THE EFFECTS OF HYDROGEN ADDITION AND INTAKE-INDUCED SWIRL ON THE CHARACTERISTICS OF NATURAL GAS COMBUSTION IN A SINGLE-CYLINDER SPARK-IGNITED ENGINE

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by
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ABSTRACT

Compressed natural gas (CNG) is an alternative fuel of interest for internal combustion engines (ICEs) in the mass transit and vocational applications. Increasingly, due to the abundant supply of shale gas, there is interest in heavy duty and in passenger vehicle applications of natural gas. CNG combustion yields significant reductions in particulate emissions compared to diesel. However, the inherently low flame speed of CNG decreases thermal efficiency and increases toxic aldehyde emissions in ICEs, requiring optimization of spark timing. Due to its increased flame speed compared to methane and liquid fuels, hydrogen has been shown to “assist” natural gas combustion in that it decreases combustion duration, reduces minimum spark advance for best torque (MBT timing), enhances combustion efficiency and can reduce emissions of unburned fuel.

The literature contains many studies that demonstrate hydrogen’s ability to burn faster than other fuels and that acknowledge hydrogen’s uniqueness compared to other fuels in terms of its mass diffusivity, wide flammability range, and minimum ignition energy, but these studies rarely attempt to explain such characteristics in a scientific manner. Most review articles focus on a particular aspect of technical implementation of hydrogen as a combustible fuel in lieu of a holistic view of hydrogen assisted combustion of hydrocarbon fuels in ICEs. The intention of the present work was to build on the understanding of the role of hydrogen in the spark-ignited combustion of natural gas, by confirming common findings in the literature, namely that the addition of hydrogen to natural gas enables spark retard due to enhanced early flame development, and that retarded spark at MBT for HCNG results in concentrated heat release near TDC, improving the efficiency compared to CNG alone. The primary objective of the present work is to perform detailed heat release analysis to evaluate the following hypothesis: while swirl can be employed to improve the sluggish early flame development of CNG, using hydrogen to
supplant swirl enables improved early flame development without compromising engine efficiency due to convective heat losses caused by enhanced fluid motion.

The present work employs a single-cylinder spark-ignited engine to study the effects of intake-induced turbulence and turbulence intensity on hydrogen assisted natural gas (HCNG) combustion. The effects with hydrogen assisted combustion are examined through comparison with combustion of CNG alone. Experiments were conducted at 2000 rpm with both fixed spark timing and adjusting spark to maintain MBT, as well as at 2750 rpm with MBT timing alone. Each study was conducted at 1.5 bar brake mean effective pressure (BMEP), stoichiometric equivalence ratio and MBT timing for each fuel; fueling rate was fixed as the throttle was opened to achieve leaner conditions (engine load is not fixed). Results with a high level of in-cylinder swirl (one intake port fully blocked) were compared to results with a quiescent in-cylinder flow (fully opened intake ports).
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Chapter 1 Introduction

Concerns regarding limited long-term availability of fossil fuels, fluctuating costs of the predominately foreign-supplied commodity of petroleum, and emissions from hydrocarbon-based fuels have generated government interest in hydrogen fuel cell development, and hence the hydrogen fueling infrastructure. Hydrogen-fueled internal combustion engines (HICE) are often referred to as the “bridge” to a hydrogen economy since utilization of hydrogen as a fuel in ICEs may facilitate the development of a hydrogen fueling infrastructure. The United States mass transit industry started to employ natural gas powered ICEs in the 1980s in an effort to meet particulate emissions requirements. Researchers and advocates who viewed burning hydrogen as a means to improve engine efficiency and to reduce emissions of oxides of nitrogen (NOx) saw the CNG-fueled engines as a natural inlet for hydrogen, given that gaseous fuel systems and infrastructure already existed in some cities. Hence demonstration projects commenced; retrofitting engines to operate with hydrogen assisted compressed natural gas (HCNG).

During his January 28, 2003 State of the Union Address, President George W. Bush proposed “$1.2 billion in research funding so that America can lead the world in developing clean, hydrogen-powered automobiles” (Bush, 2003). This proclamation heightened interest in hydrogen combustion and also fuel cell research, and The Energy Efficiency and Renewable Energy (EERE) office of the United States Department of Energy (DOE), constructed a multi-year plan (2005 – 2015) for the research, development, and demonstration of technologies as part of its Hydrogen, Fuel Cells and Infrastructure Technologies Program (Hydrogen, Fuel Cells & Infrastructure Technologies Program 2005-2015, 2007). A sharp increase in the number of
publications dedicated to hydrogen combustion has resulted; these data are portrayed in Figure 1-1.

![Figure 1-1](image)

Figure 1-1 Number of publications per year, for (○)Web of Science and (■) Elsevier ScienceDirect, and (▲) total, using “Hydrogen AND Combustion” as search terms (search date January 10, 2010).

Though natural gas-fueled spark-ignited engines emit less particulate matter than diesels, emissions of NOx are a standing issue that must be resolved to meet future emissions regulations. As of 2010, diesel engines have additional aftertreatment in place to manage emissions of NOx. While the broad flammability range of hydrogen supports lean combustion and increased rates of exhaust gas recirculation (EGR) which result in decreased combustion temperatures hence minimizing NOx emissions (Collier et al., 2005) doing so comes at the cost of decreasing engine performance.

Natural gas combustion in a spark-ignition engine exhibits a slow burn rate due to sluggish flame kernel growth, the physics of which are discussed in the next chapter. Hydrogen has been long-recognized for its fast burn rate. Langley Research Center first evaluated a hydrogen fueled turbine in 1969 for its wind tunnel in an effort to reduce the length of the turbine.
The rapid flame propagation rate of hydrogen compared to other available fuels enabled a smaller (shorter) burner. The time scales of other available fuels inhibited the length of the burner to be decreased sufficiently, compared to hydrogen (Burnett, 1969).

The burn rate is enhanced when hydrogen is added to natural gas or gasoline in a spark-ignited engine, compared to neat natural gas or gasoline (Conte and Boulouchos, 2006; D'Andrea, Henshaw and Ting, 2004; Jensen et al., 2000; Swain et al., 1993; Sita Rama Raju, Ramesh and Nagalingam, 2000; Tunestal et al., 2002; Ma et al., 2008). Additional improvements have been observed, as follows:

1. Reduced ignition delay (D'Andrea, Henshaw and Ting, 2004; Swain et al., 1993; Tunestal et al., 2002)

2. Decreased NO\textsubscript{x} emissions at lean conditions, due to leaner operation resulting in reduced combustion temperatures, and hence inhibiting the kinetics for thermal NO\textsubscript{x} generation (Akansu et al., 2004; Bauer and Forest, 2001; Collier et al., 1996; Das, Gulati and Gupta, 2000; Hoekstra, Van Blarigan and Mulligan, 1996; Huang et al., 2006; Li and Karim, 2005; Houseman and Hoehn, 1974)

3. Reduced brake specific fuel consumption (BSFC), increased brake thermal efficiency (BTE) (Bade Shrestha and Karim, 1999; Akansu et al., 2004; Cattelan and Wallace, 1995; Das, Gulati and Gupta, 2000; Finegold, 1976; Sita Rama Raju, Ramesh and Nagalingam, 2000; Soggard, Schramm and Jensen, 2000; Stebar and Parks, 1974; Huang et al., 2006).

4. Reduced CO\textsubscript{2} and CO emissions (Akansu et al., 2004; Cattelan and Wallace, 1995; Collier et al., 2005; Tunestal et al., 2002)
While basic findings in the literature with regards to burn duration, efficiency and fuel consumption are generally consistent, comprehensive fundamental explanations are lacking. Hydrogen engine review papers, one by Das and one by White, outlined the technical aspects of utilizing hydrogen in engines, but did not focus on the fundamental aspects of hydrogen combustion within the engine (Das, 1990; White, Steeper and Lutz, 2006). Das later published a paper reviewing the oxidation of hydrogen, as well as surveying hydrogen’s physical properties as well as laminar burning characteristics in burners (Das, 1996).

While many engine experiments have demonstrated enhancements to methane or gasoline combustion with hydrogen addition in terms of BSFC, pollutant emissions, efficiency, and burn rate, the literature is lacking detailed heat release analysis for hydrogen assisted combustion in ICEs to describe the effects of hydrogen on the combustion duration.

The objective of the present work is to:

1. Evaluate the results to confirm two common findings in the literature, that:
   a. HCNG improves flame development compared to CNG, and hence enables spark retard, and
   b. the addition of hydrogen shortens the main burn duration, improving the conversion of thermal to mechanical energy, thereby improving efficiency through minimizing heat loss prior to TDC improving efficiency

2. Evaluate the hypothesis of this work, which is that the addition of hydrogen supplants swirl in terms of enhancing the burn process, thereby reducing cylinder heat loss and improving efficiency.

The present work will integrate discussion of fundamentals about the burn process in conjunction with engine efficiency while considering elements of engine hardware design while examining
characteristics of the burn process. Additionally, the effects of turbulence will be studied and evaluated by blocking one intake port to induce swirl, and also by increasing engine RPM from the baseline case at 2000 RPM to enhance turbulence intensity.
Chapter 2 Literature Review

This chapter is dedicated to building a foundation for the investigation in question. Flame fundamentals for hydrocarbons and hydrogen are discussed followed by the physical properties and kinetics of hydrocarbon and hydrogen fuels. These concepts are then applied to the fundamentals of spark-ignited ICEs, specifically related to the combustion of methane and hydrogen as fuel.

2.1 Laminar flame theory

Consider a quartz tube containing a homogeneous, flammable mixture of air and fuel. Assume that the temperature of the tube, gases, and ambient environment is 25 degrees Celsius, and the system pressure is 1 atmosphere. The tube is open to the atmosphere at each end. An ignition source is introduced at one end of the tube and then removed once ignition succeeds. Figure 2-1 describes the flame, which is sustained within the tube, and is free to propagate in the direction of the unburned mixture (ahead of the flame), leaving burned gases behind the flame.

![Figure 2-1 Flame propagation in a tube](image-url)
The flame approaches the unburned gases at a velocity \(S_f\) equal to the laminar flame speed \(S_l\):

\[
S_f = S_l
\]

2-1

The density of the burned gases (hot) is less than the density of the reactants (cold). The temperature profile of the flame is shown in Figure 2-2, where \(x\) is the distance the flame has traveled and \(T\) is the temperature of the reactants and combustion products.

![Figure 2-2 Temperature profile of a model of a one dimensional planar flame](image)

Now let us consider the driving force for flame propagation. In his paper titled “Theory of Flame Propagation,” published in 1948, Zeldovich described flame propagation simply as the process of a chemical reaction in a layer that increases, leading to increased temperature of neighboring regions by heat conduction, such that further chemical reaction is initiated and hence the flame is propagated. The results of his work generated equations for flame propagation with
chemical reaction, and suggested a solution to determine velocity as function of the “arbitrary”
relation between diffusion and heat conduction (Zeldovich, 1948). Today, it seems more natural
to address ignition and flame development prior to propagation, such that ignition, in the case of
spark-ignited combustion, is an endothermic process involving an external energy source
sufficient to cleave chemical bonds of a combustible mixture. A flame develops subsequently
generating highly reactive free radicals that perpetuate exothermic chain reactions, and thus the
flame is a high temperature reaction zone which propagates toward the unburned gases.
Heywood offers a succinct description of a flame: “a flame is the result of a self-sustaining
chemical reaction occurring within a region of space called the flame front where unburned
mixture is heated and converted into products” (Heywood, 1988). A flame front comprises a
preheat zone to which heat is conducted from the reaction zone, increasing the temperature of the
unburned gas. The reaction zone exists in the region where the temperature is greatest and
extends to the hot boundary of the burned gas. These descriptions focus on two primary driving
forces of flame propagation: kinetics and heat transfer.

Equation 2-2 is a popular and simple expression that Mallard and Le Chatelier first
proposed for laminar flame speed in 1883, which depends on the diffusion of heat. Zeldovich,
Frank-Kamenetski and Semenov extended the work of Mallard and Le Chatelier by accounting
for the diffusion of species as well as heat. Glassman (1996) provides descriptions and
derivations of the work by Mallard and Le Chatelier as well as the work presented by Semenov,
which built upon Zeldovich and Frank-Kamenetski’s work. Although the latter accounted for
change in the number of moles (between the unburned and burned gases as a function of time) as
well as allowing for Lewis number (no longer constraining it to 1), the work that Semenov
presented based on Zeldovich and Frank-Kamenetski’s research reduces to the same expression that Mallard and Le Chatelier presented:

\[ S_L = \sqrt{\alpha \cdot RR} \]  \hspace{1cm} 2-2

Hence, the laminar flame speed is a function of the thermal diffusivity and the reaction rate. The oxidation reactions that support combustion are exothermic. A reaction is exothermic if the energy released during the formation of the products is greater than the energy absorbed in breaking the bonds. The heat generation from the oxidation of hydrogen and carbon based molecules is diffused from the flame to the unburned gases, heating the reactants until the temperature is high enough (the ignition temperature) to initiate the cleavage of bonds to foster chain reactions. If the reaction rate is too slow, the heat generated that diffuses to the unburned gases may dissipate to the atmosphere (via the tube), extinguishing the flame. A flame can propagate only if the reaction rate is sufficiently fast to heat the unburned gases to a point where the bonds will break (the ignition temperature). The faster the reaction rate, the faster the bond cleavage can occur, and hence more heat is available to heat up the unburned gases. Thermal diffusivity is important because the faster the heat can be transferred to the unburned gases, the faster the flame can then propagate.

The laminar flame speeds for methane in air and hydrogen in air at stoichiometric conditions and 360 K are 48 cm/s and 290 cm/s, respectively (Verhelst and Wallner, 2009). At an equivalence ratio of 0.6, the laminar flame speed for methane in air is 10 cm/s and that of hydrogen in air is approximately 100 cm/s (Dunn-Rankin, 2008). It is clear that hydrogen in air burns faster than methane in air, and hence the addition of hydrogen to methane should yield an enhanced (faster) laminar flame speed compared to methane alone.
The chemical kinetics for the oxidation of hydrogen and methane are presented below, and a discussion about the effects of kinetics on the laminar flame speeds of hydrogen, CNG and HCNG will follow.

Glassman suggests two primary initiation steps for hydrogen oxidation; the first prevails only at very high temperatures (Glassman, 1996):

\[
H_2 + M \rightarrow 2H + M \quad 2-3
\]

And the second occurs at lower temperatures:

\[
H_2 + O_2 \rightarrow HO_2 + H \quad 2-4
\]

There are four known chain-reactions for the oxidation of hydrogen, namely (Glassman, 1996):

\[
H + O_2 \rightarrow O + OH \quad 2-5
\]

\[
O + H_2 \rightarrow H + OH \quad 2-6
\]

\[
H_2 + OH \rightarrow H_2O + H \quad 2-7
\]

\[
O + H_2O \rightarrow OH + OH \quad 2-8
\]

The termination steps are thought to be:

\[
H + H + M \rightarrow H_2 + M \quad 2-9
\]

\[
O + O + M \rightarrow O_2 + M \quad 2-10
\]

\[
H + O + M \rightarrow OH + M \quad 2-11
\]

\[
H + OH + M \rightarrow H_2O + M \quad 2-12
\]

Further discussion of the roles of HO\(_2\) and H\(_2\)O\(_2\) and reverse reactions can be found in Turns (2000).

The first step in the combustion of a methane-air system is the cleavage of carbon-hydrogen bonds creating hydrogen and hydrocarbon radicals. The combustion of hydrocarbon fuels of C\(_2\) or higher is initiated by the cleavage of a C-C bond, resulting in two hydrocarbon
radicals. The chain initiation reactions for high-temperature combustion are shown below, and are classified as either low-temperature or high-temperature reactions (Glassman, 1996):

$$\text{CH}_4 + \text{O}_2 \rightarrow \text{CH}_3 + \text{H} + \text{O}_2 \text{ (low temperature)}$$  \hspace{1cm}  \text{(2-13)}

$$\text{CH}_4 + \text{M} \rightarrow \text{CH}_3 + \text{H} + \text{M} \text{ (high temperature)}$$  \hspace{1cm}  \text{(2-14)}

$$\text{RH} + \text{O}_2 \rightarrow \text{R} + \text{HO}_2 \text{ (low temperature)}$$  \hspace{1cm}  \text{(2-15)}

$$\text{RH} + \text{M} \rightarrow \text{R}’ + \text{R}'' + \text{M}$$  \hspace{1cm}  \text{(2-16)}

$$\text{CH}_4 + \text{X} \rightarrow \text{CH}_3 + \text{XH}$$  \hspace{1cm}  \text{(2-17)}

Subsequent steps involve cleaving the O-O bond, and the formation of intermediates (Glassman, 1996). Combustion is terminated when the radical pool is depleted either by interactions of the molecules with the wall, or in the case of combustion in engines, when the combustion cycle has been completed. The detailed mechanisms of hydrocarbon combustion are extensive and very complex. The main high-temperature oxidation reactions for methane are outlined as follows (Glassman, 1996):

$$\text{CH}_3 + \text{O}_2 \rightarrow \text{CH}_3\text{O} + \text{O}$$  \hspace{1cm}  \text{(2-18)}

$$\text{CH}_3 + \text{O}_2 \rightarrow \text{H}_2\text{CO} + \text{OH}$$  \hspace{1cm}  \text{(2-19)}

$$\text{CH}_3\text{O} + \text{M} \rightarrow \text{H}_2\text{CO} + \text{H} + \text{M}$$  \hspace{1cm}  \text{(2-20)}

$$\text{H}_2\text{CO} + \text{X} \rightarrow \text{HCO} + \text{XH}$$  \hspace{1cm}  \text{(2-21)}

$$\text{HCO} + \text{M} \rightarrow \text{H} + \text{CO} + \text{M}$$  \hspace{1cm}  \text{(2-22)}

The full known details of methane combustion are summarized from various sources and outlined by (Turns, 2000).

The GRI 3.0 mechanism is a kinetic model employed when simulating the combustion of methane. This mechanism contains 7 reactions for methane oxidation which rely on the radicals of O and OH, according to the GRI 3.0 mechanism (Smith et al., n.d.):

$$\text{O} + \text{CH}_4 \rightarrow \text{OH} + \text{CH}_3$$  \hspace{1cm}  \text{(2-23)}
\[
\begin{align*}
\text{OH} + \text{CH}_4 & \rightarrow \text{CH}_3 + \text{H}_2\text{O} \quad & \text{2-24} \\
\text{OH} + \text{CH}_3 (+\text{M}) & \rightarrow \text{CH}_3\text{OH} (+\text{M}) \quad & \text{2-25} \\
\text{OH} + \text{CH}_3 & \rightarrow \text{CH}_2 + \text{H}_2\text{O} \quad & \text{2-26} \\
\text{OH} + \text{CH}_3 & \rightarrow \text{H}_2 + \text{CH}_2\text{O} \quad & \text{2-27} \\
\text{O} + \text{CH}_3 & \rightarrow \text{H} + \text{CH}_2\text{O} \quad & \text{2-28} \\
\text{O} + \text{CH}_3 & \rightarrow \text{H} + \text{H}_2 + \text{CO} \quad & \text{2-29}
\end{align*}
\]

The flame thickness is a function of thermal diffusivity and laminar flame speed, and can be considered to be on the same order of thermal diffusivity divided by the laminar flame speed. The example and conditions given in Figure 2-1, the flame thickness then would be on the sub-millimeter level. Such a thickness is quite small compared to the length of a tube, as in Figure 2-1. In an engine application then, the flame thickness would be quite small compared to the engine bore, during the flame kernel growth and early flame development process.

Wang et al. studied the effects of hydrogen addition to lean, premixed natural gas-air flames both experimentally, in a constant volume vessel using Schlieren photography, and numerically using the PREMIX code in CHEMKIN II (and GRI 3.0 mechanism). They found that increasing hydrogen fraction resulted in increased mole fractions of O and OH in the reaction zone (Wang et al., 2010). Two of the 4 predominant chain-propagating steps in hydrogen oxidation (combustion) are, as noted in Equations 2-6 and 2-7. There are seven questions associated with methane oxidation that relay on O and OH for the chain-propagation reactions, namely those presented in Equations 2-23 through 2-29.

Considering the kinetics involved in hydrogen and methane oxidation as well as the results from Wang et al. (2010), it is logical to assert that the increased molar fraction of O and OH radicals in the flames of natural gas flames when hydrogen is added is the result of chemical
kinetics (or reaction rate, per Equation 2-2). Further support is offered by Priyadarshi (2006), who studied the effects of hydrogen addition to premixed, 1-dimensional methane-air flames at conditions common in spark-ignited engines (8 atm and 598 K). One portion of the study varied hydrogen fraction (0.0, 0.3 and 0.7) in the methane-air flames at equivalence ratios of 1, 0.7 and 0.5, on a constant energy basis. The GRI 3.0 mechanism resulted in a temperature profile that increased earlier (in terms of distance) and peaked higher for the hydrogen fraction of 0.7 (that for hydrogen fraction of 0.3 increased earlier and peaked higher still than without hydrogen in methane, but was much closer to the temperature profile of pure methane in air than with the hydrogen fraction of 0.7). This result is indicative of an early reaction zone due to the high hydrogen content. The introduction of hydrogen also lead to an increased mass consumption rate of methane compared to methane alone. The hydroxyl radicals increased by a factor of two when comparing the flame with a hydrogen fraction of 0.3 to that of hydrogen fraction of 0.7 (where the hydrogen fraction of 0.7 produced the most hydroxyl radicals). Priyadarshi attributes the faster OH consumption leading to CH$_3$ molecules to Equation 2-7, which results in the faster reaction in the case of hydrogen addition (Priyadarshi, 2006).

Lu et al. developed reduced mechanisms to predict flame speeds and flame structures for high temperature oxidation of CH$_4$/Air and H$_2$/Air. The reduced mechanisms produced results that aligned well with detailed mechanisms in the literature. Nitrogen is treated as a diluent in these calculations, and maximum flame temperatures are low enough that nitrogen participates thermodynamically, but not kinetically. Lu et al. (2001) presented plots in which flame speeds are portrayed as a function of pressure and stoichiometry of the fuel-air mixture, and show that the flame speed of H$_2$/Air at any equivalence ratio (at 20 atm) is at least 50% faster than CH$_4$/Air (Lu, Ju and Law, 2001).
Under stoichiometric conditions and standard temperature and pressure, the laminar flame speed of hydrogen/air is significantly greater than for that of methane/air, 170 cm/s and 43.4 cm/s (both at stoichiometric proportions), respectively (Glassman, 1996). Kinetic modeling where the Lewis number was adjusted, and preferential diffusion of H and H₂ from the reaction zone into the preheat zone of both CH₄/Air and CH₄/O₂ flames (rich) were studied. In the first case, H₂ and H did not affect the superadiabatic flame temperature significantly. Superadiabatic is a description for the temperature gradient where the hottest part has a lesser density than the relatively cooler parts, resulting in further temperature rise of the hottest portion. The suppression of preferential diffusion of H inhibited superadiabatic flame temperatures from being achieved in the CH₄/O₂ case. Additionally for the CH₄/O₂ system, suppression of H₂ and H actually increased the flame temperature (also for CH₄/O₂) (Liu and Gulder, 2005).

