numerous ratios. It was shown in fig. 3.3 that we produce in the compressed air experiments we produce syngas at ratios of 2.71 $H_2$/CO, which is at greater hydrogen concentrations than is used for fuel cells [20]. Meaning, that the detonation method is useful not only to produce syngas with low amounts of carbon dioxide but also for when the goal is to produce $H_2$ and CO that will be used to produce methanol or dimethyl ether (DME) [26]. In the second method, the spark ignition internal combustion engine, it shows that it is possible to produce a near carbon neutral energy source from a repurposed commercially available product. It should be noted that the commercially available engine managed to

have a conversion of 38% hydrogen and only 8% carbon dioxide at a $O_2/CH_4$ of 1.07, every cycle. The use of a commercial engine also shows the variability in power generation locations, it could potentially be upscaled to a factory with many engines or a single engine to produce power.

Possible places to expand this research can come in several ways, in the detonation chamber experiments, it would be beneficial to have a more expansive look at the various ratios of $O_2/CH_4$, giving a holistic view. A point of interest that is also worth looking at is the using different fuels that have shown to produce syngas for engines, such as methane enriched Biogas.

Another way to continue this research would be to push the detonation chamber to even greater pressures. For the engine method, as mentioned earlier, the presence of methane in the exhaust shows that the use of an exhaust gas recirculation (EGR) technique might not only reduce the presence of methane in the exhaust but also allow for another way to control engine/exhaust temperatures [13]. Another way to expand this research would be to expand the different types of engines to experiment with, an example of this would be using a Homogeneous Charge Compression ignition (HCCI) engine [27]. Although the HCCI engine is not as common as the SI or CI engines, it is the best of both worlds. It has been seen that the HCCI engine can perform combustions producing low NOx and resulting in a high efficiency [28].

The research done to produce this thesis shows that both old, i.e., the spark ignition ICE, and modern technology, the detonation chamber, can fill in the gap that stands between the world's current major energy resources, i.e. fossil fuels, and that of a world that relies solely on renewable energy resources, such as hydrogen, hydropower, solar, and wind energy just to name a few. Although the solution is multifaceted, syngas is one of those facets, allowing us to use old technology while looking towards future technology on the road to total carbon neutral energy.

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