The mass consumption rate is the rate at which the flame consumes the unburned mixture, and for a laminar flame can be computed as follows:

\[
\dot{m} = A \cdot \rho_u \cdot S_l
\]

where \(\dot{m}\) is the mass consumption rate expressed as mass per time, \(A\) is the flame area, \(\rho_u\) is the density of the unburned mixture, and the laminar flame speed \(S_l\). Even though the density of hydrogen is an order of magnitude smaller than methane, the mass consumption rate for H₂/air is significantly greater than for that of CH₄/air (by a factor of 3 for stoichiometric equivalence ratios, computed using flame speeds found in Glassman, 1996, and fuel densities from Heywood at 0°C, 1atm) (Glassman, 1996; Heywood, 1988).

Shock-tube investigations of hydrogen addition to methane-oxygen-argon mixtures were conducted by Lifshitz et al. (1971), and showed that hydrogen addition decreased the ignition delay time compared to the mixture without any hydrogen. Due to the apparent heat released by
the additive, the authors proposed that the effects of hydrogen addition were purely thermal in nature (that combustion chemistry was not affected) (Lifshitz et al., 1971).

Yang et al. (2010) simulated hydrogen-air flames of the following nature: freely-propagating planar flames, rich and lean premixed flames in the symmetric counterflow, counterflow diffusion flames, and rich and lean premixed flames stabilized by a counterflowing cold, nitrogen stream. The authors support the findings of Lifshitz et al. that the fast burning rate of hydrogen is a thermal effect (Lifshitz et al., 1971). They attribute the increase in flame speed to Soret diffusion (thermophoresis) of H and H₂ into the reaction zone, thereby affecting mixture properties, fuel concentration, and hence flame temperature (Yang et al., 2010).

In contrast, Wang, et al. (2010) conducted studies in an optically accessible constant volume cylindrical vessel with 130x130 diameter and length dimensions, and volume of 1.725 liters with a centrally located electrode (spark plug). Methane-air combustion was compared with methane-hydrogen-air combustion at various hydrogen fractions, and at equivalence ratios of 0.8 and 0.6. CHEMKIN (PREMIX, GRI 3.0) was used to discern the laminar premixed flame chemistry, and pressure data were employed to compute the burn durations. The authors define the “initial” combustion duration as the time period (in milliseconds) between ignition and the time when the pressure reaches 0.15 MPa. The initial combustion duration decreases significantly with increasing volume fraction of hydrogen in the fuel. The authors concluded that the maximum fraction of OH decreases with increasing H₂, and hence attributed the decreased burn duration to an increase in OH and O radicals, suggesting a chemical effect (Wang et al., 2010).
2.2 Chemical kinetics of pollutant formation

Combustion of hydrocarbons can be simplified into two parts: the fuel bonds (C-C and C-H) are first broken and carbon monoxide is formed via oxidation of its constituents (as shown in the oxidation reactions in the previous sections of this chapter), and the second step involves oxidizing carbon monoxide yielding carbon dioxide. Carbon monoxide oxidation is often slow if hydroxyl radicals are not present. During the combustion of hydrocarbons plenty of water or hydrogen is available to develop the pool of OH- radicals, hence speeding up the conversion of CO to CO₂ (Turns, 2000):

\[
\begin{align*}
\text{CO} + \text{O}_2 & \rightarrow \text{CO}_2 + \text{O} \quad 2-31 \\
\text{O} + \text{H}_2\text{O} & \rightarrow \text{OH} + \text{OH} \quad 2-32 \\
\text{CO} + \text{OH} & \rightarrow \text{CO}_2 + \text{H} \quad 2-33 \\
\text{H} + \text{O}_2 & \rightarrow \text{OH} + \text{O} \quad 2-34
\end{align*}
\]

Oxides of nitrogen generated in ICEs form via three specific pathways:

- Zeldovich mechanism (thermal NOₓ)
- Fenimore mechanism (prompt NOₓ)
- N₂O-Intermediate mechanism

Zeldovich executed a series of experiments to address whether the reaction kinetics for NOₓ were induced chemically or instead thermal in nature; more explicitly, whether the combustion reactions affected the formation of NO, or whether combustion simply provided a heat source to facilitate the chemical kinetics resulting in NO formation. He provided evidence for the latter, and presented two reactions which are known today as the Zeldovich mechanism for the formation of oxides of nitrogen (Zeldovich, 1946):

\[
\text{O} + \text{N}_2 \leftrightarrow \text{NO} + \text{N} \quad 2-35
\]
\[ \text{N} + \text{O}_2 \leftrightarrow \text{NO} + \text{O} \]  \hspace{1cm} 2-36

The Zeldovich mechanism yields what is referred to as thermal NO\textsubscript{x}. The formation of thermal NO\textsubscript{x} depends upon combustion temperature, but the formation of thermal NO\textsubscript{x} does not occur until after combustion given that nitrogen and oxygen species are present and oxygen has sufficient time to oxidize the nitrogen species (Zeldovich, 1946). While thermal NO\textsubscript{x} arises in combustion systems, it is not a formal product of combustion, meaning that the reaction rates for the oxidation of nitrogen species are significantly lower than for the oxidation kinetics of hydrocarbon and hydrogen fuels, the kinetics of which are outlined in previous sections.

Fenimore observed that the formation of nitric oxide in fuel-rich, low temperature hydrocarbon flames was larger than predicted with Zeldovich’s thermal NO\textsubscript{x} mechanism. Fenimore sought to describe a “faster, transient formation of nitric oxide in the primary reaction zone” (Fenimore, 1971).

The Fenimore mechanism yields what is referred to as prompt NO\textsubscript{x}, or NO\textsubscript{x} which is formed at the flame front. This reaction is thought to occur quickly, before thermal NO\textsubscript{x} has time to develop. The primary path to prompt NO\textsubscript{x} is also the rate-limiting step. The following series of reactions describes how prompt NO\textsubscript{x} may be formed at the flame front in hydrocarbon flames. (Fenimore, 1971):

\[ \text{CH} + \text{N}_2 \leftrightarrow \text{HCN} + \text{N} \]  \hspace{1cm} 2-37

The next aspect of the mechanism yields cyanide:

\[ \text{C} + \text{N}_2 \leftrightarrow \text{CN} + \text{N} \]  \hspace{1cm} 2-38

There is a threshold for equivalence ratio above which the prompt NO\textsubscript{x} chemistry becomes rather complex. The following reactions are the likely mechanisms for equivalence ratios below that threshold (\( \Phi \leq 1.2 \)) (Fenimore, 1971; Turns, 2000):
HCN + O ↔ NCO + H \hspace{1cm} 2-39
NCO + H ↔ NH + CO \hspace{1cm} 2-40
NH + H ↔ N + H \hspace{1cm} 2-41
N + OH ↔ NO + H \hspace{1cm} 2-42

The N$_2$O-intermediate mechanism is prevalent in low temperature conditions where the equivalence ratio is rather lean (<0.8):

O + N$_2$ + M ↔ N$_2$O + M \hspace{1cm} 2-43
H + N$_2$O ↔ NO + NH \hspace{1cm} 2-44
O + N$_2$O ↔ NO + NO \hspace{1cm} 2-45

It is important to mention that both NO and NO$_2$ can be formed within the combustion chamber and NO easily oxidizes in the atmosphere to become NO$_2$, hence the expression NO$_x$.

The reaction by which NO is converted to NO$_2$ before exiting the combustion chamber is:

NO + H$_2$O ↔ NO$_2$ + OH \hspace{1cm} 2-46

Additionally, NO$_2$ may be reduced to NO before exiting the combustion chamber via:

NO$_2$ + H ↔ NO + OH \hspace{1cm} 2-47
NO$_2$ + O ↔ NO + O$_2$ \hspace{1cm} 2-48

The formation of oxides of nitrogen in spark-ignited hydrogen or hydrocarbon combustion predominantly is due to thermal NO$_x$ formation (Heywood, 1988; Schobert, 1990).

2.3 Thermophysical properties of air and select fuels

It is imperative to understand the thermophysical properties of a given fuel, or air-fuel system, when aiming to analyze the fundamental flame characteristics of a given system. These
concepts will be employed in the upcoming discussion regarding experimental determination of laminar flame speeds. Table 2-1 summarizes several key parameters for hydrogen and methane.

Table 2-1 Thermophysical properties of hydrogen-air and methane-air mixtures. (Verhelst and Wallner, 2009)

<table>
<thead>
<tr>
<th>Property</th>
<th>H₂-air</th>
<th>H₂-air</th>
<th>CH₄-air</th>
<th>C₈H₁₈-air</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume fraction fuel (%)</td>
<td>29.5</td>
<td>9.5</td>
<td>9.5</td>
<td>1.65</td>
</tr>
<tr>
<td>Mixture density (kg/m³)</td>
<td>0.850</td>
<td>1.068</td>
<td>1.123</td>
<td>1.229</td>
</tr>
<tr>
<td>Kinematic viscosity (mm²/s)</td>
<td>21.6</td>
<td>17.4</td>
<td>16</td>
<td>15.2</td>
</tr>
<tr>
<td>Autoignition temperature (K)</td>
<td>858ᵃ</td>
<td>&gt; 858ᵃ</td>
<td>813ᵃ</td>
<td>690ᵃ</td>
</tr>
<tr>
<td>Adiabatic flame temperature (K)</td>
<td>2390</td>
<td>1061</td>
<td>2226</td>
<td>2276</td>
</tr>
<tr>
<td>Thermal conductivity (10⁻² W/mK)</td>
<td>4.97</td>
<td>3.17</td>
<td>2.42</td>
<td>2.36</td>
</tr>
<tr>
<td>Thermal diffusivity (mm²/s)</td>
<td>42.1</td>
<td>26.8</td>
<td>20.1</td>
<td>18.3</td>
</tr>
<tr>
<td>Ratio of specific heats</td>
<td>1.401</td>
<td>1.400</td>
<td>1.354</td>
<td>1.389</td>
</tr>
<tr>
<td>Speed of sound (m/s)</td>
<td>408.6</td>
<td>364.3</td>
<td>353.9</td>
<td>334.0</td>
</tr>
<tr>
<td>Air-to-fuel ratio (kg/kg)</td>
<td>34.2</td>
<td>136.6</td>
<td>17.1</td>
<td>15.1</td>
</tr>
<tr>
<td>Mole ratio before/after combustion</td>
<td>0.86</td>
<td>0.95</td>
<td>1.01</td>
<td>1.07</td>
</tr>
<tr>
<td>Laminar burning velocity, ~360 K (cm/s)</td>
<td>290</td>
<td>12</td>
<td>48</td>
<td>45</td>
</tr>
<tr>
<td>Gravimetric energy content (kJ/kg)</td>
<td>3758</td>
<td>959</td>
<td>3028</td>
<td>3013</td>
</tr>
<tr>
<td>Volumetric energy content (kJ/m³)</td>
<td>3189</td>
<td>1024</td>
<td>3041</td>
<td>3704</td>
</tr>
</tbody>
</table>

Hydrogen is a linear molecule composed of a covalent bond referred to as a molecular orbital; molecular orbitals belong to an entire molecule instead of an individual atom. The bond dissociation energy of the hydrogen molecule is 436 kJ/mol (McMurry, 1995).

Methane comprises four covalent C-H bonds. The energy associated with the formation of four C-H bonds excites the carbon atom to an sp³ valence state, and these four equivalent tetrahedral sp³ bond to produce a profoundly stable molecule (Karplus, Porter and Karplus, 1971). The bond dissociation energy of the carbon-methyl bond (C-CH₃) of the methane molecule is 438 kJ/mol (McMurry, 1995).
2.4 Experimental determination of laminar flame characteristics

Assumptions about the laminar flame characteristics of a given air-fuel system are often employed when discussing turbulence within an ICE. The laminar flame characteristics for conventional liquid fuels are well understood, and much empirical data has been generated and correlated with turbulent flames in engines, hence the overall contribution of the laminar flame characteristics to turbulence in a conventional air-fuel ICE system is generally agreed upon. Due to the differences in thermophysical properties between gaseous fuels and liquid fuels, specifically hydrogen, a thorough analysis of flame characteristics, beginning with those for laminar flames, is important. This section focuses on experiments that involve outward propagating spherical flames at constant pressure, or flames in a constant volume combustion bomb.

The following equation is used to deduce the unstretched burning velocity for flames influenced by small stretch rates at low pressures (at or near atmospheric). When rates of flame stretch are low, there exists a linear relationship between flame stretch and the corresponding unstretched burning velocity, and hence the equation below can be employed. The unstretched burning velocity is computed by the following equation, with three of the terms discerned experimentally as described below (Clavin, 1985):

\[ u_n = u_l - L \cdot \kappa \]  

(2-49)

Where \( u_l \) is the unstretched laminar burning velocity, \( u_n \) is the stretched laminar burning velocity, \( L \) is the Markstein length (of the burned gases), and \( \kappa \) is the rate of flame stretch. Flame stretch is determined by the rate of change in flame radius, \( r \), as a function of time, which can be measured in fundamental flame experiments:
\kappa = \frac{2}{r} \cdot \frac{dr}{dt} \quad 2-50

The Markstein length is determined experimentally using the slope of the stretched flame speed plotted as a function of the stretch rate of the flame. Markstein length is a function of reaction kinetics as well as molecular transport, which can be affected by flame stretch and differential diffusion of both heat and species (Haworth, 2010).

The Markstein number, \( Ma \), is the Markstein length, \( L \), divided by the flame thickness, \( \delta \):

\[ Ma = \frac{L}{\delta} \quad 2-51 \]

The Karlovitz number is a measure of the flame stretch through curvature of the laminar flame due to turbulence, expressed as the ratio of flame thickness and laminar flame speed multiplied by the rate of flame stretch.

\[ Ka = \frac{\delta L}{S_l} \cdot \kappa \quad 2-52 \]

Employing the relationships for Karlovitz number and Markstein number into the original equation for stretched burning velocity, we obtain:

\[ \frac{u_l}{u_n} = 1 + MaKa \quad 2-53 \]

In the case of hydrocarbon-air flames, a negative Markstein number indicates that laminar burning velocity increases as flame stretch increases, suggesting instabilities in the flame with effects of preferential diffusion. Likewise, positive Markstein numbers show a decrease in laminar burning velocity when the stretch rate increases, indicating a flame that is stable (Tseng, Ismail and Faeth, 1993).

Tseng et al. (1993) studied the effects of positive flame stretch on the laminar burning velocity of low-range hydrocarbon fuels in outward propagating spherical flames at atmospheric pressure. Linear correlations between Markstein numbers and equivalence ratios are assumed,
but the slope for methane-air flames is opposite in direction compared to those for ethane, ethylene and propane (Figure 2-3).

The Markstein numbers \((Ma)\) for propane were discussed in detail; where \(Ma < 0\), the flame radius increases more slowly and produces less stable flames than for \(Ma > 0\), where \(Ma > 0\) yields more stable flames that grow more quickly as a function of time. When comparing
mixtures of various stoichiometry for a given set of $Ma$ (where $Ma < 0$ or $Ma > 0$), in both cases richer mixtures show flames growing more rapidly than for leaner mixtures (Tseng, Ismail and Faeth, 1993).

Spherical laminar Methane-air flames were simulated at atmospheric conditions by Bradley et al. (Bradley, Gaskell and Gu, 1996). Burning velocities and Markstein lengths were computed and discussed. The findings show that Markstein lengths based on stretch rates from strain differ from stretch rates due to flame curvature.

Hydrogen behaves in a manner opposite of liquid hydrocarbon fuels in the sense that the stability of a hydrogen-air flame is greatest in lean regions (where Markstein number $< 0$), and decreases with increasingly rich air-fuel mixtures. Liquid hydrocarbon fuels are typically less stable at lean and stoichiometric proportions (where Markstein number $> 0$), and increase in stability as the air-fuel mixture becomes richer. Typically, for hydrocarbon fuels, positive Markstein lengths indicate a diffusionally stable flame whereas negative Markstein lengths indicate an unstable flame. For hydrogen, however, the behavior is opposite, and hydrogen is most stable in the case of negative Markstein lengths (Aung, Hassan and Faeth, 1998; Miao et al., 2009; Najt, 2010).

Aung et al. (1998) studied the effects of pressure and diluent concentration on the interactions of flame stretch for laminar premixed outward propagating spherical hydrogen flames at normal temperatures. Markstein numbers determined at various equivalence ratios for pressures of 0.35 – 1 atmosphere were in reasonable quantitative agreement with one another, with Markstein numbers increasing with increasing richness of the flame. In lean conditions, the Markstein number just becomes negative. At 1 atmosphere, the Markstein number increases more so than at lower pressures. At pressures from 2-4 atmospheres, Markstein numbers increase
for richer flames more significantly than at lower pressures, and on the lean side become more negative with increasing pressure. The slopes of the higher pressure curves of Markstein length versus equivalence ratio are much steeper with increasing pressure. The resulting effects of flame stretch on laminar burning velocities were significant (Aung, Hassan and Faeth, 1998). Kwon and Faeth also studied outwardly propagating spherical hydrogen flames and found that flames were indeed very sensitive to flame stretch (Kwon and Faeth, 2001).

Verhelst and Wallner (2009) discussed the results of Aung et al. in greater depth in their recent review paper, commenting that in the high pressure (4 atmosphere) condition of their study, the laminar flame speed increases more than linearly with a decrease in the flame stretch rate (which means that the Markstein lengths for hydrogen in this particular region are unique compared to liquid fuels). This invalidates the use of equation (2-53) above, which assumes a linear relationship. While it is agreed that at low rates of flame stretch (low pressures) hydrogen follows the linear trend of burning velocity as a function of stretch rate, this is not the case at higher pressures. Hence, present work discerning burning velocities and flame speeds for hydrogen that use the linear relationship may not be accurate. This is an important consideration for ICE work, and will be discussed further later; Verhelst and Wallner also suggest this as a topic of much needed investigation (Verhelst and Wallner, 2009).

One recent publication offers insight into the impact of pressure (0.8 – 2 bar) on the laminar burning velocities and Markstein lengths in a constant volume combustion bomb for various blends of methane and hydrogen fuel with air in stoichiometric proportions (Miao et al., 2009). Both unstretched flame speed and unstretched burning velocity decrease when initial pressure is increased for methane/hydrogen mixtures from 20-60%. The maximum pressure of this work is near 2 bar, which may allow the assumption of linear relationships for burning
velocity and stretch rate to be considered, even though Verhelst and Wallner (2009) have found that the Markstein lengths for hydrogen to behave contrary to Equation 2-53.

2.4.1 Turbulent burning velocity

Turbulent flames consist of a laminar flame front that becomes wrinkled due to the influence of instabilities and vortical structures, resulting in a fully developed turbulent flame (if in fact the conditions for a given air-fuel mixture can be supported in this environment). Hence, the characteristics of the laminar flame become a part of the equation for overall combustion rate.

Turbulence is an important attribute of a combustion system. A turbulent flame yields a greater mass consumption rate than a laminar flame due to the increased flame (surface) area achieved by wrinkling of the flame, thereby enhancing the energy release rate from chemical reactions and resulting in improved power or output of the system (Glassman, 1996). Turbulent flow quantities fluctuate as a function of time, and hence statistical approaches are used to describe properties of turbulent flow, such as velocity (Lancaster, 1976). The complex structure and broad range of length scales makes computations for fully reacting turbulent flow demanding, even with modern computing technology. It is for this reason that basic relationships often deduced from fundamental flame studies are employed to quantify relationships for turbulent combustion systems.

The relationship between turbulent flame speed and laminar flame speed is given as:

\[ S_t \cdot A_l = S_l \cdot A_t \]  \hspace{2cm} 2-54

where \( S_t \) is the turbulent flame speed, \( A_l \) the laminar flame area, and so forth (with the subscript “\( l \)” indicating laminar and “\( t \)” turbulent). The mass consumption rate for a turbulent flame is
similar for a laminar flame and is approximated as the density of the unburned gas times the turbulent flame speed:

\[ \dot{m} = A_t \cdot \rho_u \cdot S_t \]  \hspace{1cm} 2-55

The turbulent flame speed is a useful quantity in that it is required to calculate the mass consumption rate of the turbulent flame in an engine. The turbulent burning velocity depends on mixture properties and also on the flow, the engine geometry, and the history of the flame, unlike the laminar burning velocity which depends on mixture properties and the apparatus used during the measurement.

Flow characteristics may alter the chemical reactions in a combustion system where a turbulent flame exists. The extent to which flow conditions may affect combustion is dependent on characteristic times associated with the fluctuating components of density, velocity, pressure, temperature and species concentrations (Kuo, 2005). Damköhler number is a dimensionless parameter employed to evaluate whether fluid mechanics influences the chemical reaction rate (Turns, 2000):

\[ Da = \tau_f / \tau_c \] \hspace{1cm} 2-56

where \( \tau_f \) is the characteristic flow time and \( \tau_c \) the characteristic time for chemical reaction. The faster the chemical reaction rate, the smaller the characteristic chemical time resulting in \( Da >> 1 \); in this case the system is said to contain a “fast-chemistry regime” (Turns, 2000). When \( Da << 1 \), turbulence has the potential to affect the fluid mechanics such they affect the chemical reaction rate, energy release rates and flame structure (Glassman, 1996).

While it is complex to measure the turbulent flame speed, it is generally accepted that \( S_t \) is always greater than \( S_l \), and that \( S_t \) increases when the turbulence intensity ahead of the flame is increased (Glassman, 1996). Inducing turbulence in a combustion system in order to enhance the
rate of combustion is a common practice. The benefits of swirl in an engine, such as reducing carbon monoxide emissions and improving the burn process must be balanced against other characteristics of the combustion process, as excessive turbulence can induce quenching of the flame and increase heat loss due to convection (Heywood, 1988).

2.4.2 Quenching

Flame propagation relies on radical generation and heat transfer from the reaction zone to the unburned gases. A flame will quench if radicals are removed, such as near a surface, or if radical generation is slowed, such as when temperature declines due to heat losses or when homogeneous inhibition of radical formation or enhanced radical removal takes place.

Quenching can also occur due to extensive stretching of the flame (Glassman, 1996). Quenched regions can develop during the end of the combustion process in an ICE resulting from locally slow burning mixtures, and contribute substantially to the emission of unburned hydrocarbons (Hadjiconstantinou, Min and Heywood, 1996). The quench layers and cylinder wall crevices are the source of unburned hydrocarbons, in cases of normal engine operation and otherwise complete combustion (Cheng et al., 1993; Heywood, 1976).

2.5 Spark-ignition combustion

The laminar burning velocity ($u_l$) is a function of pressure, temperature, stoichiometry and also the concentration of diluent in the combustion system, and affects the rate of combustion in the cylinder as well as the tolerance of an air-fuel mixture to EGR. Since flames in the
combustion chamber of a spark ignition engine are considered to be laminar flames that are wrinkled due to in-cylinder turbulence, the influence of stretch rate on the laminar burning velocity is an important concept (Verhelst and Wallner, 2009).

2.5.1 Flame development in an internal combustion engine

Ignition of the compressed air-fuel mixture relies on chain-initiation reactions outlined above for hydrogen and methane (natural gas). An energy source is necessary to foster ignition, and in the case of a spark-ignited ICE that source is a spark plug. A spark plug is the conduit via which an electric discharge is generated by a high voltage coil and results in arcing between the electrode and ground of the spark plug. The energy of the arc is dictated by the coil and the gap between the electrode and the ground.

The energy release from the spark plug is sufficient to create an instantaneous plasma state of the fluid, breaking molecular bonds of the mixture within the combustion chamber, in the vicinity of the arc. The rate at which a flame kernel develops by subsequent propagation of chemical reactions is primarily governed by the minimum ignition energy for a given fuel. Hydrogen has quite a low minimum ignition energy compared to methane, and this serves to foster a more rapid flame kernel development compared to methane.

Ignition delay is a term used to characterize the time scale for autoignition of non-premixed flames and premixed fuel-air mixtures. This time period (or number of crank angle degrees) is an important consideration, particularly for methane. Spadaccini and Colkett (1994) summarized the literature for sensitivity analysis evaluating the relative contribution of kinetics on the ignition delay of methane and fuels containing methane plus low molecular weight
hydrocarbons (similar to natural gas), specifically from fundamental autoignition studies of stoichiometric air-fuel mixtures in shock tubes. Frenklach and Bornside (1984) concluded that ignition delay hinges heavily on reactions previously outlined for the methyl radical with an oxygen molecule, and the reaction of a hydrogen atom with an oxygen molecule (Frenklach and Bornside, 1984). The latter is said to be most significant at high temperatures (Spadaccini and Colket III, 1994). It is important to note that even small concentrations of ethane, propane or butane (regardless of isomer) in a mixture with methane will shorten ignition delay times relative to neat methane. At very lean equivalence ratios, significant free radicals such as OH, H, O and CH$_3$ accelerate the ignition process (Spadaccini and Colket III, 1994).

The term “ignition delay” should not be used to describe phenomenon in a spark-ignited engine. Instead a fraction of the combustion duration (typically considered ignition to 5%) accounts for the period of time (or number of crank angle degrees) between the crank angle degree at which the spark was fired and the onset of a fully developed flame.

Flame development in a spark-ignited engine follows the ignition process and is controlled by the stoichiometry and the motion of the local air-fuel mixture, particularly near the spark plug during the discharge. During the early flame development process, the laminar flame is under the strong influence of flame curvature (Boulouchos, Steiner and Dimopoulos, 1994). Cycle-to-cycle variations result from differences in flame development (and propagation) from one combustion cycle to the next and must be acknowledged and minimized (Bianco, Cheng and Heywood, 1991; Heywood, 1976).

In 1957, Mayer proposed an energy balance for one-dimensional steady state laminar flames, and ultimately asserted that the flame speed generally depends on the chemical mixture and the mechanism by which heat loss occurs (i.e. via convection or radiation) (Mayer, 1957).
Propagation of the developed flame is the physical movement of the flame from the vicinity of the spark plug across the combustion chamber toward the unburned air-fuel mixture, consuming the unburned portion (unburned gases) as it moves, leaving behind combustion products (the burned gases). Flame propagation is governed by the diffusion of both heat and mass to the unburned mixture. In the case of the present work, the ICE has a central spark plug; therefore the flame propagates downward and outward from the top of the combustion chamber. It is during the propagation processes that chain-propagating reactions take place, consuming fuel species and air to produce combustion products. Expressions for the laminar and turbulent flame quantities were discussed in the previous sections.

There is a significant difference between the densities of the burned and unburned gas mixtures; for gasoline fuel the density of the unburned mixture is about four times greater than the burned gases. Combustion chamber geometry, spark plug location, flow field characteristics and the state and composition of the unburned mixture govern the flame propagation process (Heywood, 1988).

### 2.5.2 Combustion duration

The combustion duration describes the number of crank angle degrees between that where 10 percent of the fuel mass was burned, and that where 90 percent of the fuel mass was burned. The pressure trace during combustion is measured as a function of crank angle degrees (CAD), and that curve is integrated to compute the cumulative heat release based on the ratio of specific heats, the lower heating value of the fuel, and the stoichiometry of the air-fuel mixture. The heat release computation assumes CAD at which the spark is fired to be start of combustion
(SOC), and subsequently compares the computed cumulative energy released for each CAD to the total amount of fuel energy contained in the combustion chamber for that combustion cycle in order to discern percent of heat released. The early flame development period is expressed between SOC (or 0% heat released) and 10% of the heat released (or 10% of the fuel mass burned).

Burn duration is an important quantification in the combustion process. Efficiency of the combustion process requires a balance between heat loss and timing loss (spark advance). Spark advance, required for slow burning fuels such as methane, increases heat losses to the surroundings, but reduces losses associated with timing since more of the fuel mass burns near top dead center (TDC). Significant heat loss results can decrease efficiency and may lead to less complete combustion, hence increasing unburned hydrocarbons and carbon monoxide (CO) emissions.

For a gasoline-fueled spark-ignited ICE, it has been shown that there is a weak relationship between the initial flame kernel behavior (or speed with which the early flame development occurs) and the 10-90% combustion duration where flame kernel development was quantified using a fiber-optic spark plug (Bianco, Cheng and Heywood, 1991).

2.5.3 Role of turbulence in a spark-ignited engine

Boulouchos presented a description of the laminar to turbulent transition in an engine, at the 1st Ignition Symposium in 2004 (Boulouchos, 2004). Figure 2-4 was reproduced from the conference proceedings from that presentation.
A flame progresses from a spark discharge, where the spark event creates a plasma state of the air-fuel mixture that breaks molecular bonds (Boulouchos, 2004). In a lean hydrocarbon flame, the flame speed decreases when the flame is stretched, whereas for lean hydrogen flames stretch increases the flame speed. The flame gets bigger and, once large enough, it will become impacted by turbulence. Turbulence results in the wrinkling of the flame, which increases the surface area of the flame thereby increasing the mass consumption rate. In ICEs, the transition from laminar to wrinkled turbulent flame occurs when the diameter of the flame kernel is on the order of 4-5 mm (Najt, 2010). The time that it takes the flame to evolve from the onset of the spark to development of a wrinkled turbulent flame is often referred to as “ignition delay,” however Boulouchos describes this simply as the transition of “a baby flame growing into an adult” (Boulouchos, 2004).
Lancaster (1976) conducted an experimental study in a CFR engine using a hot-wire anemometer to measure in-cylinder turbulence data that provided turbulence intensity and turbulence scale quantifications at various operating conditions for gasoline fuel. The primary conclusion was that turbulence is isotropic near TDC of the compression event, and the turbulence intensity near TDC of the compression event is a linear function of the intake volume flow rate (Lancaster, 1976). This means that as engine speed increases, and hence the mean piston speed increases, the turbulence intensity increases as well. Turbulence intensity is the root mean square value of the fluctuation about the mean velocity of the fluid motion and can be expressed as follows:

\[ u' = \sqrt{u'^2} \] 

Intake-generated turbulence is a design factor in modern spark-ignition engines, as rotating flow increases turbulence intensity, leading to gains in combustion stability and enhanced mass consumption rate. Imparting swirl in the intake flow also serves to improve air and fuel mixing. Improved mixing and improved combustion stability permit leaner combustion. In the case of hydrogen-fueled ICEs, flame stability can be sustained even with significant quantities of EGR which effectively lowers peak cylinder temperatures and reduces thermal NOx emissions (Hill and Zhang, 1994; Nagayama, Araki and Iioka, 1977).

Tumble and swirl are terms used to describe rotating flow. Swirl describes the rotational component about the axis parallel to the cylinder; the component about the axis perpendicular to the cylinder is called tumble. Ultimately, swirl and tumble increase the turbulence intensity within the combustion chamber; turbulence intensity increases burn rate and convection of the flame zone, and also affects flame area by flame-holding on the spark plug (Hill and Zhang, 1994).
Intake-generated swirl provides turbulence inside the combustion chamber, resulting in increased flame development and flame propagation, as the turbulent flame speed is higher, resulting in a shorter combustion duration, which enables spark to be retarded. During flame development this faster flame-growth results in less variation within the center of the flame, which reduces changes in the flame shape from interactions with the wall. Increased burn rate decreases cycle-to-cycle variation, and indicates that burning ends earlier in the expansion stroke, therefore reducing the chance for misfire (Heywood, 1988).

If combustion phasing is appropriate for a given fuel, an increase in the mass burn rate may suggest higher peak cylinder temperature, thereby increasing NOx emissions. However, rotating flows may increase convective heat transfer to the cylinder walls (Heywood, 1988), and during very lean operation peak temperatures may decrease enough to suppress thermal NOx production (Hill and Zhang, 1994; Pazinauskas, Wilson and Evans, 2000). However, significant heat loss can compromise thermal efficiency.

The laminar burning velocity of natural gas is about 50-60% lower than that of gasoline. Slow burn rate increases heat losses from the flame front via conduction to the electrode, thereby leading to cool flame temperatures where formaldehyde is produced (Pazinauskas, Wilson and Evans, 2000). Slow flame development contributes to cycle-to-cycle variations and also pollutant emissions formation (such as aldehydes and ketones) from natural gas combustion (Ayala et al., 2003; Bianco, Cheng and Heywood, 1991).

Swirl also serves to increase the flame speed, by virtue of improving homogeneity of the air-fuel mixture. Mixture quality may be the most important factor in combustion, as it can improve flame speed, subsequently improving burn rate and other responses. Providing a homogeneous air-fuel mixture is more difficult with gaseous fuel than with liquid fuel as the
momentum with which liquid fuel flows through an injector allows the droplets to penetrate the air charge prior to vaporization. Gaseous fuels, however, begin to diffuse at the surface of the airflow (Pazinauskas, Wilson and Evans, 2000).

Turbulence in ICEs results in a faster burn rate and permits lean combustion in spark-ignited combustion engines (Hill and Zhang, 1994; Nagayama, Araki and Iioka, 1977). Higher burn rate achieved with turbulence decrease combustion duration, which effectively completes combustion in a shorter period near TDC. Hence, effects of cycle-to-cycle variation of the expansion ratio and cyclic work output are minimized, leading to more efficient combustion.

Conte and Boulouchos (2006) quantified laminar flame speeds using ion sensors and an optical spark plug combined with heat release analysis in a gasoline-fueled spark-ignited engine. When hydrogen was added to gasoline, the laminar flame speed was found to increase by as much as four times compared to gasoline combustion alone. The effects on the turbulent phase of combustion were not proportional to the increase in laminar flame speed, however, though the turbulent flame speed was increased in the presence of hydrogen (Conte and Boulouchos, 2006).

2.5.4 Engine geometry

Engine geometry has a direct effect on the combustion process and thermal efficiency. As such, it is important to address the limitations of the comparisons made in this work.

In the automotive world, engine design is optimized around a specified fuel; fuel quality is also a consideration, i.e., octane number. Engine compression ratio and mixture properties (such as the ratio of specific heats for the air-fuel mixture) are also critical considerations when choosing engine hardware.
As a first point, let us consider compression ratio. The compression ratio of a given engine is chosen based on the required engine performance, but is limited by ignition quality of the fuel. Modern, conventional gasoline applications in the United States (an important distinction, since fuel quality in the United States is sub-par to European fuels, for example) are likely to have compression ratios between 9-10, given that modern engines must be able to operate knock-free at octane numbers as low as 89. Performance engines may have a compression ratio as high as 11 or 12. Natural gas has an octane number of 105, and hence can realize higher compression ratios (approximately 13). A difference in compression ratio results in a difference in bore and stroke sizes, and potentially stroke to bore ratio (S/B), and also the ratio of the surface area of the combustion chamber (with piston at TDC) to the volume (S/V). The higher the S/V ratio, the more thermally inefficient the engine becomes. At a given S/B, S/V increases as a function of increasing compression ratio. The higher the S/B, the lower the S/V is at a given CR, meaning that increasing S/B decreases thermal losses. However, increased S/B slows the burn process. Hence, everything needs to be balanced, for a specific fuel and desired performance level of an engine.

In addition to engine geometry, valve opening and closing is tuned for a given geometry and fuel, to maximize efficiency. Failure to tune valve-timing for a given engine geometry and fuel application results in a poor thermal efficiency.

Engine design and manufacturing is extremely expensive, especially for a custom engine. Hence, the present work did not employ an engine that was designed nor optimized for natural gas. The present work uses a Ricardo Hydra single-cylinder test engine with S/B of unity, and 10.44:1 compression ratio (additional specifications are provided in the Experimental section). Since the Ricardo Hydra was not optimized for CNG, the thermal efficiency is expected to be
quite low. And given that the valve timing is generic, or in other words, not tuned, valve timing is another contribution to the presumed low efficiency when burning natural gas in this engine.

The ratio of specific heats ($\gamma$) is the other factor contributing to thermal efficiency. For a given fuel, gamma changes as a function of equivalence ratio. Gamma is different for the burned gases and unburned gases. And gamma is different for CNG than for HCNG. The indicated thermal efficiency increases as gamma increases. At the stoichiometric equivalence ratio, gamma for methane-air is 1.354, and 1.401 for hydrogen-air (Verhelst and Wallner, 2009). A sample calculation is shown in Table 2-2, and demonstrates the potential to increase the indicated thermal efficiency by changing compression ratio and accounting for the ratio of specific heats of the fuel. The results are theoretical, and must be balanced against the characteristics of the burn process, bore-to-stroke ratio, etc.

Table 2-2 Example of the effects of compression ratio and gamma on thermal efficiency.

<table>
<thead>
<tr>
<th>$\gamma$</th>
<th>10.44</th>
<th>11</th>
<th>11.5</th>
<th>12</th>
<th>12.5</th>
<th>13</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.35</td>
<td>0.56</td>
<td>0.57</td>
<td>0.57</td>
<td>0.58</td>
<td>0.59</td>
<td>0.59</td>
</tr>
<tr>
<td>1.4</td>
<td>0.61</td>
<td>0.62</td>
<td>0.62</td>
<td>0.63</td>
<td>0.64</td>
<td>0.64</td>
</tr>
</tbody>
</table>

2.6 Summary of literature and statement of research objectives

Hydrogen is unique compared to liquid hydrocarbon fuels. The wide flammability range of hydrogen enables extremely lean combustion, which supports high rates of EGR that can be used to minimize NOx emissions in ICEs. Hydrogen has a high mass diffusivity in air (or nitrogen, an important distinction since many models assume diffusivity into the diluent alone), which fosters a faster flame development. The low minimum ignition energy of hydrogen also facilitates enhancements in early flame development compared to hydrocarbon fuels. These
physicochemical properties contribute to the fast laminar flame speed of hydrogen compared to hydrocarbon fuels.

Laminar flame speed itself is one component of a very intricate process of combustion, whether in an outward propagating spherical flame or in an ICE. Laminar burning velocity, for example, while a function of laminar flame speed, is also a function of the density ratio of burned to unburned gas in the system. The density of the unburned mixture for fuels that include hydrogen as a constituent is lower due to the low density of hydrogen. Therefore, in conjunction with hydrogen’s fast laminar flame speed, the lower unburned density accounts for an increase in the laminar burning velocity.

The existing methods used to determine unstretched laminar burning velocities require a linear relationship between flame speed and flame stretch rate, and hence are not applicable at pressures near engine conditions when hydrogen is a component of the fuel, as the flame speed responds more than linearly as a function of flame stretch. Hence, the literature does not provide high-integrity data for laminar flame speeds and burning velocities at engine conditions for hydrogen. This makes it difficult to further quantify the relative contribution of laminar flame properties to the overall combustion duration or to the turbulent burning parameters in a combustion system. The data that exist, however, show that at moderate pressures (2-4 bar) the stretched and unstretched flame speeds and velocities decrease compared to those at lower pressures, for methane/hydrogen flames (Miao et al., 2009).

It has been shown that the relative increase in flame speed during the turbulent phase of combustion when hydrogen is added to gasoline is lower than the increase observed on the laminar flame speed (Conte and Boulouchos, 2006). It was shown for gasoline that the early flame development contributed only slightly to the overall combustion duration (Bianco, Cheng
and Heywood, 1991). The primary conclusion of the literature suggests that improved BSFC is achieved with HCNG compared to CNG alone, and is an indication that the mass consumption rate is faster for HCNG than CNG, hence leading to an improved overall burn rate as reported by many studies (Collier et al., 1996; Conte and Boulouchos, 2006; D'Andrea, Henshaw and Ting, 2004; Hassaneen et al., 1998; Sita Rama Raju, Ramesh and Nagalingam, 2000; Soggard, Schramm and Jensen, 2000; Swain et al., 1993). The first objective of the present work is to confirm that the present work aligns with literature with regards to two specific findings:

- Hydrogen addition speeds up the early flame development process of natural gas, enabling spark retard
- The spark retard achieved with hydrogen addition to natural gas effectively results in heat release concentrated near TDC, improving the thermal to mechanical efficiency

While many engine experiments have demonstrated enhancements to methane or gasoline combustion with hydrogen addition in terms of BSFC, pollutant emissions, efficiency, and burn rate, much of the literature is lacking detailed heat release analysis for hydrogen assisted combustion in ICES to describe the effects of hydrogen on the combustion duration. Hence, the second and primary objective of the present work is to perform detailed heat release characterization of hydrogen assisted natural gas combustion in a spark-ignited engine, and compare the combustion characteristics with those for natural gas specifically, to address the following hypothesis: hydrogen addition to natural gas supplants swirl, resulting in an improved early flame development without incurring thermal losses attributed to swirl.

The Experimental section, provided in the next chapter, provides information about the test facilities and specifications of them. The Results chapter presents the findings, and the discussion of those results ensues in the subsequent chapter. The Discussion chapter addresses
three primary topics, aligned with each aspect of the aforementioned hypothesis. The conclusions
and recommendations follow. Additional data is shown in Appendix A, and the Matlab code for
the heat release model is presented in Appendix B.
Chapter 3 Experimental

3.1 Ricardo Hydra engine test bench and instrumentation

Figure 3-1 shows the engine test cell and instrumentation configuration. The Ricardo Hydra engine configured with an advanced control system and dynamometer with absorbing and motoring capabilities, was acquired for the hydrogen assisted combustion project.

Figure 3-1 Schematic of the test bench and instrumentation.
Figure 3-2 shows a photograph of the Ricardo Hydra test bench. The Hydra is a 0.5 L, single-cylinder, 4-valve, naturally aspirated, port-injected, spark ignition engine. The control system allows the user independent control of RPM (or torque), load, stoichiometry, and spark timing.

Table 3-1 summarizes the engine specifications for the Ricardo Hydra, and Table 3-2 shows the valve timing. Note that the stroke to bore ratio is unity; also note that 10.44:1 compression ratio is on the high-side for a conventional commercial spark-ignited engines. Natural gas is composed of methane, predominantly, and as such has a sufficiently high octane number, and hence engine-knock (from pre-ignition) will not be a concern for the present study.
Table 3-1 Ricardo Hydra engine geometry and technical specifications.

<table>
<thead>
<tr>
<th>Engine Type</th>
<th>Four stroke</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aspiration</td>
<td>Normally aspirated</td>
</tr>
<tr>
<td>CR</td>
<td>10.44:1</td>
</tr>
<tr>
<td>Bore</td>
<td>86 mm</td>
</tr>
<tr>
<td>Stroke</td>
<td>86 mm</td>
</tr>
<tr>
<td>Con Rod Length</td>
<td>143 mm</td>
</tr>
<tr>
<td>Rated Speed</td>
<td>6000 RPM</td>
</tr>
<tr>
<td>Minimum Speed</td>
<td>1000 RPM</td>
</tr>
<tr>
<td>Maximum Speed</td>
<td>6500 RPM</td>
</tr>
<tr>
<td>Coolant outlet T</td>
<td>85 °C</td>
</tr>
<tr>
<td>Oil Inlet T</td>
<td>85 °C</td>
</tr>
</tbody>
</table>

Table 3-2 Valve timing for the Ricardo Hydra engine.

<table>
<thead>
<tr>
<th>Valve Timing</th>
<th>CAD BTDC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intake Valve Open</td>
<td>2</td>
</tr>
<tr>
<td>Intake Valve Close</td>
<td>44</td>
</tr>
<tr>
<td>Exhaust Valve Open</td>
<td>42</td>
</tr>
<tr>
<td>Exhaust Valve Close</td>
<td>4</td>
</tr>
</tbody>
</table>

The associated data acquisition system encompasses thermocouples, pressure transducers, shaft encoder, lambda sensor, mass flow controller, as indicated in Figure 3-1. All are integrated into a LabView PXI system, using a SCXI chassis. LabView version 7 was used to create a data monitoring and collection system, complete with MFB calculations, and heat release code. A Meriam laminar flow element and a plenum chamber were integrated for accurate charge airflow measurement.

The Hydra exhaust is outfitted with a heated canister filter coupled to a heated sample line, both kept at 190°C, in order to preserve emissions in their gaseous state as they travel to the analytical equipment and remove particulates prior to gas analysis. Emissions analysis was achieved using an AVL CEB II emissions bench, composed of analyzers for CO, CO₂, NOₓ, HC (low and high) and O₂, Figure 3-3.
The same storage tank was used for CNG and HCNG. Between fueling of each fuel, the tank was purged several times by first evacuating the tank to atmosphere, followed by 2 partial fills (to 1000 psi) with the new fuel of interest and subsequent evacuation to atmosphere. The tank was then filled to 3600 psi with the fuel of interest to be used for testing. After fueling, a fuel sample was collected with a bag and later fed to the GC with a syringe. The syringe was filled and emptied 3 times with the fuel in the bag before acquiring the sample for analysis.

### 3.2 Intake port modification for intake-induced swirl

The Hydra possesses a quiescent combustion chamber. Components were fabricated and employed to partially or fully block one of the intake ports to generate intake-induced swirl, shown in Figure 3-4.
Figure 3-4 Threaded components of various bore used to block one intake port incrementally or fully, to create intake-induced swirl.

Figure 3-5 shows a picture of the intake with one port opened and one port fully blocked. An internally threaded aluminum component was manufactured to press into one of the intake ports, to accept components to partially or fully block the intake port.

Figure 3-5 Photograph of intake port of Ricardo Hydra engine, with one port fully blocked.

3.3 Development of custom gaseous fueling system

A gaseous fueling system was designed, fabricated, and employed, according to natural gas vehicle requirements per the Department of Transportation (DOT) and the National Highway
and Transportation Safety Administration (NHTSA). In order to introduce compressed natural
gas and hydrogen into the engine safely, a gaseous fueling system was designed and integrated.

A Hazard and Operability (HAZOP) analysis was performed on the system during the
design phase, to examine the safety of the system and to determine the overall risk associated
with it. The analysis identified critical locations for pressure regulators, vents, gas detectors,
hard-plumbed lines vs. the use of connectors, and the need for a breakaway hose at the connection
between the fuel tank and the feed line to the engine. Furthermore, it lead to a decision to place
the storage tank outdoors, which resulted in a significant project where the Office of Physical
Plant (OPP) at the university poured a concrete pad (for tank storage), trenched a line from the
pad to the building, and drilled through the building exterior to plumb the fuel line into the
laboratory.

The system is composed of a 3600 psi, glass-wrapped steel cylinder with an 80L capacity
(Figure 3-6). The tank includes manual shut-off valves on each end. One valve is also outfitted
with a fueling receptacle, shown in Figure 3-7. The other valve is fitted with quick disconnects,
to easily and safety detach the tank from the fueling system, so that the tank can be transported to
the hydrogen fueling station on campus. The quick disconnect is attached to a hose, which is
connected to a break-away line that was installed for safety, to protect the system if the tank was
moved without first disconnecting the tank.
The break-away enters a pneumatic valve, which is opened to allow fuel to flow from the tank into the building when a solenoid valve is switched on to permit compressed air to flow outside to the pneumatic valve. A pressure regulator sits inline downstream of the pneumatic valve, and drops the pressure from 3600 psi down to 200 psi so that low-pressure fuel is entering the fueling system in the building. The outlet of the pressure regulator has a pressure relief device to ensure low-pressure delivery to the laboratory, in the event that the pressure regulator fails or becomes damaged. A more thorough schematic of the fueling system is shown in Appendix C.
The pressure of the gaseous fuel is regulated down to 75psi once it reaches the engine test stand, and then enters a Sierra Instruments mass flow controller for flow control and measurement. A vent hood is positioned above the engine, and is outfitted with a hydrogen sensor to collect hydrogen that may leak from the system and detect its presence.

3.3.1 Test Conditions

Table 3-3 presents the summary of test conditions employed for the present work.

<table>
<thead>
<tr>
<th>RPM</th>
<th>Spark timing</th>
<th>Intake configuration (q = base port configuration) (s = one port fully blocked)</th>
<th>(\Phi) range</th>
</tr>
</thead>
<tbody>
<tr>
<td>2000</td>
<td>Fixed</td>
<td>(s, \text{ ns})</td>
<td>0.6 - 1</td>
</tr>
<tr>
<td>2000</td>
<td>MBT</td>
<td>(s, \text{ ns})</td>
<td>0.6 - 1</td>
</tr>
<tr>
<td>2750</td>
<td>MBT</td>
<td>(s, \text{ ns})</td>
<td>0.6 - 1</td>
</tr>
</tbody>
</table>

3.4 Heat release model

Predictions of burn duration were achieved using a heat release model developed previously by Szybist (Szybist, 2005). This code was modified later for use with gaseous fuels, namely HCNG, by Clark (Clark, 2008). The heat release model uses measured, in-cylinder pressure data to discern the rate of energy released throughout the four-stroke cycle. It is also possible to employ schemes to predict the mass fraction of fuel burned as a function of CAD throughout the cycle, from which burn duration can be assumed (i.e. the period between 0-10\% mass fraction burned (MFB), is considered to be the early flame development period, and 10-90\% MFB is considered the bulk burn duration).
The heat release model comprised a zero dimensional single zone model and direct numerical solution was possible. The following assumptions were employed in the present work, and are typical for streamlined engine heat release analysis:

- Homogeneous mixture with uniform properties
- Treats $\gamma$ (ratio of specific heats) the same for both CNG and HCNG fuels, and is assumed to be that of air (Heywood, 1988). This assumption is consistent with other works investigating the pressure-based burn characteristics of hydrogen assisted natural gas combustion (Kornbluth, McCaffrey and Erickson, 2009; Huang et al., 2007).
- Heat release due to combustion is considered to be heat added to the cylinder
- Heat transfer to the walls and to the crevice volumes is neglected

The heat release model was coded according to the following equations. The gross heat release rate (release of chemical energy of the fuel) is quantified as:

$$\partial Q_{ch} = \partial U_s + \partial Q_{ht} + \partial W + \sum h_i dm_i$$  \hspace{1cm} 3-1

The net heat release rate is often referred to as the apparent heat release, and is quantified as the chemical heat release rate less the heat losses associated with blow-by and crevice volumes. This quantity is neglected (assumed to be zero) in the present work, due to lack of instrumentation to quantify the losses.

$$\partial Q_{ch} = \partial Q_n - \partial Q_{ht} - \sum h_i dm_i$$  \hspace{1cm} 3-2

The net energy is determined via Equation 3-3, and is a function of the net work and the sensible energy. The net energy can also be determined from measured variables, namely the mixture mass, constant-volume specific heat, and change in temperature, cylinder pressure, and change in volume.

$$\frac{dQ_n}{dt} = mc_v \frac{dT}{dt} + p \frac{dV}{dt}$$  \hspace{1cm} 3-3
The differentiated ideal gas law is shown as:

\[ PdV + VdP = mRdT \]  \hspace{1cm} 3-4

And then combined with the net heat release from measured parameters Combine the two to get:

\[ \frac{dQ_n}{dt} = \left(1 + \frac{c_v}{R}\right) \cdot P \frac{dv}{dt} + \frac{c_v}{R} V \frac{dP}{dT} \]  \hspace{1cm} 3-5

The relationship for gamma relative to the constant-volume specific heat and universal gas constant is:

\[ \frac{c_v}{R} = \frac{1}{\gamma - 1} \]  \hspace{1cm} 3-6

Substituting into equation 3-6 gives:

\[ \frac{dQ_n}{dt} = \frac{\gamma}{\gamma - 1} P \frac{dv}{dt} + \frac{1}{\gamma - 1} V \frac{dP}{dT} \]  \hspace{1cm} 3-7

The ratio of specific heats (\( \gamma \)) is then computed based on the temperature (in Kelvin), for \( T < 1000 \):

\[ \gamma = 1.3 + 6.0 \times 10^{-5} \times T - 1.5 \times 10^{-7} \times T^2 \ldots \]  \hspace{1cm} 3-8

\[ \ldots - 5.6 \times 10^{-11} \times T^3 + 9.2 \times 10^{-14} \times T^4 \]

And for \( T > 1000 \):

\[ \gamma = 1.4 + 2.5 \times 10^{-4} \times T - 1.4 \times 10^{-7} \times T^2 \ldots \]  \hspace{1cm} 3-9

\[ \ldots - 3.7 \times 10^{-11} \times T^3 + 3.7 \times 10^{-15} \times T^4 \]

The cylinder temperature was not measured in the present work, and hence it is estimated from thermodynamic properties. The bulk cylinder temperature is a function of air and fuel mass, the specific heat, cylinder volume and energy as a function of CAD:

\[ \frac{dT}{d\theta} = \frac{1}{(m_{air}+m_{fuel})c_v} \left( \frac{dQ_n}{d\theta} - P \frac{dv}{d\theta} \right) \]  \hspace{1cm} 3-10
Cylinder pressure data was collected at every crank angle degree and resolved to 0.1 CAD. For every test, 200 cycles were collected sequentially, and then averaged. The averaged pressure data were then smoothed via “smooth” in Matlab, which smooths the data using a moving average filter with a span of 5. Due to the memory-intensive nature of collecting 200 data files for each test condition, only the averaged pressure data was saved for a given test point.

Start of combustion is assumed to be the time of spark (Najt, 2010). The mass fraction burned is estimated using normalized values of the cumulative heat release (in lieu of Weibe function or Rassweiler & Withrow) relative to the fuel energy input for the combustion cycle (Rassweiler and Withrow, 1938). The cumulative heat release then is estimated by the following equation:

$$Q(\theta_i) = \int_{\theta_{soc}}^{\theta_i} \frac{dQ_n}{d\theta} d\theta$$  \hspace{1cm} 3-12

And the mass fraction burned is represented by:

$$Q\% = \frac{q_i}{Q_{max}}$$  \hspace{1cm} 3-13

Referring back to Equation 3-6 shows that the volume is an important quantity used to discern heat release.

The volume of the combustion chamber at a given CAD depends on the engine geometry, namely bore ($B$), stroke ($S$), compression ratio (cr), connecting rod length ($l_{rod}$) and the radius of the crank travel ($r_{crank}$). The change in volume is ultimately computed and used in the heat release calculation, specifically in equations 3-4, 3-5, 3-6, 3-8, and 3-11, above. The following equations summarize the method by which delta volume is computed. The displacement volume is a function of the bore diameter and length of the stroke:

$$V_d = \pi \cdot B^2 \cdot \frac{S}{4}$$  \hspace{1cm} 3-15

The clearance volume is the displacement volume divided by the compression ratio minus 1:
The cylinder volume is then computed as:

\[ V_c = \frac{V_d}{(cr - 1)} \]  

The cylinder volume is then computed as:

\[
cylVol = V_c + \left( \frac{\pi \cdot B^2}{4} \right) \cdot \left( r_{crank} \cdot (1 - \cos(CA(radians))) \right) \ldots \]

\[
\ldots + \frac{r_{crank}}{4l_{rod}} \cdot (1 - \cos(2 \cdot CA(radians))) \quad \text{3-17}
\]

And the delta is then computed by:

\[
\Delta V_i = \frac{(cylVol_{i+1} - cylVol_{i-1})}{2 \cdot \Delta CA} \quad \text{3-18}
\]

### 3.5 Confirming TDC

The location of TDC was confirmed in a rudimentary way which involved evaluating the peak pressure of the motored pressure trace at both engine speeds from the present work (2000 and 2750 RPM). The coolant inlet temperature was confirmed to be stable and greater than 80 degrees Celsius. The location (crank angle) of peak pressure was taken to be TDC. Matlab was used to find the maximum pressure and return the index of the maximum pressure in the pressure matrix, as well as the pressure value to confirm TDC, i.e. the location of peak pressure was not determined visually. The method used provides the dynamic TDC, which is superior to static TDC. In both cases (at both engine speeds: 2000 & 2750 RPM), the location of peak pressure was at 360 CA.

### 3.6 Propagation of error

The propagation of error was computed for all variables (such as brake specific energy consumption) that were computed as a function of at least two measured variables (such as torque
and mass fuel flowrate). The variance of a given measured variable was computed as a first step. Then the following equations (3-15 and 3-16) were employed, where \( \sigma \) refers to the variance, \( y \) represents the computed variable for which the error is being discerned, \( x \) represents the measured variable with subscript \( i \), for \( i \) number of variables, and \( m \) is the multiplier for a given variable (\( x_i \)):

\[
m_i = \left. \frac{x_i \, \partial y}{y \, \partial x_i} \right| \tag{3-14}
\]

\[
\frac{\sigma_y^2}{y^2} \approx \sum_i m_i^2 \frac{\sigma x_i^2}{x_i^2} \tag{3-15}
\]
Chapter 4 Results

The first objective of this research was to confirm that present findings correlate with those in the literature, specifically that:

1. The addition of hydrogen improves flame development, and hence enables spark retard
2. The addition of hydrogen shortens the main burn duration, improving the conversion of thermal to mechanical energy, thereby improving efficiency through minimizing heat loss prior to TDC improving efficiency

The second and primary objective of this work was to evaluate a hypothesis via performing heat release characterization of hydrogen assisted natural gas combustion in a spark-ignited engine, and compare the combustion characteristics with those for natural gas, specifically, to address deficiencies in the hydrogen assisted combustion literature. The hypothesis of this work is not found in the literature to-date, and states that the addition of hydrogen supplants swirl in terms of enhancing the burn process, thereby reducing cylinder heat loss and improving efficiency.

Studies were designed and performed to confirm common findings in the literature, and to test the hypothesis. The results for each experiment are described in the following sections. The term “quiescent” is used to describe the engine configuration without any modifications; this configuration is “quiescent” (meaning very low levels of in-cylinder swirl) in terms of its charge motion in its base configuration and is denoted in the data label suffix as “-q.” For comparison, experiments were performed with increased swirl, which was generated by fully blocking one of the two intake ports, generating some amount of intake-induced swirl, and denoted as “-s” in the data label suffix (i.e CNG-q, CNG-s, HCNG-q, HCNG-s).
This chapter serves to present the data resulting from this research. The following chapter contains an in-depth discussion of the findings.

4.1 Base engine (quiescent) studies at 2000 RPM

Tests were conducted at 1.5 bar brake mean effective pressure (BMEP) at stoichiometric air fuel ratio (AFR) at fixed spark timing and at MBT timing without intake-induced swirl. The spark timing required to attain MBT at stoichiometric AFR and 1.5 bar BMEP for both non-swirl compressed natural gas (CNG) and hydrogen assisted compressed natural gas (HCNG) cases was held constant as a function of stoichiometry for the fixed spark timing studies. The fueling rates at these conditions were fixed as throttle was opened incrementally to vary stoichiometry. The throttle was adjusted incrementally at a constant fueling rate to sweep AFR in the lean direction, and spark timing (ST) was adjusted to MBT at each new AFR.

4.1.1 Fixed spark timing

The BSEC is higher for CNG than for HCNG for the lean conditions near stoichiometric, as shown in Figure 4-1, indicating that HCNG is more efficient overall than CNG. However, the difference in BSEC is small, and may not be statistically significant for stoichiometric conditions.
Figure 4-1 Brake specific energy consumption (BSEC) as a function of equivalence ratio ($\Phi$) for (○) HCNG-q, (□) CNG-q, for fixed spark timing (15.6 CA BTDC for HCNG-q, and 26.6 CA BTDC for CNG-q) at 2000 RPM with base port configuration (quiescent).

The emissions index (EI) normalizes engine-out combustion product species with the quantity fuel consumed, and is used in the present work to report carbon monoxide, unburned hydrocarbons, and oxides of nitrogen emissions.

The emissions index of carbon monoxide (EICO) decreases as a function of increasingly lean equivalence ratio, for both CNG and HCNG, and is depicted in Figure 4-2. The trends in the present work are expected, as carbon monoxide generation is known to be a function of fuel-rich combustion, and trends downward as the amount of excess air in the air-fuel mixture increases (Heywood, 1988).
As seen in Figure 4-3, the emissions index of total hydrocarbons (EITHC) is similar for both HCNG and CNG. The EITHC increases as a function of increasingly lean conditions for both CNG and HCNG for conditions leaner than stoichiometric. Lower temperatures lead to premature quenching of reactions, and hence CO formation is increased.
The addition of hydrogen to CNG (via HCNG fuel) provides an improvement in the emissions index of oxides of nitrogen (EINOx), as shown in Figure 4-4.
The brake thermal efficiency (BTE), shown in Figure 4-5, of HCNG is higher (better) than for CNG. The BTE for both fuels increases as the equivalence ratio decreases (becomes more lean). The trend for CNG plateaus near $\Phi = 0.6$, as it approaches the lean limit.

The NMEP is plotted for CNG and for HCNG in Figure 4-6. The CNG achieves a higher NMEP over all equivalence ratios compared to HCNG in this fixed spark timing scenario.
Figure 4-6 Net mean effective pressure (kPa) as a function of equivalence ratio (Φ), for (○) HCNG-q, (□) CNG-q, for fixed spark timing (15.6 CA BTDC for HCNG-q, and 26.6 CA BTDC for CNG-q) at 2000 RPM with base port configuration (quiescent).

The burn duration is presented in crank angle degrees (CA), and represents the time required to progress from 10% to 90% of the mass fraction burned of the fuel. The early flame development period occurs prior to the 10% mass fraction burned point. The end of combustion is difficult to model, hence the 90% mass fraction burned point is chosen as the end of the main burn duration period (it has proven to be a reasonable representation of the combustion duration) (Stone, 1999).

The burn duration for HCNG is faster between 0.9 ≤ Φ ≤ 0.8 than for CNG, as shown in Figure 4-7. The values for burn duration for both fuels are quite close together at stoichiometric, but diverge at Φ < 0.8. The burn duration for both fuels level out as the mixtures become more lean.
Figure 4-7 Burn duration, 10-90% mass fraction burned (CA) as a function of equivalence ratio (Φ), for (○) HCNG-q, (□) CNG-q, for fixed spark timing (15.6 CA BTDC for HCNG-q, and 26.6 CA BTDC for CNG-q) at 2000 RPM with base port configuration (quiescent).

Figure 4-8 shows that the midpoint of the burn process, CA50, is after TDC for both fuels, where CA50 is closer to TDC for CNG than for HCNG. The difference between the fuels is consistently approximately 6-8 CAD.
Figure 4-8 Crank angle at 50% mass fraction burned point as a function of equivalence ratio ($\Phi$), for ($\circ$) HCNG-q, ($\square$) CNG-q, for fixed spark timing (15.6 CA BTDC for HCNG-q, and 26.6 CA BTDC for CNG-q) at 2000 RPM with base port configuration (quiescent).

The quantity plotted in Figure 4-9 is the cumulative energy released (from fuel burning) during the compression stroke, before the piston reaches TDC. HCNG releases less energy prior to TDC than for CNG, across the range of equivalence ratios tested.
4.1.2 Minimum spark advance for best torque (MBT) timing

Another means of comparing the combustion behavior of CNG and HCNG is to operate the engine at each test condition with optimized spark timing. This is referred to as the “minimum spark advance for best torque” or MBT timing. Operating the engine at MBT timing serves to optimize the phasing of combustion such that the expansion stroke can benefit from optimal thermal-to-mechanical energy conversion. In this way, the phasing of the heat release rate is best suited to produce useful work, which implies both less pumping losses due to negative work from too advanced spark timing and less lost work in the form of excess exhaust enthalpy.

The spark timing values are shown in Table 4-1, for each equivalence ratio, for both HCNG and CNG. The values are reported in CAD, relative to top dead center (TDC), such that the negative value indicates that spark timing occurred before TDC. The values reported for HCNG are retarded compared to those for CNG, and the degree of retard increases as equivalence ratio becomes leaner.
Table 4-1 Values for spark timing, relative to top dead center (TDC), for each equivalence ratio

<table>
<thead>
<tr>
<th></th>
<th>( \Phi )</th>
<th>1</th>
<th>0.9</th>
<th>0.8</th>
<th>0.7</th>
<th>0.6</th>
</tr>
</thead>
<tbody>
<tr>
<td>HCNG-q</td>
<td>Spark timing (CAD)</td>
<td>-16.0</td>
<td>-17.2</td>
<td>-17.9</td>
<td>-19.2</td>
<td>-24.8</td>
</tr>
<tr>
<td>CNG-q</td>
<td></td>
<td>-24.0</td>
<td>-25.4</td>
<td>-28.1</td>
<td>-33.0</td>
<td>-48.5</td>
</tr>
</tbody>
</table>

Figure 4-10 shows that the brake specific energy consumption (BSEC) improves with leaner conditions for both HCNG and CNG fuels. HCNG (at MBT timing) is less efficient at stoichiometric conditions than CNG, but then becomes more efficient, consistently, for equivalence ratios < 1.0 compared to CNG.

Figure 4-10 Brake specific energy consumption as a function of equivalence ratio (\( \Phi \)), for ○ HCNG-\( q \), □ CNG-\( q \), for minimum spark advanced for best torque at 2000 RPM with base port configuration (quiescent).

The EICO are shown in Figure 4-11, showing that CO is higher for HCNG than for CNG.
The emissions index of hydrocarbons (EITHC) is greater for CNG at MBT timing (Figure 4-12) than for fixed spark timing (Figure 4-3), at a given equivalence ratio. The EITHC is lower for HCNG than for CNG in the very lean region, but closer to stoichiometric (1.0 ≤ Φ ≤ 0.9) it is higher for HCNG than for CNG.
Figure 4-12 Emissions index of unburned hydrocarbons (kg HC/kg fuel), as a function of equivalence ratio ($\Phi$), for (○) HCNG-q, (□) CNG-q, for minimum spark advanced for best torque at 2000 RPM with base port configuration (quiescent).

The emissions index for oxides of nitrogen (EINO$_x$) is shown in Figure 4-13. The EINO$_x$ of HCNG at $\Phi \leq 0.8$ increases substantially (almost two times as much) compared to CNG at those equivalence ratios, indicative of the higher flame temperatures achieved for HCNG (with hydrogen) compared to CNG.

The EINO$_x$ is lower for MBT timing (Figure 4-13) than for fixed spark timing for CNG (Figure 4-4). The EINO$_x$ of HCNG is approximately the same for HCNG in the case of both fixed and MBT timing scenarios, until $\Phi \leq 0.8$, where the MBT timing results for EINO$_x$ are larger than those for fixed spark timing.
The addition of hydrogen to CNG results in substantial improvements to BTE, compared to CNG alone, for all equivalence ratios, except stoichiometric (see Figure 4-14). Comparing the results from the MBT timing study to those from fixed spark timing, the BTE is lower for MBT timing (for both fuels). In the present work, when spark timing is held fixed as a function of equivalence ratio, it means that spark timing becomes more retarded as stoichiometry becomes leaner.
The NMEP is shown in Figure 4-15. Both fuels realize a lower NMEP at stoichiometric, and NMEP increases as the air-fuel mixture becomes leaner. Recall that during the fixed spark timing study shown in Figure 4-6, HCNG suffered from lower NMEP than for CNG. In the case of optimum combustion phasing (MBT timing), shown in Figure 4-15, the NMEP for HCNG is higher than for CNG at all equivalence ratios, which highlights the efficiency gained by introducing hydrogen to the fuel.
Figure 4-15 Net mean effective pressure (kPa) as a function of equivalence ratio (\(\Phi\)), for (○) HCNG-q, (□) CNG-q, for minimum spark advanced for best torque at 2000 RPM with base port configuration (quiescent).

The main burn duration (10-90% mass fraction burned) is shown in Figure 4-16, where HCNG exhibits a faster rate of burning than does CNG. This is quite different than for fixed spark timing (Figure 4-7), where the burn durations are similar for both fuels until the leanest conditions. Comparing the results for MBT timing (Figure 4-16) to those from the fixed spark timing study (Figure 4-7), the burn duration for CNG is longer for MBT than for fixed spark timing. Regarding HCNG, the burn duration at MBT timing is shorter at each equivalence ratio compared to the burn duration for HCNG at fixed spark timing, except at the stoichiometric condition.
Figure 4-16 Burn duration, 10-90% mass fraction burned (CA) as a function of equivalence ratio (Φ), for (○) HCNG-q, (□) CNG-q, for minimum spark advanced for best torque at 2000 RPM with base port configuration (quiescent).

The CA50 is presented in Figure 4-17 and is approximately the same for both CNG and HCNG, at Φ ≤ 0.8, despite the significant difference in spark timing (more than 10CAD, see Table 4-1). This data shows that HCNG burns faster (in terms of fewer CAD) than CNG. This finding, along with the shortened 10-90% MFB duration from Figure 4-16, suggest that hydrogen addition to CNG enhances the burn rate. HCNG’s improved burn process compared to CNG is well documented in the literature, and additional analysis in subsequent sections will continue to evaluate the benefits of adding hydrogen to CNG, to confirm the literature findings.
Figure 4-17 CA50 as a function of equivalence ratio (Φ), for (○) HCNG-q, (□) CNG-q, for minimum spark advanced for best torque at 2000 RPM with base port configuration (quiescent).

The energy released between the SOC and TDC is shown in Figure 4-18, and demonstrates that CNG loses more energy before TDC than HCNG for all equivalence ratios.

Figure 4-18 Energy released between start of combustion and top dead center (%) as a function of equivalence ratio (Φ), for (○) HCNG-q, (□) CNG-q, for minimum spark advanced for best torque at 2000 RPM with base port configuration (quiescent).
4.2 Intake-induced swirl studies: 2000 RPM, MBT and fixed spark timing

The intake-induced swirl testing was conducted similarly to the quiescent studies, at an engine speed of 2000 RPM. One intake port was blocked completely, but the procedure and test set up were the same otherwise. Achieving a BMEP of 1.5 bar was the target for each stoichiometric test point, at MBT timing, for each fuel. In the case of the fixed spark timing studies, the spark timing was held constant, at the value of MBT timing for $\Phi = 1$, as the throttle was opened incrementally to achieve leaner equivalence ratios. The fueling rate was held constant for each equivalence ratio. This same approach was followed for the MBT study, except that the spark timing was swept to achieve the minimum spark advance for best torque, at a given equivalence ratio. The BMEP of 1.5 bar was found at stoichiometric, but then load was allowed to vary as throttle was opened to achieve leaner conditions.

4.2.1 Fixed spark timing

Figure 4-19 shows that the brake specific energy consumption (BSEC) for CNG is higher (worse) than it is for HCNG. BSEC decreases as mixtures become more lean, and the difference in BSEC between CNG and HCNG becomes more pronounced with increased leanness.
The trend of EICO is generally the same for both fuels, except that EICO for HCNG remains quite high (>0.1 kg CO/kg fuel) until the air-fuel mixture is leaner than 0.9 equivalence ratio. This is similar to the trends that were shown in the quiescent case, for fixed spark timing (see Figure 4-2).
The emissions index of hydrocarbons (EIHC) is shown in Figure 4-21 for CNG and HCNG, and shows that CNG results in higher overall hydrocarbon emissions than for HCNG. Comparing the results of EIHC in the case of intake-induced swirl with those from the quiescent study (as shown in Figure 4-3), the EITHC for CNG is higher in the presence of swirl than in the quiescent conditions, for a given equivalence ratio.

Comparing CNG swirl to CNG quiescent, at fixed spark timing, shows that even at retarded spark timings (such as $\Phi < 0.7$), swirl fosters better combustion, as the EIHC is less with swirl than without. In the case of HCNG, the EITHC is generally the same at a given equivalence ratio, both when swirl is present and when the intake flow is quiescent.
Figure 4-21 Emissions index of unburned hydrocarbon (kg HC/kg fuel), as a function of equivalence ratio ($\Phi$), for (◊) HCNG-s, (▽) CNG-s, for fixed spark timing (15.6 CA BTDC for HCNG-q, and 26.6 CA BTDC for CNG-q) and 2000 RPM with modified port configuration (swirl).

Figure 4-22 shows that EINO$_x$ for CNG is higher than for HCNG, at all equivalence ratios. EINO$_x$ for CNG is higher, for lean conditions, in the case of swirl than in the quiescent case. EINO$_x$ for HCNG combustion is generally the same at a given equivalence ratio, in both the swirl and quiescent study.
Figure 4-22 Emissions index of oxides of nitrogen (kg NOx/kg fuel), as a function of equivalence ratio (Φ), for (◊) HCNG-s, (▼) CNG-s, for fixed spark timing (15.6 CA BTDC for HCNG-q, and 26.6 CA BTDC for CNG-q) and 2000 RPM with modified port configuration (swirl).

Figure 4-23 shows that brake thermal efficiency for HCNG is higher than for CNG in all lean conditions. The values of BTE for CNG in the presence of swirl are comparable to those in the quiescent case (Figure 4-5). The same is generally true for HCNG.
Figure 4-23 Brake thermal efficiency (%) as a function of equivalence ratio (Φ), for (◊) HCNG-s, (▼) CNG-s, for fixed spark timing (15.6 CA BTDC for HCNG-q, and 26.6 CA BTDC for CNG-q) and 2000 RPM with modified port configuration (swirl).

The data shown in Figure 4-24 portrays the NMEP for natural gas, as well as for hydrogen assisted natural gas combustion, in the presence of intake-induced swirl. The NMEP is similar for HCNG and CNG, a trend consistent with the quiescent case (Figure 4-6). CNG sees higher NMEP for a given equivalence ratio compared to HCNG in the presence of swirl, as is true in the case of quiescent intake flows as well. The values of NMEP for HCNG are comparable in both the swirl and quiescent cases.
Figure 4-24 Net mean effective pressure (kPa) as a function of equivalence ratio ($\Phi$), for (◊) HCNG-s, (◇) CNG-s, for fixed spark timing (15.6 CA BTDC for HCNG-q, and 26.6 CA BTDC for CNG-q) and 2000 RPM with modified port configuration (swirl).

The burn duration, shown in Figure 4-25, is similar for both fuels, though the burn duration is faster for HCNG than for CNG under lean conditions. This trend is consistent with the results from the quiescent case as well (see Figure 4-7). The actual values of burn duration are lower (faster) in the case of swirl, compared to quiescent, for each fuel, at a given equivalence ratio.
Figure 4-25 Burn duration, 10-90% mass fraction burned (CA), as a function of equivalence ratio ($\phi$), for (◊) HCNG-s, (▼) CNG-s, for fixed spark timing (15.6 CA BTDC for HCNG-q, and 26.6 CA BTDC for CNG-q) and 2000 RPM with modified port configuration (swirl).

The crank angle degree at which fifty percent of the fuel is burned (CA50), based on fifty percent heat release, is given in Figure 4-26. The midpoint of the burn process (CA50) is earlier for CNG than for HCNG, which is expected, given that the timing of CNG compared to HCNG is more advanced (starts earlier relative to TDC). This trend is consistent with the quiescent case (Figure 4-8).
Figure 4-26 CA50 (CA), as a function of equivalence ratio (Φ), for (◊) HCNG-s, ( ▽) CNG-s, for fixed spark timing (15.6 CA BTDC for HCNG-q, and 26.6 CA BTDC for CNG-q) and 2000 RPM with modified port configuration (swirl).

More energy is released prior to TDC in the case of CNG without hydrogen, as shown in Figure 4-27. This trend is consistent with the quiescent case, though the magnitude of percent energy released prior to TDC is greater (for a given fuel, at a given equivalence ratio), in the case of swirl. It is important to reiterate that hydrogen assisted natural gas combustion results in fewer energy losses, at a given equivalence ratio, than burning natural gas alone. It should be noted that load varies as a function of increased leanness due to the way the tests were conducted (fixed fueling, adding more air). Adding more air leads to improved oxidation (since, in practice, stoichiometric conditions in an engine do not provide enough air to oxidize all of the fuel), which will result in more heat released. Hence, the trends for both fuels increase with decreasing equivalence ratio. The trend for CNG falls off after Φ < 0.7, likely because combustion instabilities are increasing, specifically because the timing is retarded compared to MBT in this particular case.
Figure 4-27 Energy released between start of combustion and top dead center (%) as a function of equivalence ratio (Φ), for (◊) HCNG-s, (▼) CNG-s, for fixed spark timing (15.6 CA BTDC for HCNG-q, and 26.6 CA BTDC for CNG-q) and 2000 RPM with modified port configuration (swirl).

4.2.2 Minimum spark advance for best torque

The spark timing for both fuels at each equivalence ratio is shown in Table 4-2. The minimum spark advance for best torque is more retarded for HCNG than for CNG at each equivalence ratio. Although the timing becomes more advanced as a function of decreasing equivalence ratio, it is noteworthy that the trends between the two fuels diverge increasingly. In comparing the spark timing values for the quiescent flow configuration, it is clear that swirl enables more retarded timings to achieve MBT than in the quiescent case. This is true for both fuels, at all comparable equivalence ratios (refer to Table 4-1).

Table 4-2 Spark timing values, relative to top dead center (TDC), for HCNG and CNG in the case of intake-induced swirl, for each equivalence ratio.

<table>
<thead>
<tr>
<th></th>
<th>Φ</th>
<th>1</th>
<th>0.9</th>
<th>0.8</th>
<th>0.7</th>
<th>0.6</th>
</tr>
</thead>
<tbody>
<tr>
<td>HCNG-s</td>
<td>Spark timing (CAD)</td>
<td>-13.1</td>
<td>-14.0</td>
<td>-14.4</td>
<td>-15.8</td>
<td>-18.9</td>
</tr>
<tr>
<td>CNG-s</td>
<td>-17.1</td>
<td>-17.2</td>
<td>-19.9</td>
<td>-27.2</td>
<td>-39.9</td>
<td></td>
</tr>
</tbody>
</table>
The brake specific energy consumption is shown in Figure 4-28, and exemplifies the benefits of hydrogen assisted combustion compared to natural gas alone, as the values of BSEC are lower (better) for hydrogen assisted combustion of natural gas, compared to CNG alone. This trend is consistent with that from the quiescent study (refer to Figure 4-10), except at the stoichiometric equivalence ratio.

![Figure 4-28 Brake specific energy consumption (%) as a function of equivalence ratio (Φ), for (◊) HCNG-s, (▼) CNG-s, at minimum spark advance for best torque and 2000 RPM with modified port configuration (swirl).](image)

The results of the EICO for natural gas with and without hydrogen-assist are shown in Figure 4-29; hydrogen assisted combustion yields more carbon monoxide than CNG alone for equivalence ratios richer than 0.7. The trends for EICO are the same for HCNG in both the swirl and quiescent cases, as well as for CNG in both swirl and quiescent cases (Figure 4-11).
The results for EIHC in Figure 4-30 show that natural gas combustion produces more hydrocarbons, at the same equivalence ratio, than for hydrogen assisted natural gas (HCNG). Comparing the findings for the swirl condition to those from the quiescent case (Figure 4-12), both CNG and HCNG show consistent trends, though the magnitude of the EIHC peaks at a higher value for CNG in the quiescent case than in the swirl condition. HCNG results in higher EIHC in the presence of swirl compared to the quiescent condition (Figure 4-12).
The EINO$_x$ is higher when natural gas is assisted by hydrogen than for natural gas alone, as shown in Figure 4-31. Compared to the quiescent case (Figure 4-13), the EINO$_x$ from HCNG is higher with swirl than without swirl. The same comparison is true of the EINO$_x$ for CNG. It is notable that, in the fixed spark timing case (recall Figure 4-22) where swirl is present, CNG combustion results in higher EINO$_x$ than does HCNG. The trends for HCNG and CNG are consistent (for MBT in the swirl condition) when comparing back to MBT timing in the quiescent configuration (Figure 4-10). The values at a given equivalence ratio are the same for CNG in both the swirl and quiescent studies (for MBT timing).
The brake thermal efficiency, shown in Figure 4-32, is higher (better) for HCNG compared to CNG alone. The trend of increased BTE for HCNG compared to CNG at the same equivalence ratio is true in the case of fixed spark timing (Figure 4-23) as well as for MBT, though the difference between CNG and HCNG is greater in the MBT case than when the timing is fixed. The trends for BTE in the case where swirl is induced are consistent with those from the quiescent configuration, for both fuels, across the equivalence ratio range. The values of BTE for CNG are similar in both cases (swirl and quiescent), where as HCNG generally provides incremental improvement in BTE when swirl is present compared to the quiescent case, at a given equivalence ratio.
Figure 4-32 Brake thermal efficiency (%), as a function of equivalence ratio ($\Phi$), for (◊) HCNG-s, (▼) CNG-s, at minimum spark advance for best torque and 2000 RPM with modified port configuration (swirl).

Figure 4-33 shows the net mean effective pressure for CNG and HCNG in the intake-induced flow configuration, where the hydrogen addition offers higher NMEP than for natural gas alone. Natural gas sees a consistent trend for NMEP when comparing the results with swirl to those in the quiescent study (Figure 4-15), the values of which are nearly identical in both cases (swirl and quiescent). Also consistent with the quiescent conditions, HCNG achieves higher NMEP compared to CNG in the presence of swirl.

The trends for NMEP are quite different, for both fuels, when the results from MBT timing are compared to those when spark timing was fixed (Figure 4-24). The trends from the fixed spark timing case are linear and nearly the same for CNG and HCNG at a given equivalence ratio, which contrasts with the results in the case of swirl, where HCNG results in a much higher NMEP than does CNG, at a comparable equivalence ratio.

Natural gas results in a lower value of NMEP in the case of swirl (Figure 4-33) compared to the fixed spark timing study, where HCNG sees a better NMEP when swirl is present.
compared to fixed spark timing (recall the results of NMEP for fixed spark timing in Figure 4-24).

The results for burn duration are given in Figure 4-34 for HCNG combustion as well as for CNG alone, where hydrogen addition results in improved (lower) burn durations for natural gas. The difference in CA between CNG and HCNG increases as the conditions become leaner, meaning that the disparity in burn rate becomes more significant, as a function of decreasing equivalence ratio. These results are in sharp contrast with the results from the fixed spark timing study (refer to Figure 4-25), where burn duration is nearly the same for both fuels at a given equivalence ratio (with CNG burning somewhat slower than HCNG, but not significantly).

The main duration is lower overall for hydrogen assisted combustion, when MBT is induced, compared to the fixing timing. CNG burns more slowly in the MBT case than in the fixed spark timing study. The trends for burn duration are consistent for both fuels, meaning that the difference in burn duration between the quiescent configuration and swirl case (faster in the
case of swirl) is true both for CNG (CNG-q compared to CNG-s) and for HCNG (HCNG-q compared to HCNG-s). Both fuels see an improved burn duration when swirl is present compared to the quiescent case, but the improvement with hydrogen addition is more substantial, comparatively. Hence, HCNG burns faster with swirl than without swirl, compared to CNG with and without intake-induced swirl.

There is a perceived benefit of hydrogen addition in conjunction with lean conditions compared to CNG, specifically according to Figure 4-33, but this is because load is increasing as a function of leaner equivalence ratio. The increasing load with decreasing equivalence ratio is the reason NMEP increases for both fuels as conditions become leaner. In addition, hydrogen requires more air than CNG to meet the same stoichiometry, and hence there is more air for HCNG compared to CNG; given that hydrogen realizes and increased O and OH pool compared to CNG, and that those radical pools foster flame development and flame propagation, HCNG effectively outputs more work at the same stoichiometric condition as CNG.

![Figure 4-34 Burn duration, 10-90% mass fraction burned (CA), as a function of equivalence ratio (Φ), for (◊) HCNG-s, (▼) CNG-s, at minimum spark advance for best torque and 2000 RPM with modified port configuration (swirl).](image)
Figure 4-35 shows that CA50 for HCNG occurs earlier than for CNG. Recall that the spark timing for CNG is advanced compared to that for HCNG, meaning that the first half of the burn process occurs significantly faster for HCNG than for CNG (Table 4-2).

This trend is quite different in comparison to the results for CA50 in the quiescent study, where CA50 for HCNG combustion occurs later than for CNG alone for the conditions at and near stoichiometric, and then becomes quite similar at more lean conditions (equivalence ratio less than or equal to 0.8).

The percent of energy released prior to TDC is presented in Figure 4-36, and shows that HCNG releases more energy prior to TDC than CNG alone. There is no significant difference in the energy released BTDC at stoichiometric air-fuel proportions between CNG and HCNG. There is more available oxidant in the case of HCNG at the same equivalence ratio than for CNG. This is significant because it serves to increase the load for HCNG (due to the study having been conducted at fixed fueling) compared to CNG at the same equivalence ratio.
4.3 Turbulence intensity study: 2750 RPM, MBT timing

The following studies were conducted at 1.5 bar brake mean effective pressure (BMEP) at stoichiometric air fuel ratio (AFR) and maximum brake torque (MBT) spark timing without intake-induced swirl. The fueling rates at these conditions (for CNG and for HCNG) were then fixed as throttle was opened incrementally to vary stoichiometry, and timing adjusted for minimum spark advance for best torque at each new AFR. The same fueling rates were adopted for the cases where intake-induced swirl was introduced via full blockage of one intake port; the same process was employed to adjust AFR and MBT timing as described above. The starting point of 1.5 bar BMEP was achieved at 2750 RPM, at the stoichiometric, MBT condition. The MBT timing is reported in Table 4-3. The MBT timing for HCNG was always more retarded than CNG at the same condition. However, HCNG-q and CNG-s have nearly identical MBT timings.
Table 4-3 The minimum spark advance for best torque (MBT) timing summary for CNG and HCNG, in both the quiescent and swirl configurations, as a function of equivalence ratio, at an engine speed of 2750 RPM.

<table>
<thead>
<tr>
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<th>Φ</th>
<th>1</th>
<th>0.9</th>
<th>0.8</th>
<th>0.7</th>
<th>0.6</th>
</tr>
</thead>
<tbody>
<tr>
<td>HCNG-q</td>
<td>Spark timing (CAD)</td>
<td>-24.0</td>
<td>-24.7</td>
<td>-26.0</td>
<td>-26.7</td>
<td>-28.1</td>
</tr>
<tr>
<td>CNG-q</td>
<td>-31.8</td>
<td>-34.5</td>
<td>-34.6</td>
<td>-38.4</td>
<td>-40.6</td>
<td></td>
</tr>
<tr>
<td>CNG-s</td>
<td>-24.0</td>
<td>-24.7</td>
<td>-26.0</td>
<td>-27.2</td>
<td>-30.3</td>
<td></td>
</tr>
</tbody>
</table>

The brake specific energy consumption is shown for both CNG and HCNG, in the quiescent and swirl configurations, at a higher engine speed than the previous studies, 2750 RPM (Figure 4-37). The BSEC for both fuels, as well as for CNG-s, decreases with decreasing equivalence ratio. Overall, CNG-s results in the highest (worst) BSEC of all cases, across the range of equivalence ratios. The best BSEC (lowest) is achieved by CNG-ns at phi > 0.8, and by HCNG-ns at phi < 0.8. When CNG for the quiescent case is compared to that when swirl is present, there is a distinct increase in BSEC for swirl at the same equivalence ratio.

Figure 4-37 Brake specific energy consumption (kJ/kW-hr) as a function of equivalence ratio (Φ), for (○) HCNG-q, (□) CNG-q, (♦) CNG-s, at minimum spark advance for best torque and 2750 RPM (both base port configuration and modified port configuration (swirl) are tested).
The emissions index of carbon monoxide (EICO) is shown in Figure 4-38. For the CNG fuel, the EICO results in the same value at the same equivalence ratio when comparing the quiescent to the case with swirl. The addition of hydrogen results in increased EICO until equivalence ratio is less than 0.8. The levels of in-cylinder turbulence in this study do not affect the production of carbon monoxide, as seen by the identical EICO results for CNG-s and CNG-q.

![Figure 4-38 Emissions index of carbon monoxide (kg CO/kg fuel) as a function of equivalence ratio (Φ), for (○) HCNG-q, (●) CNG-q, (▼) CNG-s, at minimum spark advance for best torque and 2750 RPM (both base port configuration and modified port configuration (swirl) are tested).](image)

Figure 4-39 shows the emissions index of unburned hydrocarbons (EIHC) for each fuel at 2750 RPM and MBT timing. Similar to the results above for EICO (Figure 4-38), there is little difference between CNG-q and CNG-s. Furthermore, at Φ > 0.8, all cases have comparable EIHC. Intake-induced swirl effectively has no impact on emissions, at 2750 RPM with MBT timing. Hydrogen addition offers a benefit in terms of reducing EIHC at lean conditions, compared to CNG alone.
Figure 4-39 Emissions index of unburned hydrocarbons (kg HC/kg fuel) as a function of equivalence ratio (Φ), for (○) HCNG-q, (□) CNG-q, (▼) CNG-s, at minimum spark advance for best torque and 2750 RPM (both base port configuration and modified port configuration (swirl) are tested).

The EINOx is shown in Figure 4-40, for CNG in the quiescent case, CNG with intake-induced swirl, and CNG with hydrogen added (HCNG) in the quiescent case at 2750 RPM with MBT timing. The EINOx is higher for CNG-s compared to CNG-q at the same equivalence ratio. Hydrogen addition results in the lowest EINOx, except at Φ < 0.7.

Increased engine speed (compared to 2000 RPM) results in increased NOx for CNG, for both the quiescent case and when intake-induced swirl is present (compares Figure 4-40 to Figure 4-31). EINOx for HCNG is slightly higher at some equivalence ratios, but generally the same, indicating that increased RPM does not influence thermal NOx production when hydrogen is present. This is expected since the comparison is being made at the same stoichiometry, residence time is not increasing (it is decreasing), and combustion temperatures should not increase significantly due to faster movement of the piston. It may be possible for the temperature to increase slightly due to a smaller time scale, affecting the heat transfer from the cylinder to the coolant, but not substantially.
Figure 4-40 Emissions index of oxides of nitrogen (kg NOx/kg fuel) as a function of equivalence ratio (Φ), for ○ HCNG-q, □ CNG-q, ( ) CNG-s, at minimum spark advance for best torque and 2750 RPM (both base port configuration and modified port configuration (swirl) are tested).

The brake thermal efficiency is shown in Figure 4-41, and shows that CNG in the presence of intake-induced swirl performs worse than the other cases. HCNG in the quiescent configuration performs better than all cases for equivalence ratios < 0.8, and CNG in the quiescent case performs better than all cases for equivalence ratios > 0.8.

In the case of swirl, CNG generally results in a higher BTE for the same equivalence ratio at 2750 RPM than at 2000 RPM (both at MBT timing), except at stoichiometric. CNG in the quiescent condition performs better or the same at higher engine speed compared to the quiescent case at lower engine speed, both at MBT timing.
Figure 4-41 Brake thermal efficiency (%) as a function of equivalence ratio (Φ), for (○) HCNG-q, (□) CNG-q, (▼) CNG-s, at minimum spark advance for best torque and 2750 RPM (both base port configuration and modified port configuration (swirl) are tested).

The NMEP is shown in Figure 4-42. In the case of CNG, the NMEP is consistently lower for swirl than for quiescent operation, at the same Φ. The NMEP improves, overall, as a function of decreasing equivalence ratio, for all cases. Hydrogen addition results in values of NMEP higher than for CNG-q or CNG-s when Φ < 0.8. Overall, CNG in the quiescent case is the most efficient for equivalence ratios > 0.8, and HCNG is the most efficient at equivalence ratios < 0.8.
Figure 4-42 Net mean effective pressure (kPa) as a function of equivalence ratio (Φ), for (○) HCNG-q, (□) CNG-q, (▼) CNG-s, at minimum spark advance for best torque and 2750 RPM (both base port configuration and modified port configuration (swirl) are tested).

The main burn duration is given in Figure 4-43. The trends for CNG, both in the quiescent and swirl cases, result in the same burn duration, except at stoichiometric and at Φ = 0.6, where the quiescent configuration results in main burn durations that are longer than in the case of swirl. The main burn duration for HCNG is shorter (faster) than for CNG in the quiescent or swirl configurations.

Comparing the MBT timing burn duration at 2750 RPM to that at 2000 RPM (refer to Figure 4-16 and Figure 4-34) for each fuel and intake port configuration, each fuel burns faster (achieves a shorter burn duration) at 2750 RPM compared to 2000 RPM at the same equivalence ratio.
Figure 4-43 Burn duration, 10-90% mass fraction burned (CA) as a function of equivalence ratio ($\Phi$), for (○) HCNG-q, (□) CNG-q, (▼) CNG-s, at minimum spark advance for best torque and 2750 RPM (both base port configuration and modified port configuration (swirl) are tested).

The CA50 results are shown, as a function of equivalence ratio, in Figure 4-44. The overall trend for the midpoint of the burn process is CNG-s < CNG-q < HCNG-q. The trend for the main burn duration (refer to Figure 4-43) is HCNG-q < CNG-s < CNG-q. The point here is that CNG-s reaches its CA50 much earlier than the other cases (at 2750 RPM), even though the main burn duration of CNG-s is longer than HCNG, and the SOC of CNG-s is the same as HCNG, and later than CNG-q. This indicates that the early flame development for CNG-s must be rapid.
The results in Figure 4-45 show the percent of energy released prior to the piston reaching TDC, as a function of equivalence ratio. Hydrogen addition results in the least amount of heat lost prior to TDC, compared to CNG at either the quiescent or swirl configurations. Comparing these results with those from 2000 RPM and MBT timing in the quiescent configuration, hydrogen addition reduces the amount of heat lost compared to CNG (Figure 4-18) at both engine speeds.
Figure 4-45 Energy released between start of combustion and top dead center (%) as a function of equivalence ratio ($\Phi$), for (○) HCNG-q, (■) CNG-q, (▼) CNG-s, at minimum spark advance for best torque and 2750 RPM (both base port configuration and modified port configuration (swirl) are tested).
Chapter 5 Discussion

5.1 Hydrogen addition and early flame development

The first objective of this work is to confirm that hydrogen addition improves the early flame development of compressed natural gas (CNG), allowing the minimum spark advance for best torque (MBT) to be retarded compared to CNG alone. This section will review the fundamentals of flame development in an ICE, and evaluate pertinent data from the results chapter and draw from the literature to compare and confirm them.

Lancaster conducted motored studies to discern the effects of engine variables on turbulence, using hot-wire anemometry in a CFR engine at 8.72 compression ratio (Lancaster, 1976). A follow-up study was conducted using the same engine (spark-ignited CFR, with spark plug located tangential to the plane of the piston), where Lancaster et al. acquired in-cylinder pressure measurements from propane-air mixtures to quantify the effects of turbulence on flame propagation (Lancaster et al., 1976). Both the motored and fired data were correlated using a two-zone heat release model (Lancaster et al., 1976).

Lancaster et al. concluded that approximately 35% of the overall combustion duration is allocated to the flame development period (Lancaster et al., 1976). Hence, the early flame development comprises a substantial fraction of the overall burn process. This finding highlights the significance of the early flame development process. From this finding, one can assert that early flame development is a critical factor in MBT timing, i.e., a slower (longer) early flame development period requires advanced spark timing, such that a fully developed flame can be established prior to TDC, whereas a faster (shorter) early flame development period enables retarded spark timing while still allowing the establishment of a fully developed flame prior to TDC.
Figure 5-1 The ratio of turbulent flame speed to laminar flame speed plotted as a function of flame radius, computed based on a CFR engine at 8.72 compression ratio with side-fired spark. Laminar flame speeds were computed at engine temperature and pressures based on flame speed measurements at lower temperature and pressures, according to an equation derived by DeSoete and Brasselet (DeSoete and Brasselet, 1969). A geometric model for flame propagation coupled with a heat release model was used to compute the turbulent flame speed. A visual description of the burn progress is presented (Lancaster et al., 1976).

The data presented in Figure 5-2 is a summary of the data discussed in the results section, and includes additional details about the combustion process for each case. The chart represents the combustion process from SOC through the crank angle at which 90% of the fuel is considered burned (CA90, or the 90% MFB point). To interpret the chart, start with the 2000 RPM and fixed spark timing case with quiescent configuration for CNG (the left most line on the chart), and proceed up the y-axis from the bottom to the top of the chart.

1. The spark timing, which is the same as SOC, for CNG in the quiescent configuration at 2000 RPM and fixed spark timing occurs at 333 CA

2. The next value is the CA10
3. The value (highlighted with a rectangular border) between SOC and CA10 represents the 0-10% MFB duration.

4. The next value is 385, which is the value of CA50.

5. The last data point (at the top of the y-axis) is CA90 at 385 CA

The data are grouped in pairs, with each pair surrounded by a colored box, such that the first result is for CNG, and the second is for HCNG at the same condition (i.e., same RPM, intake configuration, and timing – fixed or MBT).

![Figure 5-2](image_url)

**Figure 5-2 Summary of the combustion process as a function of crank angle degree, for all cases (CNG, HCNG, quiescent, swirl, both 2000 RPM and 2750 RPM, for the equivalence ratio 0.9. The value encased in a dashed box represents the duration of the early flame development period (0-10% mass fraction burned) in crank angle degrees (CA). The symbols are defined as follows: ( ) SOC, ( ) CA10, ( ) CA50, ( ) CA90. (refer to Figure 4-7, Figure 4-16, Figure 4-25, Figure 4-34 and Figure 4-43)**

The summary in Figure 5-2 highlights that hydrogen addition results in a shorter early flame development period, which is a portion of the 0-10% mass fraction burned duration (or the
number of crank angle degrees between SOC and CA10). Recall that the 0-10% portion of the burn process comprises the SOC, the establishment of the flame kernel, and then flame growth and propagation until the flame becomes fully developed (refer to Chapter 2).

In Figure 5-2, the quiescent configuration at 2000 RPM and fixed spark timing is shown in the first box (the left side of the plot). Recall that the data are presented for an equivalence ratio of 0.9, which means that both fuels suffer from poor combustion phasing relative to MBT. Hydrogen addition offers a shorter flame development period than CNG alone by 5 CAD. The timing for HCNG is retarded in comparison to CNG, by 11 CAD. This same trend, both retarded timing and faster flame development period, prevails for the four remaining comparisons. The initial portion of the early flame development period is considered to be a laminar process in the ICE, specifically the development of the flame kernel. The laminar burning velocity is governed by the laminar flame speed and the mixture properties (Equation 2-1).

Conte and Boulouchos (2006) investigated the effects of hydrogen addition to a 2-cylinder, 0.5L port-fuel-injected gasoline-fueled spark-ignited engine with 8.7:1 compression ratio with 62mm stroke and 72mm bore. Flame speed and flame front propagation characteristics were discerned via pressure measurement, ion-sensing devices and an optical spark plug. Their results showed that laminar flame speed increased more than four times with hydrogen addition compared to gasoline alone, and that the increase was a linear function of the energy fraction of hydrogen in the fuel mixture (Conte and Boulouchos, 2006). Furthermore, recall from the literature review that Boulouchos had found the flame speed of hydrogen to increase with flame stretch, whereas the flame speed of hydrocarbon flames decreases with flame stretch (Boulouchos, 2004). This is a key to understanding why hydrogen addition presents a benefit to increasing flame speed in engine conditions.

Huang et al. (2006) studied the effects of hydrogen addition to natural gas flames in a constant volume combustion bomb. The results showed that unstretched laminar burning velocity
increased with the increase of hydrogen fraction in natural gas (Huang et al., 2006). Laminar flame speed governs the early flame development process in an ICE. Laminar flame speed has been shown to increase with hydrogen addition. It is then reasonable to suggest that the increased laminar flame speed resulting from hydrogen addition is responsible for the shorter (faster) early development period of the burn process for HCNG combustion compared to CNG in the present work. Recall per Wang et al. (2010) that the increased O and OH concentrations early in the burning process are attributed to the faster burning of hydrogen compared to methane. Hence this increase is largely due to an increase in the reaction rate (refer back to the literature review to revisit oxidation mechanisms for hydrogen and methane).

In the case of 2750 RPM with MBT timing for the quiescent intake configuration (Figure 4-45) the spark timing for both CNG and HCNG under the influence of swirl is more retarded than the same fuel in the quiescent case, compared to the same equivalence ratio.

Bauer and Forest (2001) studied the effects of varying hydrogen fraction in CNG from 0% (neat CNG) to 60% (40% CNG) in a 0.61 L single-cylinder engine with 8.5:1 compression ratio. A full load study was conducted at engine speeds of 700 and 900 RPM, where equivalence ratio was swept, and MBT plotted for each equivalence ratio and hydrogen fraction (0%, 20%, 40% and 60%). In both cases (at both engine speeds), increasing hydrogen fraction results in more retarded timing compared to CNG alone and lower hydrogen fractions, at all equivalence ratios (Bauer and Forest, 2001). Note that there is a typo in the caption for Figure 4 of the referenced work. The caption states, “Full load MBT spark advance BTDC increases with hydrogen addition.” The plot clearly shows that the spark timing, in terms of CA bTDC decrease (spark set at fewer degrees prior to TDC, and hence more retarded) as hydrogen fraction increases.

Huang et al. (2007) studied the effects of hydrogen addition to natural gas in a three-cylinder spark-ignited natural gas engine with bore and stroke of 68.5 and 72 mm, respectively,
0.8L displacement and 9.4 compression ratio. Hydrogen fraction was varied and equivalence ratio swept from rich to lean at 2000 RPM, MBT timing and at wide open throttle (WOT). Pressure data was measured and post-processed to compute burn characteristics. The resulting data showed that MBT was retarded with hydrogen addition compared to natural gas alone, without compromising the burn duration (Huang et al., 2007), which supports the findings of the present work.

The results of the present work, that hydrogen addition shortens the early flame development period (0-10% MFB), as highlighted in Figure 5-2, agree with the findings in literature, as presented above. It is clear that the early flame development period is decreased when hydrogen is present, enabling retarded spark timing compared to CNG.

5.1.1 NOx emissions for HCNG and CNG

The results in Figure 4-13 show the EINOx at 2000 RPM and MBT timing for the quiescent configuration. The EINOx for HCNG at $\Phi \leq 0.8$ is higher than that for CNG, where at relatively richer equivalence ratios the EINOx is lower for HCNG than for CNG. The data from the fixed spark timing study (Figure 4-4, comparable study to Figure 4-13 except that spark timing is held constant) shows that the EINOx is lower for HCNG than CNG. In the case where MBT timing was used, the combustion phasing was more optimal, and hence results in higher flame temperatures, which likely accounts for the increase in NOx. Spark timing is effectively retarded (in the case where spark timing was fixed) for all equivalence ratios less than stoichiometric, which impedes the combustion temperature, reducing the potential for thermal NOx formation.

Ma et al. studied the effects of varying the hydrogen fraction in HCNG in a 6.2 L, turbocharged spark-ignited engine with a 10.5:1 compression ratio. Spark timing was swept from
0 to 25 crank angle degrees before TDC for all studies, at 1200 and 2400 RPM, both for lambda values of 1.3 and 1.5 (or equivalence ratios of 0.76 and 0.66, respectively). The idle condition (800 RPM) was studied as well, at lambda of 1.1 (or equivalence ratio of 0.9). Compressed natural gas was studied, along with HCNG with 20%, 30% and 40% hydrogen by volume in the fuel. The resulting BSNOx (at each equivalence ratio for both 1200 and 2400 RPM) is lowest for CNG in all cases, at all spark timings compared to HCNG, where 40% HCNG produces the highest BSNOx. The 20% and 30% HCNG trend to lower NOx as hydrogen content is reduced, but in the case of 1200 RPM and 1.3 lambda, and then 2400 RPM at 1.5 lambda, the BSNOx trends overlap at more advanced timing (Ma et al., 2009). Comparing BSNOx at a given spark timing, CNG produces less NOx than HCNG. However, this also shows that retarding timing for HCNG results in reduced BSNOx, and given that HCNG can be retarded significantly compared to CNG, HCNG may have the potential to produce less NOx than CNG at comparable conditions.

Collier et al. studied the effects of hydrogen addition to CNG in a 4.6L engine with 9:1 compression ratio, with bore and stroke of 90.2 mm and 90 mm, respectively (Collier et al., 1996). A timing sweep with HCNG (30% H2) and equivalence ratio of 0.8, at 2350 RPM and 420 kPa BMEP shows significant decrease in BSNOx emissions with retarded timing. The resulting BSNOx at 10 CA bTDC is approximately 30 times less than at 40 CA bTDC.

Hence, the results of the present work are in line with literature findings. Ultimately, the retarded timing of HCNG compared to CNG alone can allow reduced EINOx emissions simultaneously with improved BTE.

5.2 Hydrogen addition and thermal to mechanical energy conversion

The next objective of the present work builds on the first, and asserts that the ability to achieve retarded timing with hydrogen addition compared to CNG alone results in a
concentration of the heat release near TDC, which effectively increases the conversion of thermal to mechanical energy. The BSEC, BTE and NMEP will be employed to evaluate the hypothesis at greater depth. The objective is to confirm the findings in literature.

### 5.2.1 Impact on hydrogen addition on the brake specific energy consumption (BSEC) of CNG

The BSEC is a measure of the engine efficiency in that it quantifies the energy consumption relative to the brake specific output of the engine, on a kilojoule of fuel per kilowatt-hour of engine output basis. The “real-world” importance of BSEC in a vehicle application is fuel economy. The lower the BSEC, the higher the fuel economy, or the farther one can drive per unit of fuel consumed.

It is customary to report brake specific fuel consumption (on a gram of fuel per kilowatt-hour of output of the engine) for conventional liquid fuels, the density of which varies modestly. BSFC has commonly been reported in work on gaseous fuels (Akansu et al., 2004; Bauer and Forest, 2001; Das, Gulati and Gupta, 2000; Ma et al., 2008; Ma et al., 2009; Mohammed et al., 2011). The existing state of technology requires that gaseous hydrogen and natural gas be stored in the gaseous state on-board vehicles, and hence the volume of the fuel is a primary consideration. Using BSFC, on a mass basis, may be misleading for gaseous fuels, as the densities of gaseous fuels can vary significantly from one to the other, such as in the case of methane in comparison to hydrogen. One example from the present work is shown below, comparing BSEC to BSFC, in Figure 5-3. The BSEC is higher for CNG than for HCNG, as shown in Figure 5-3, (a). The results for BSFC (Figure 5-3, (b)) are consistent with the BSEC, in the sense that CNG results in greater fuel consumption than HCNG. However, the disparity between the values is greater when the data are presented as BSFC compared to BSEC, since
BSEC accounts for the lower heating values (LHV) of the fuels, as the LHV for CNG is approximately 48,000 kJ/kg, where that for HCNG is approximately 53,000 kJ/kg. A comparison at Φ = 0.9 reveals that BSFC of CNG is approximately 16% higher than that of HCNG, where the BSEC of CNG is only approximately 6% higher than that of HCNG. The finding that values of BSEC and BSFC trend similarly from the above comparison (Figure 5-2) suggests that it is reasonable to compare BSEC and BSFC on a qualitative basis (i.e. comparing the BSEC trends between CNG and HCNG of this work with BSFC trends for CNG and HCNG from the literature).
Figure 5-3 (a) Brake specific energy consumption (BSEC) as a function of equivalence ratio ($\Phi$) for (○) HCNG-q, (□) CNG-q, for fixed spark timing (15.6 CA BTDC for HCNG-q, and 26.6 CA BTDC for CNG-q) at 2000 RPM with base port configuration (quiescent). (b) Brake specific fuel consumption (BSFC) as a function of equivalence ratio ($\Phi$) at the same conditions as (a).

The information in Table 5-1 provides a qualitative summary of the effects of hydrogen addition on CNG, for the present study, in terms of several primary variables (namely BSEC, BTE and NMEP). This section will focus on the BSEC. Whether spark timing is fixed or set for MBT, the effect of hydrogen clearly results in an improvement in BSEC compared to CNG alone. Since BSEC is the ratio of the measured engine output to the energy input to the engine,
decreased BSEC is a measure of improved conversion of thermal energy (fuel) to mechanical energy (work output). These findings are consistent with the literature, as explained below.

Table 5-1 Summary of the effects of hydrogen addition on natural gas, at 2000 RPM, with fixed and MBT timing, in the quiescent configuration. Legend: (↑) increase, (↓) decrease, (•) neutral/no change (refer to Figure 4-1, Figure 4-10, Figure 4-5, Figure 4-14, Figure 4-6, and Figure 4-15,)

<table>
<thead>
<tr>
<th>Effects of H₂ + on CNG (fixed timing)</th>
<th>BSEC</th>
<th>BTE</th>
<th>NMEP</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>↓</td>
<td>↑</td>
<td>↓</td>
</tr>
<tr>
<td>Effects of H₂ + on CNG (MBT timing)</td>
<td>↓</td>
<td>↑↑</td>
<td>↑↑</td>
</tr>
</tbody>
</table>

Brake specific energy consumption (in lieu of brake specific fuel consumption) has been used in other studies to quantify fuel consumption relative to engine output. Examples include Mohammed et al. (2011) and Cattelan and Wallace (1995). Mohammed et al., studied the effects of hydrogen addition in small quantities (0-8 % H₂) to CNG in a single-cylinder, spark-ignited engine where the hydrogen was direct-injected. The engine had a displacement of approximately 0.4L with a high compression ratio (CR) (high as far as spark-ignited engines are concerned) of 14:1. The studies were conducted at stoichiometric conditions over a range of engine speed (2000 – 4000 RPM) and combustion phased optimally via MBT timing. The BSEC data for 2000 RPM for that work resulted in 1.3 – 1.4 kJ/kW-hr (Mohammed et al., 2011). The values are considerably lower than that for the results of the present work at stoichiometric (2.0 – 2.4 kJ/kW-hr), shown in Figure 4-10, perhaps due to the significant difference in compression ratio (14:1 in the cited work compared to 10.44:1 in the present work). This assertion is plausible given that spark-ignited engines are known to exhibit improved efficiency for high compression ratios (14-20) compared to lower compression ratios (Stone, 1999).

Cattelan and Wallace (1995) studied the effects of hythane (20% volume H₂ in CNG) compared to neat CNG in a 3.1 liter multi-cylinder engine (MCE) with a CR of 8.8:1 and under slightly richer-than-stoichiometric air-fuel proportions (equivalence ratio = 1.015). They swept
spark timing close to MBT to 8-10 CAD more advanced, for engine speeds of 1200 and 1800 RPM; BSEC quantities between 2.3-2.4 kJ/kW-hr were reported at 1800 RPM (Cattelan and Wallace, 1995). These values correspond more closely with the findings of the present work (2.0 - 2.4 kJ/kW-hr, as seen in Figure 4-10).

The study by Bauer and Forest (described previously) varied hydrogen fraction and swept equivalence ratio at engine speeds of 700 and 900 RPM, both at part load and full load. The resulting BSFC decreases (improves) with increasing hydrogen fraction, across the all measured equivalence ratios (Bauer and Forest, 2001).

These examples from the literature highlight the improvement to brake specific energy (fuel) consumption realized by combing hydrogen with CNG combustion, compared to burning CNG alone. These results support the finding of this work.

Error! Reference source not found. provides the mass of fuel (in grams) per cycle for CNG and HCNG with MBT timing at both engine speeds. At 2000 RPM, there is a small difference in the fuel quantity per cycle (0.0002 grams), and this difference is considered to be insignificant. In the case of 2750 RPM, however, the difference is much larger, in that CNG requires nearly 15% more fuel per cycle (on a mass basis) than HCNG.

| Table 5-2 Mass of fuel per cycle for each test case, at engine speeds of 2000 and 2750 RPM, and MBT spark timing. |
|--------------------------------------------------|----------------|----------------|----------------|----------------|
| 2000 RPM, MBT | 0.0087 | 0.0087 | 0.0085 | 0.0085 |
| 2750 RPM, MBT | 0.0081 | 0.0081 | 0.0093 | 0.0093 |
It is important to consider the difference in the lower heating value (LHV) between CNG and HCNG when comparing the efficiency. Hence the brake thermal efficiency, which accounts for the lower heating value, is examined in the next section.

5.2.2 Impact of hydrogen addition on the brake thermal efficiency (BTE) of CNG

The BTE is a measure of the engine efficiency. This quantity accounts for the measured work at the output shaft of the engine, the amount of fuel energy per combustion cycle. BTE is essentially the BSEC while accounting for the LHV. Engine geometry is a significant contributor to the thermal efficiency, specifically the stroke-to-bore ratio (S/B).

Filipi and Assanis conducted studies to measure the effect of the S/B ratio on combustion, heat transfer and efficiency in a single-cylinder spark-ignited engine. They fixed engine displacement at 0.4 L, and varied the S/B ratio (0.7, 1.0 to 1.3), with corresponding bore sizes of 90, 80, and 73 mm, respectively. A quasi-dimensional model was employed to comprehend whether effects of S/B ratio were due to engine geometry, or due to bulk flow and turbulence. MBT timing was used for all conditions, at engine speeds of 1500, 3000 and 4500 RPM, for both 262 and 500 kPa BMEP.

The results were nonlinear, in that the difference between the results at 0.7 and 1.0 S/B ratio were smaller than the difference between 1.0 and 1.3 S/B ratio. The burn duration (from SOC to 90% MFB) increased as S/B decreased, meaning that the longest stroke resulted in the shortest burn duration (for 1500 RPM at part load, and 3000 RPM at wide-open throttle (WOT), both with stoichiometric air-fuel proportions). The rate of heat loss as a function of crank angle was shown for each S/B ratio; the S/B ratio in order from slowest to fastest rate of heat loss is 1.3 < 1.0 < 0.7. The heat loss for each case was reported normalized against that at S/B ratio of 0.7, and they found a 5% difference in normalized heat loss between the S/B of 1.0 and 1.3, with the
S/B ratio of unity suffering from higher heat losses than S/B ratio of 1.3. Load contributed a small difference in normalized heat loss for a given S/B ratio. The normalized indicated efficiency was better (higher) for the longest stroke (S/B ratio of 1.3), due to lower heat loss and faster burning (Filipi and Assanis, 2000).

The authors concluded that heat loss variations with S/B ratio impacts the thermal efficiency more significantly than variations in burn durations, and for the longest stroke nearly 80 percent of the efficiency gains is attributed to reduced heat loss (Filipi and Assanis, 2000).

The engine geometry of the present work has an S/B ratio of unity. Since the engine geometry is fixed, the “inherent” heat loss of the test engine is the same for all cases. Thermal efficiency gains or losses then, between the two fuels at the same conditions in the present work, must be associated with burn duration (assuming combustion is phased according to MBT timing).

Stone (1999) modeled the effects of burn duration on the MBT ignition timing and engine performance, based on a Rover K16 spark-ignited engine with a 10:1 compression ratio. The “early burn period” is represented by the 0-10% MFB, and the main combustion duration is the 10-90% MBF period. The spark timing is adjusted for MBT in all cases.

The results are summarized in Table 5-3. Consider the first line as the base case, where MBT timing is 17 CA bTDC, and both the 0-10% MFB and 10-90% MFB are 20 CA in duration. The variable is highlighted in yellow for the two remaining cases. When the main burn duration is doubled (from 20 to 40 CA) and the early burn period is fixed at 20 CA, the MBT timing advances by 6 CAD. Both the brake efficiency and maximum cylinder pressure decrease relative to the base case where the main burn duration was shorter. This shows a clear effect of main burn duration on engine performance (efficiency improves with shorter main burn duration).
Table 5-3 The effect of burn durations on the MBT timing and engine performance for stoichiometric operation at 1000 RPM, in a Rover K16 engine with 10:1 compression ratio. (Reproduced from Stone, 1999, page 147)

<table>
<thead>
<tr>
<th></th>
<th>0-10% (CA)</th>
<th>10-90% (CA)</th>
<th>MBT timing (CA bTDC)</th>
<th>Brake efficiency</th>
<th>(P_{\text{max}}) (bar)</th>
<th>Angle of (P_{\text{max}}) (CA aTDC)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>20</td>
<td>17</td>
<td>0.266</td>
<td>38.5</td>
<td>21</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>40</td>
<td>23</td>
<td>0.250</td>
<td>30.2</td>
<td>18</td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>20</td>
<td>37</td>
<td>0.266</td>
<td>38.3</td>
<td>22</td>
<td></td>
</tr>
</tbody>
</table>

In the last case (third line Table 5-3), the 0-10% MFB period is doubled to 40, the spark timing adjusts for MBT (37 CA bTDC) and is advanced by 20 CA. The main burn period remains the same as before (20 CA bTDC), and the brake efficiency and maximum cylinder pressure do not change. This suggests that delays in the early flame development period, as categorized by 0-10% MFB, do not affect the overall engine performance, as long as spark timing is adjusted to MBT (Stone, 1999).

Now that we have established the impact of main burn duration on the thermal efficiency (given the constraints of the system in the present work), let us discuss the results from the present work in more detail.

Figure 4-9 gives the percentage of energy released prior to TDC for the quiescent condition at 2000 RPM and fixed spark timing. The results show that hydrogen addition releases less energy prior to TDC compared to CNG, consistently, for varying equivalence ratio. The timing in this case is fixed, which means that the timing is retarded relative to MBT at equivalence ratios leaner than stoichiometric. The poor engine performance in terms of BSEC (Figure 4-1), BTE (Figure 4-5) for CNG compared to HCNG are likely due to slower burning during the main burn duration period and are a function of the ill-phased timing. This is supported by Filipi and Assani (2000), and Stone (1999), as reported previously, and exemplifies the need to employ MBT timing to optimize the burn process in order to maximize thermal efficiency (Filipi and Assanis, 2000; Stone, 1999).
Figure 5-4 depicts the burn process from SOC to CA90 at $\Phi = 0.9$, and shows the effects of hydrogen addition to natural gas at 2000 and 2750 RPM, and fixed and MBT timings. The pair of results (Figure 5-4) highlighted with a red oval shows at 2000 RPM and MBT timing under the influence of intake-induced swirl. Recall that Figure 4-32 shows the resulting BTE at that the same conditions, and shows that BTE is consistently higher for HCNG than for CNG. These data illustrate several points. The first is that MBT timing is retarded for HCNG compared to CNG (346 compared to 343 CA). Secondly, the main burn duration (from CA10-CA90 in Figure 5-4) is shorter for HCNG than for CNG. Higher BTE with hydrogen addition is then expected when considering the retarded timing of HCNG in conjunction with a quick burn process, even though the percentage of energy released prior to TDC is slightly higher for HCNG compared to CNG (Figure 4-36). This is because the quantity of energy released prior to TDC is balanced with other losses and gains, through the phasing of combustion according to MBT. Reducing the length of the main burn process reduces the heat losses (Stone, 1999), and hence hydrogen addition to CNG improve efficiency.
Figure 5-4 Summary of the burn process as a function of crank angle degree, for all cases (CNG, HCNG, quiescent, swirl, both 2000 RPM and 2750 RPM, for the equivalence ratio 0.9. The burn process for the case at 2000 RPM and MBT timing with intake-induced swirl is highlighted with a red oval. The value encased in a dashed box represents the duration of the early flame development period (0-10% mass fraction burned) in crank angle degrees (CA). The symbols are defined as: (**) SOC, (**) CA10, (**) CA50, (**) CA90.

The energy consumption per cycle is summarized in
Table 5-4, and shows that CNG requires more fuel energy than HCNG to reach the same output at stoichiometric conditions and MBT timing (recall that the fueling rate was determined based on 1.5 bar BMEP at stoichiometric, and MBT timing, at both engine speeds, for each fuel, and then held constant as equivalence ratio was adjusted by opening the throttle). This supports the observation of improved thermal efficiency with HCNG compared to CNG.
Table 5-4 Energy consumption per cycle for each fuel at engine speeds of 2000 and 2750 RPM, both at MBT timing.

<table>
<thead>
<tr>
<th></th>
<th>HCNG-q (J/cycle)</th>
<th>HCNG-s (J/cycle)</th>
<th>CNG-q (J/cycle)</th>
<th>CNG-s (J/cycle)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2000 RPM, MBT</td>
<td>410</td>
<td>412</td>
<td>439</td>
<td>438</td>
</tr>
<tr>
<td>2750 RPM, MBT</td>
<td>432</td>
<td>447</td>
<td>459</td>
<td>480</td>
</tr>
</tbody>
</table>

The assertion that hydrogen addition improves BSEC and BTE compared to CNG alone, is well-supported by the preceding discussion. Let us now turn to the resulting NMEP to explore this assertion further.

Figure 5-5 illustrates the portions of the combustion cycle (from a pressure/volume perspective) that contribute to indicated mean effective pressure (IMEP) and pumping mean effective pressure (PMEP). The NMEP is a measure of the work done on the piston by the gases over the entire four-stroke engine cycle, divided by the displaced volume of the cylinder. The significance of evaluating NMEP is that it accounts for pumping work. This quantity (NMEP = IMEP + PMEP) is of particular importance given that HCNG in the present work has a higher mass-based stoichiometric air-to-fuel ratio (18.2) than CNG (17.1). Hence, for the same AFR, HCNG requires more air, and subsequently less throttling, which may reduce the pumping losses relative to CNG. It is expected then, for the present work, that HCNG will achieve higher values for NMEP than CNG, and higher thermal efficiency as well.
The pumping losses represent the work done on the gases by the piston during the intake and exhaust strokes, and is a negative quantity (as it does not contribute, positively, to engine output) when the pressure during the intake stroke is less than the pressure during the exhaust stroke. (Heywood, 1988; Stone, 1999; Ferguson and Kirkpatrick, 2001).

Driving the pressure during the expansion stroke too high will cause higher pressure during exhaust stroke, which increases pumping losses. So while it might seem intuitive to maximize the pressure during the expansion stroke, it must be balanced to preserve engine efficiency. Stone asserts that MBT timing is an optimized balance of high pressure during compression with an increased pressure during expansion (Stone, 1999). The optimization of setting the minimum spark advance for best torque for HCNG offers an enhanced benefit compared to CNG alone, since it can be retarded, concentrating the heat release close to TDC, which also confirms a common finding of the literature.
Figure 4-15 (2000 RPM, MBT timing, with a quiescent intake configuration) shows that hydrogen addition results in a higher NMEP than CNG, due to optimum combustion phasing (MBT timing), which is retarded significantly for HCNG compared to CNG (meaning, spark timing is much closer to TDC than for CNG). This phasing of combustion produces more positive work, compensating for the inefficiency that inhibited HCNG during the fixed spark timing study (Figure 4-6). Advanced timing (for CNG compared to HCNG) leads to an increase in pressure before TDC, resulting in an increase in compression (or negative) work (evident by lower NMEP compared to HCNG, Figure 4-15). The increased pressure before TDC also increases pressure during the expansion stroke (or positive work), but not necessarily enough to offset the negative work. Figure 4-18 provides further insight into the differences between CNG and HCNG combustion, as the percent of energy released prior to TDC is higher for CNG compared to HCNG, which suggests that CNG must lose more heat to the cylinder walls, whereas HCNG, with more retarded timing, has heat release concentrated close to TDC, which helps to improve the brake thermal efficiency. Refer back to Figure 5-4 to compare the 10-90% MFB durations for CNG compared to HCNG at 2000 RPM and MBT timing at an equivalence ratio of 0.9. The 10-90% MFB duration for HCNG is approximately 25 CA where that of CNG is 31 (this is in the quiescent case); for intake-induced swirl at 2000 RPM, MBT, the 10-90% MFB duration is 22 for HCNG, and 31 for CNG. These data show that the bulk burn process for HCNG is more efficient (occurs faster, with less time for heat loss to the cylinder walls) than for CNG. This is substantiated further by Figure 4-14, which shows significantly higher BTE for HCNG than for CNG. Hence, the retarded timing results in higher cylinder pressures during the expansion stroke, improving the conversion of thermal to mechanical energy. These results are in agreement with those in the literature, which report improved thermal efficiency with hydrogen addition compared to natural gas alone.
The study concludes that hydrogen addition (at 0.8 ≤ Φ ≤ 1.0) provides a combination of faster burn, better efficiency and lower EINO\textsubscript{x} emissions than CNG alone at 2000 RPM, with MBT timing, and without intake-induced swirl (Figure 4-13, Figure 4-14 and Figure 4-16), supporting findings commonly reported in the HCNG literature.

### 5.3 Hydrogen addition, engine speed, and swirl effects on natural gas

As discussed in the previous sections, there are benefits in adding hydrogen to natural gas in terms of improving the flame development period and overall burn process, and also improving the thermal efficiency. The literature has not suggested utilizing hydrogen as a trade off with engine (hardware) design, specifically regarding bulk fluid motion (turbulence), in an effort to enhance the combustion process. The hypothesis of the present work is that hydrogen addition supplants swirl. In short, this leads to the ability to eliminate swirl, which reduces heat loss, leading to improved efficiency. Intake-induced swirl at sufficient levels increases turbulence in the combustion chamber. In-cylinder turbulence promotes flame propagation and reduces cycle-to-cycle variations, and hence swirl is a design factor in IC\textsubscript{E}s. There is a limit to the benefits of in-cylinder turbulence, as rotating flows can enhance the rate of convective heat loss to the cylinder walls, and hence turbulence (and therefore, swirl) must be balanced against overall engine performance and efficiency when designing an engine.

#### 5.3.1 Natural gas and intake-induced swirl

The present work has shown that intake-induced swirl reduces the main burn duration for CNG (recall Figure 4-25, Figure 4-34) compared to CNG at comparable conditions in the quiescent configuration (recall Figure 4-7, Figure 4-16). This finding holds at 2000 RPM and
both fixed and MBT spark timing, across the examined equivalence ratio range. A comparison of the impact of swirl on the burn process for CNG at engine speeds of 2000 and 2750 RPM (both at MBT timing) is shown below.

The burn process has been shown to shorten (burn faster) with hydrogen addition to natural gas, in a spark-ignited ICE, in various studies in the literature (Conte and Boulouchos, 2006; D'Andrea, Henshaw and Ting, 2004; Jensen et al., 2000; Sita Rama Raju, Ramesh and Nagalingam, 2000; Swain et al., 1993; Tunestal et al., 2002; Ma et al., 2008). The main burn duration (10-90% MFB) for both CNG and HCNG is often shown to increase (become slower) as a function of decreasing (leaner) equivalence ratio. Swain et al. held load constant at 1.03 bar BMEP across the equivalence ratio range. The present work holds fueling constant across the equivalence ratio range, opening the throttle incrementally to achieve leaner air-to-fuel ratios. Less throttling of the air improves volumetric efficiency, and thereby increases the load, and results in increased NMEP as the equivalence ratio decreases (NMEP results of the present work are shown in Figure 4-6, Figure 4-15, Figure 4-24, Figure 4-33, and Figure 4-42). Comparing the present work (fixed fueling and variable load with decreasing equivalence ratio) to others (with fixed load, or varying fuel quantity across equivalence ratio range) is still appropriate in terms of evaluating the effects of hydrogen addition on natural gas (in all cases, hydrogen addition reduces the burn duration compared to natural gas alone). One must be careful to avoid comparing a trend of burn duration quantitatively across equivalence ratio from a fixed-load study with the present fixed-fueling/variable load study.

Hassaneen et al. (1998) studied the flame development process of natural gas combustion in a 4.6 L V-8 spark-ignited engine with 10.6:1 compression ratio and a bore and stroke of 90.2 and 90.0 mm, respectively. Load was fixed and equivalence ratio swept for engine speeds of 1500, 2100, 2500 and 3000 RPM. MBT timing was employed, and spark was also swept at intervals of 4 CA plus MBT, and 4 CA minus MBT. In short, for a given equivalence ratio
sweep, load was held constant. The early burn process (0-10% MFB) and the main burn duration were assessed. The results showed that the burn processes for 0-10% and 10-90% increase (are longer) with decreasing equivalence ratio, with fixed load. However, they found that increased NMEP served to decrease (shorten) the burn durations (Hassaneen et al., 1998). In the case of fixed fueling, load is permitted to vary and results in increased NMEP with decreasing equivalence ratio, as discussed in the previous paragraph. Hence, increased load enables burn durations to decrease even as equivalence ratio decreases, as is the case in the present work.

Figure 5-6 highlights that the addition of swirl allows retarded MBT timing (compared to the quiescent configuration) for CNG. The overall burn process is therefore shifted. At an engine speed of 2000 RPM, the overall burn process shifts, but CA90 is only 3 degrees later for CNG with swirl compared to the quiescent case. This means that the overall burn process, in addition to early flame development, is faster under the influence of intake-induced swirl.
Figure 5-6 Summary of the burn process as a function of crank angle degree, CNG in the quiescent configuration compared to intake-induced swirl, with MBT timing at engine speeds of 2000 and 2750 RPM. The value encased in a dashed box represents the duration of the early flame development period (0-10% mass fraction burned) in crank angle degrees (CA). The symbols are defined as: (⊙) SOC, (●) CA10, (〇) CA50, (△) CA90.

It has been shown that for lean, spark-ignited combustion in an ICE that the early flame development of natural gas can be enhanced by increasing the turbulence intensity (Hall, 1989). Heywood (1988) showed that for a central spark-fired engine with a compression ratio (CR) of 10 operating at 1500 RPM at approximately 4 bar IMEP, high swirl from the intake resulted in a higher predicted turbulence intensity than for a case with no swirl generated during the intake (swirl generation controlled via valve lift) (Heywood, 1988)

While Heywood was correct that swirl effectively leads to an increase in turbulence intensity, it is important to acknowledge that swirl motion leads to an increase in the turbulence kinetic energy, which subsequently increases the turbulence intensity.
The Ricardo Hydra test engine employed for the present work was modeled by Bhattacharjee and Haworth (2010). The cylinder mesh comprises 246532 hex cells, divided into layers. During simulation, piston travel results in cell deformation. The maximum cell volume of 4.6888 $\text{e}^{-8}$ mm$^3$ and minimum cell volume is 2.58227 $\text{e}^{-11}$ mm$^3$ with a total model volume of 7.62684 $\text{e}^{-4}$ mm$^3$. Figure 5-7 shows one view of the three dimensional model used for the Ricardo Hydra.

![Figure 5-7 View of the Ricardo Hydra Geometry per the CFD grid (Bhattacharjee and Haworth, 2010)](image)

The computational fluid dynamics (CFD) simulation software used to model the Hydra is called ACFlux, developed initially by General Motors, and further by Haworth’s research group at Penn State University (Bhattacharjee and Haworth, 2010). The turbulent combustion model is a flamelet model and uses information on the laminar flame speed and thickness from detailed chemistry calculations. A characteristic time scale model with single step global chemistry was used in conjunction with a turbulence Re-normalization group (RNG) k-epsilon model (TKE) (Bhattacharjee and Haworth, 2010).
Figure 5-8 shows the modeled turbulence kinetic energy in the flow divided by the turbulence kinetic energy estimated from the mean piston speed as a function of crank angle degree for the Ricardo Hydra engine used in the present work. The influence of intake-induced swirl clearly results in more turbulence kinetic energy in the flow field, certainly during the intake stroke (0-180 CA), but prevails during the compression stroke (180-360 CA) as well, compared to the quiescent case. Hence, the presence of intake-induced swirl results in a faster flame propagation period for CNG than in the quiescent case (compare 2000 RPM, MBT for CNG-q and CNG-s in Figure 4-16 and Figure 4-34, respectively, and compare CNG-q with CNG-s at 2750 RPM and MBT, Figure 4-43). This is because increased turbulence intensity has been shown to improve the early flame development of CNG, and turbulence intensity is a function of increased turbulence kinetic energy which results from imparting swirl (Lancaster et al., 1976). Turbulent burning velocity is thought to govern the burn rate (Turns, 2000), and since turbulence (via swirl, in this case) distorts the flame front, resulting in wrinkling (increased flame area), turbulence intensity can be thought to increase the turbulent burning velocity. Another method of increasing the turbulence kinetic energy (instead of imparting swirl in on the intake flow) and subsequently elevating the level of turbulence intensity is to increase engine speed.
Figure 5-8 The ratio of turbulence kinetic energy to kinetic energy based on mean piston speed as a function of crank angle in the Ricardo Hydra Engine used in the present work. The data were produced from a CFD model based on the dimensional geometry of the engine. The curve for (---) the quiescent case in the present work, and (- - - - - ) for the intake-induced swirl condition (Bhattacharjee and Haworth, 2010).

5.3.2 Engine speed and engine performance

Now we consider the impacts of increased engine speed on the performance of CNG. Figure 5-6 shows the burn characteristics at 2750 RPM for CNG in the quiescent and swirl configurations as well as those at 2000 RPM. The MBT timing at 2750 RPM is advanced compared to the same case (quiescent or swirl) at 2000 RPM. This is because higher engine speed reduces the amount of time that the flame has to develop before TDC is reached. The CA90 at 2750 RPM (Figure 4-43) occurs much earlier compared to the same case at 2000 RPM (Figure 4-34). The CA90 for CNG at 2750 RPM in the quiescent configuration is at 383 CA,
which is 7 CA before CA90 at 2000 RPM. Similarly, CA90 for CNG in the swirl configuration occurs at 382 CA, which is 11 CA earlier than at 2000 RPM (CA90 = 392 CA).

Figure 5-9 shows the burn durations plotted as time (ms) instead of CA, for an absolute comparison. At 2000 RPM, intake-induced swirl clearly provides shortened burn duration for both CNG and for HCNG. The improvement is more consistent for HCNG than for CNG. In the case of 2750 RPM, swirl addition to CNG has little to no effect on the burn process, supporting the notion that the increased turbulence provided from an increase in mean piston speed (higher RPM) reduces the need for intake-induced swirl. The most important aspect of the comparison in Figure 5-9 is that at higher RPM, the burn durations are shorter than for any of the cases at 2000 RPM. This is not expected. Although turbulence intensity scales with mean piston speed, and that increased turbulence enhances mixing and can improve the burn process, the time available for the flame to propagate across the cylinder is decreased. Hence, one would expect the absolute time for the flame to propagate to be approximately the same at both 2000 and 2750 RPM. But the data show that the burn process is shortened at higher RPM.
A comparison of stoichiometric spark-ignited engine operation on propane and on hydrogen showed that the turbulent flame speed for propane was significantly higher than its laminar flame speed (Heywood and Vilchis, 1984). Since turbulent flame speed is a function of the flame area, which is affected (increased) significantly due to turbulence (via wrinkling, for example), one can assume that raising the turbulence intensity increases the turbulent flame speed, even if a fuel has a slow laminar flame speed of a fuel (such as methane, or CNG in the present work). The present work shows, when comparing the burn durations of CNG-q at 2000 and 2750 RPM both with MBT timing (in Figure 4-16 and Figure 4-43, respectively), that the burn duration at 2750 RPM is shorter (faster) than at 2000 RPM. Flame speed has been shown to increase as a function of engine speed, such that increasing engine speed results in faster flame
speeds (Bouchard, Taylor and Taylor, 1937). Lancaster et al. (1976) found that increased turbulent flame speed as a function of engine speed was due to increased turbulence of the mixture (Lancaster et al., 1976).

In order for turbulence to influence flame propagation, the size of the flame kernel must be of the same order as the magnitude of the turbulence scale (Lancaster et al., 1976; Taylor and Taylor, 1970; Stone, 1999). Lancaster et al. (1976) provided a concise and informative description of how turbulence affects flame speed, based on an assessment of the literature in conjunction with the findings of their study (described in previous sections of the present work),

“As discussed previously, turbulence increases flame speed by increasing the surface area of the flame through distortion by wrinkling or entrainment. When the flame kernel is small, only small-scale eddies can provide this distortion; larger scale eddies displace the flame kernel without distorting it. As the flame kernel grows, the flame front can be distorted by increasingly larger eddies.” The distortion of the flame front and the flame speed both increase with time (Lancaster et al., 1976). Perhaps this helps to explain why the CA90 for CNG at higher engine speed (Figure 4-43) occurs ahead of that at 2000 RPM (Figure 4-16 for quiescent and Figure 4-34 with intake-induced swirl), even though the initial flame development period starts earlier and takes longer at higher engine speed. The increased spark advance for higher speed operation is due to the early flame kernel growth not speeding up enough to offset the reduced time allowed for combustion as engine speed increases. But after the initial growth, the higher turbulence level at higher engine speeds compensates for the reduced time and keeps the overall burn duration essentially constant, in terms of number of crank angle degrees.
5.3.3 Hydrogen addition versus swirl

While it is advantageous to reduce the main burn duration, since faster burn (in CA) minimizes the amount of heat release that will occur after the piston begins to travel downward (during the expansion stroke), it is important to acknowledge the cost of employing swirl. This is because heat release that occurs too far beyond TDC is not productive, in terms of doing work on the piston.

Table 5-5 summarizes the effects of intake-induced swirl on BSEC, BTE, NMEP and the percentage of heat released prior to TDC when CNG is burned and MBT timing is employed, at both 2000 and 2750 RPM. The summary at 2000 RPM shows that BSEC and BTE suffer as a result of intake-induced swirl, and yet the percent of energy released prior to TDC is either unaffected or lower than in the quiescent case. Increases in BSEC will impact fuel economy (in a vehicle) negatively. We know from the previous section (5.2) that efficiency losses can be a function of the main burn duration (10-90% MFB), for a given engine (Filipi and Assanis, 2000; Stone, 1999).

Table 5-5 Summary of the effects of intake-induced swirl on CNG, for key parameters, relative to the quiescent configuration, with MBT timing, at specified RPM. Legend: (↑) increase, (↓) decrease, (•) neutral (Figure 4-10, Figure 4-14, Figure 4-15, Figure 4-18, Figure 4-28, Figure 4-32, Figure 4-33, Figure 4-36, Figure 4-37, Figure 4-41, Figure 4-42, Figure 4-45)

<table>
<thead>
<tr>
<th>RPM</th>
<th>BSEC</th>
<th>BTE</th>
<th>NMEP</th>
<th>% Q bTDC</th>
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<tr>
<td>2000</td>
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It is now well established that while swirl helps to improve the burn process for CNG, it comes at the loss of efficiency. This is where hydrogen addition offers the greatest benefit to CNG: hydrogen addition can improve the burn process without experiencing efficiency losses at the same magnitude as CNG. In other words, HCNG increases the burn rate compared to CNG,
as does swirl when added to CNG, but HCNG achieves better burn rates without the negative consequences on efficiency.

5.3.3.1 The effects of hydrogen addition on the combustion and engine performance of CNG

Figure 5-10 provides a summary of the burn processes for CNG and HCNG for 5 cases (2000 RPM with and without swirl, at fixed spark timing and MBT, and for 2750 RPM MBT). The early flame development period, represented by the SOC-10% MFB, is always longer for CNG than for HCNG at the same conditions. Natural gas (methane) is known to suffer from slow flame development.

Figure 5-10. Summary of main burn processes of CNG compared to those with hydrogen addition.
Groff and Matekunas (1980) showed that bulk mixing and large-scale flow prior to TDC causes wrinkling of the flame that persists and wrinkles the flame at a later point in the burn process, and must be accounted for in order to predict flame behavior in an engine. The wrinkling can increase the flame area, hence increasing turbulent burning velocity (Groff and Matekunas, 1980). Recall that the disadvantage of spark advance is that it produces higher pressures before TDC and increased compression work (which is negative work), and is the motivation for employing MBT timing, since MBT timing provides optimized efficiency at a given condition compared to advanced timing (Stone, 1999). This highlights a benefit of hydrogen addition, which shortens the burn process without the cost of increased negative work that can reduce the overall efficiency.

Figure 4-27 shows the percent of energy released prior to TDC for CNG and HCNG under the influence of intake-induced swirl. It is clear that CNG releases more energy before TDC than HCNG. This is expected due to the advanced spark timing of CNG compared to that of HCNG. Revisiting Figure 4-9 (percent energy released prior to TDC at 2000 RPM and fixed spark timing, quiescent) highlights that the magnitude of the heat release before TDC is significantly higher in the case of swirl than in the quiescent configuration. This is expected given the discussion in the previous section, and because it is known that swirl can increase the convective heat transfer to the cylinder wall, resulting in heat loss through the coolant (Heywood, 1988).

Figure 5-11 shows the heat release for the same case. Evaluating the quiescent case reveals a shift in combustion phasing with hydrogen addition, such that the bulk of the heat release occurs after TDC (CA = 360). Recall that the spark timing was held constant for CNG (26.6 CA before TDC) and for HCNG (15.6 CA before TDC) at all equivalence ratios and for both quiescent and swirl configurations. Comparing the quiescent and swirl cases for natural gas shows that swirl serves to improve the early flame development, resulting in earlier heat release.
such that peak heat release occurs just before TDC. HCNG also experiences faster heat release in the case of swirl compared to the quiescent intake configuration, but the timing is retarded such that the bulk of the heat release still occurs after TDC. Recall that the spark timing for CNG and HCNG were chosen based on MBT timing at stoichiometric conditions and 1.5 bar BMEP in the quiescent condition. In summary, evaluating the heat release (Figure 5-11) in conjunction with the percent of heat released prior to TDC (Figure 4-9 and Figure 4-27) emphasizes the inefficiencies associated with swirl addition to both fuels; CNG suffers more than in the case of hydrogen addition, due to the relatively advanced spark timing. Furthermore, hydrogen addition offers faster burn durations without the addition of intake-induced swirl, which offers an opportunity to improve efficiency. This finding supports the hypothesis of this work, that hydrogen addition supplants swirl in terms of improving the early flame development period, and does so with better thermal efficiency than CNG with swirl.
Figure 5-11 Instantaneous heat release plotted in kJ/CA as a function of crank angle for (—) HCNG-q, (—-—- )HCNG-s, (······)CNG-q, and (······)CNG-s, at an equivalence ratio of $\Phi = 0.9$ at 2000 RPM, fixed spark timing.

Table 5-6 Summary of the effects of intake-induced swirl, and hydrogen addition, on CNG in the quiescent configuration, at 2750 RPM, MBT timing. Legend: (↑) increase, (↓) decrease, (•) neutral

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<th>BSEC</th>
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Figure 5-12 highlights that HCNG consistently has retarded MBT timing compared to CNG at MBT timing, shown as the SOC, a shorter early flame development period (0-10% MFB) than CNG, and a shorter main burn duration (10-90% MFB) compared to CNG. Figure 5-12 shows that the burn process from the SOC through the 90% MFB point (CA90) at an equivalence ratio of 0.9. The overall trend, at 2750 RPM, for the 0-50% burn duration (fastest to slowest) is
CNG-s < HCNG-q < CNG-q. At 2750 RPM and an equivalence ratio = 0.9, both HCNG and CNG in the quiescent configuration achieve the longest 0-50% burn period (33.2 and 41.3, respectively), compared to any other RPM or intake configuration, for the same fuel. Conversely, under the influence of intake-induced swirl, CNG (at 2750 RPM) achieves the shortest 0-50% burn period (22.7 CA) compared to any other configuration.
Figure 5-12 Summary of the combustion process as a function of crank angle degree, for all CNG and HCNG in the quiescent configuration, as well as CNG under the influence of intake-induced swirl, at MBT timing, at both 2000 RPM and 2750 RPM, for the equivalence ratio 0.9. The value encased in a dashed box represents the duration of the early flame development period (0-10% mass fraction burned) in crank angle degrees (CA). The symbols are defined as: ( ) SOC, ( ) CA10, ( ) CA50, ( ) CA90. [refer to Figure 4-16, Figure 4-34 and Figure 4-43]

While CNG-s achieves the fastest burn process, CNG suffers from a reduction in efficiency compared to HCNG-q at 2750 RPM. Figure 4-37 shows that the BSEC at 2750 RPM and MBT timing is higher for CNG with swirl than for CNG or HCNG in the quiescent case. This is expected since swirl, when compared to cases in the quiescent condition, increases convective heat loss at the cylinder wall, reducing the available energy to do positive work on the piston. This point can be verified further by evaluating the resulting BTE (Figure 4-41), which is lowest for CNG with swirl compared to either CNG or HCNG in the quiescent case. These results show that although the burn process can be improved for CNG with swirl addition, doing so comes at the cost of a decrease in thermal efficiency. This finding lends credence to the
hypothesis of this work, because there is a need to understand whether hydrogen might be capable of improving the burn process without a reduction in thermal efficiency.

Figure 4-45 shows the percent of energy released prior to TDC, ordered from the most energy released prior to TDC to lowest is CNG-s > CNG-q > HCNG-q. At the same equivalence ratio, the timing for CNG under the influence of swirl is more retarded than the same fuel in the quiescent case. This means that in the case of swirl, CNG released more heat in less CAD than CNG or HCNG in the quiescent case. Furthermore, inducing swirl by blocking one intake port increases pumping losses, and hence decreases NMEP. As a consequence, the NMEP is lower for both fuels in the swirl case compared to quiescent, and the BSEC is higher for CNG in the case of swirl compared to the quiescent case.

Table 5-7 Summary of the effects of hydrogen addition on CNG, for key parameters, relative to the quiescent configuration, with MBT timing, at specified RPM. Legend: (↑) increase, (↓) decrease, (•) neutral (refer to Figure 4-10, Figure 4-14, Figure 4-15, Figure 4-18, Figure 4-37, Figure 4-41, Figure 4-42 and Figure 4-45)

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Figure 4-16 shows the main burn duration for the quiescent condition and MBT timing at 2000 RPM. HCNG results in faster burn duration than CNG, which is a direct result of the advanced spark timing of CNG compared to HCNG, which means that CNG needs more time for flame kernel growth and early flame development than does HCNG. Figure 4-18 shows that both fuels require more fuel energy to be consumed prior to TDC as equivalence ratio becomes leaner. This is because in lean conditions (where fueling rate is fixed for each equivalence ratio, and the throttle is opened to allow more air to achieve lean equivalence ratios), a higher volume of air/fuel mixture means that more heat is lost to the unburned gas from the burned gas early in the
flame development process. Overall, however, hydrogen assisted combustion releases less heat
prior to TDC than CNG, due to its retarded MBT timing, while achieving faster burn, and better
efficiency (BTE is higher for HCNG, Figure 4-14). Hence, swirl is not required to improve the
burn process of HCNG, particularly since hydrogen addition improves the burn process
(supplants swirl) without compromising the efficiency.

Tunestal et al. (2002) studied the effects of hydrogen addition to natural gas in a 0.6 L
single-cylinder engine, and compared engine performance and burn characteristics with two
engine heads. One combustion chamber was classified as a turbine and generated lower
turbulence than the quartette chamber, which provided fast burning (high turbulence). The 4-
valve engine had a compression ratio of 12:1 with stroke and bore of 140 mm and 120.65 mm,
respectively (Tunestal et al., 2002). Studies were conducted at 1200 RPM and 1.5 bar IMEP at
MBT timing, sweeping equivalence ratio from stoichiometric to lean. This work is of particular
interest since it is parallel to the present work, in that increased turbulence levels are induced, and
the effects on burn characteristics with CNG and HCNG are evaluated. The primary difference
between that work and the present studies is that the present studies were conducted at higher
engine speeds, and the present studies also considered the effects of higher RPM (2750 compared
to 2000) in order to understand the effects of turbulence intensity. Tunestal et al. (2002) held
load constant at 1.5 bar IMEP (which means that fueling was reduced as a function of decreasing
equivalence ratio). The present work started at a load of 1.5 bar BMEP, but the load varies as
equivalence ratio becomes leaner (constant fueling was used).

Tunestal et al. (2002) conducted experiments at several fuel combinations, including neat
CNG, and CNG with hydrogen added from 5% to 20% of the fuel, by volume. The findings for
the turbine (slower burning) combustion chamber reveal that hydrogen addition resulted in
shorter main burn durations (10-90% MFB) and higher net indicated efficiencies than CNG alone,
across the range of equivalence ratios. The quartette (fast burning chamber) resulted in higher
indicated efficiency for hydrogen addition than CNG, but the disparity was most pronounced at lean conditions. The main burn duration for the fast chamber did not result in faster burn periods until conditions were leaner than $\Phi = 0.7$ (Tunestal et al., 2002). These results agree with the findings of the present work (recall the case at 2000 RPM at MBT timing), as hydrogen addition decreases the main burn duration in both the quiescent and swirl cases (Figure 4-16 and Figure 4-34, respectively), and results in increased brake thermal efficiency (recall Figure 4-14 for the quiescent case and Figure 4-32 for swirl).

In summary, intake-induced swirl can facilitate shorter early burn duration for CNG, but does so at the cost of increasing the heat loss, which leads to loss of thermal efficiency and increased brake specific energy consumption. Hydrogen addition to natural gas also achieves shorter early burn durations, without compromising thermal efficiency.
Chapter 6 Conclusions & Recommendations

The two objectives of this research were:

1. To confirm two findings regarding the role of hydrogen in CNG combustion that are prevalent in literature
   a. Hydrogen addition improves the burn process of CNG
   b. Hydrogen addition provides an improvement in the thermal efficiency compared to CNG

2. To evaluate a hypothesis unique to this research
   a. Hydrogen supplants swirl when comparing the combustion performance of HCNG to CNG

These objectives are described in more detail below, and the results of the present work specific to each objective are presented, accordingly.

The objective to confirm pertinent findings from the literature were successful. The first item, that the addition of hydrogen improves flame development, enabling spark retard, was shown to be true in at two engine speeds (2000 and 2750 RPM), across the range of equivalence ratios examined (stoichiometric to $\Phi = 0.6$), when comparing the fuels at MBT spark timing. The early flame development period (0-10% MFB) is consistently shorter in CA (faster) for HCNG compared to CNG. The bulk burn period (10-90% MFB) of HCNG is also shorter than for CNG. Furthermore, the MBT spark timing for HCNG is consistently retarded compared to the timing for CNG at a given engine speed and equivalence ratio, by virtue of the faster burn process.

The assertion that the shorter burn duration of HCNG serving to minimize heat loss and improve thermal to mechanical energy conversion (BTE) compared to CNG was also confirmed, both at engine speeds of 2000 and 2750 RPM with MBT timing, where HCNG generally results in a higher BTE (and lower BSEC) than CNG at the same engine speed and equivalence ratio.
The second and primary objective of this work was to evaluate a hypothesis via performing heat release characterization of hydrogen assisted natural gas combustion in a spark-ignited engine, and compare the combustion characteristics with those for natural gas, specifically. That hypothesis, *the addition of hydrogen supplants swirl by enhancing the burn process, thereby reducing cylinder heat loss and improving efficiency, compared to the burn process and BTE of CNG in the case of intake-induced swirl*, was shown to be true for both engine speeds studied (2000 and 2750 RPM) and at MBT spark timing for the equivalence ratio range tested (1.0 < $\Phi < 0.6$). HCNG provides a faster early flame development period and faster main burn process, while also achieving values of BTE higher than those for CNG.

### 6.1 Confirmation of hypothesis

The present work presented a new hypothesis and showed evidence that hydrogen can be used to improve the burn process of CNG, instead of using swirl to make the flame development occur faster, and that it does so without incurring losses in BTE, as is observed when intake-induced swirl is imparted on CNG to improve the burn process. Experiments covering a full engine operating map (idle – 4500 RPM, MBT timing, at stoichiometries from slightly richer than stoichiometric to rather lean (perhaps $\Phi = 0.6$), at both light and high loads (WOT) would add clarification and understanding to the findings of the present work. Is the effect shown in this research limited once higher loads are imposed? Will the hypothesis hold up when comparing HCNG and CNG at the same load? These are two important questions that need to be addressed.
6.2 Influence of load and air mass

The present study addresses idle conditions at two engine speeds (2000 and 2750 RPM) and low loads (1.5 bar BMEP at stoichiometric conditions, with load varying as fueling is held constant and throttle opened to achieve leaner conditions). WOT studies, as well as moderate loads are of interest, since normal engine operation in a vehicle application varies from idle to WOT depending on driving conditions. A parametric study varying spark timing, load, engine speed and stoichiometry for both CNG and HCNG would be a significant contribution to the literature.

The present work showed improvement in the burn process at 2750 RPM compared to 2000 RPM. Conducting studies at a fixed load, 1.5 bar BMEP, with MBT timing at both engine speeds (2000 and 2750 RPM), would help to explain the findings of the present work. Are the current findings significant and do they merit further investigation? Or does load somehow come influence the burn process and convolute the results?

Fixing the hydrogen fraction in natural gas and varying equivalence ratio resulted in a greater influence on the stretched flame speed than hydrogen addition (Huang et al., 2006). This finding does support the present work, in that hydrogen addition increases the flame speed compared to natural gas alone, and it also raises a question about the influence of air-to-fuel ratio when hydrogen is present in the fuel mixture. Evaluating the performance of CNG compared to HCNG on an equivalence ratio basis may be flawed, given that more air is required in the case of HCNG, which reduces pumping losses (less throttling). It would be informative to evaluate the data as a function of torque, or perhaps air-to-fuel ratio, to improve the basis for comparison. Does HCNG achieve better efficiency and fuel consumption than CNG at the same AFR?
6.3 Fundamental data applicable to engine conditions

The literature lacks fundamental flame information specific to ICEs, at pressures relevant to engine operation. A characterization of the flame in an ICE for both CNG and HCNG, with and without intake-induced swirl is a needed contribution to the field of gaseous fuel combustion in ICEs. Optically accessible engine studies would provide substantive information to the literature.

The explosion limit curves at a given air-to-fuel ratio for H₂/air and CH₄/air are quite different, due to the differences in flammability limits and physical properties of the fuels. The unburned gas densities and expansivity of the burned gases will be different as well. A fundamental investigation into these parameters and their effect on combustion, specifically the burn process at engine conditions, would be meaningful.

An investigation of the overall emissions, including full hydrocarbon speciation and radical concentrations using laser diagnostics along with empirical quantifications of the Damkohler number could be telling of the relative contribution of kinetics versus fluid mechanics on the burn rate.

6.4 Ion-sensing head gasket and optical spark plug

The Ricardo Hydra engine was outfitted with an ion-sensing head gasket (6 ion sensors), and an optical spark plug. Data from the ion sensors in the head gases were collected at the 2000 RPM, MBT case with and without the influence of intake-induced swirl, for both CNG and HCNG. It may be valuable to harvest this data, to evaluate the sensor readings at SOC, to discern whether spark timing really is an appropriate assumption for SOC with these fuels, in the given
engine set-up. The data could be examined further to draw assertions about the early flame development period.

Figure 6-1 shows a head gasket equipped with 6 ion probes that has been designed and fabricated for the Hydra engine which enables detecting the flame arrival along the plane of head gasket. The related signal conditioning board and data acquisition are in place and functional.

![Figure 6-1 Ion probe head gasket for the Ricardo Hydra engine](image)

Another in-cylinder flame detector, optical sensor equipped spark plug, has also been obtained which allows the flame detection on the top of the combustion chamber (Figure 6-2 and Figure 6-3). Follow-up studies could employ this device to ascertain important characteristics about the spark event and subsequent SOC.
The fueling process used required purging the high-pressure cylinder with the fuel to be used and emptying it to atmosphere several times prior to fueling with the fuel to be tested. The ambient temperature varied considerably throughout the time period that the tanks were fueled, purged, and used in the tests. As such, there was no real consistency of the fuel from test to test.
Given the low volume of fuel in the 80L cylinder, many re-fueling events took place. Furthermore, the blending at the fueling station was not 100% repeatable, according to Air Products, as the station was new and being developed during the time fuel was being acquired and consumed for the present work. Hence, the HCNG composition may have been variable from fill to fill.

Bag samples were collected from the tank after each fueling, and ran through a GC in an effort to comprehend the true constituents of the fuel from each fill. However, the calibrations for species aside from methane and hydrogen were not sufficient, and some samples yielded nonsensical compositions of the constituents. Hence, the composition of CNG and HCNG used in the present work was assumed to be the same for all fuels. This is not desirable, and the data quality would be enhanced with improved fueling conditions and fuel sampling/analysis. A suggestion would be to procure multiple tanks or a larger volume tank so that many tests could be run on a single batch of fuel. Obviously it is also imperative to calibrate the GC properly for broad ranges of low-range hydrocarbons (methane, ethane, propane, butane, etc.), as well as nitrogen. Standardized fuels for both CNG and HCNG would be ideal.

6.6 Basic requirements for pressure-based heat release

The pressure data generated from the present work is noisy (meaning that the signal quality, was not optimum, and may even be questionable in terms of accuracy). The following steps are proposed to enhance the integrity of pressure data; these steps should be followed when setting up pressure sensing systems on a given test article and integrity confirmed periodically:

- Integrate proper cables/isolate from spark noise or other disturbances
- Determine TDC
• Employ a pegging technique (to reference the pressure sensor data to a measured absolute pressure)

• Employ sensor gains properly

• Employ data quality checks (i.e. to assess whether thermoshock may be affecting the cylinder pressure data)

A paper by Davis and Patterson (2006) is recommended for review regarding methods to evaluate the quality of cylinder pressure data and provides tactics to improve data accuracy (Davis and Patterson, 2006).

6.7 Investigation of thermodynamic properties and development of more sophisticated heat release model is required for gaseous fuels

Log plots of pressure as a function of cylinder volume throughout the four-stroke cycle were plotted for each fuel at the same operating point (i.e. 2000 RPM, MBT timing, equivalence ratio = 0.8) for the present work. Figure 6-4 shows the slope of the compression curve for each fuel, and indicates that gamma needs to be treated specifically for each fuel, since there is a significant difference between the slopes for CNG compared to HCNG.
This finding necessitates further evaluation; a sensitivity study for gaseous fuels, in terms of the use of gamma (air) compared to air including the fuel, should be conducted to determine whether an enhanced heat release code is required.

Separate from concerns specific to the handling of gamma is the interest in evaluating early flame development between CNG and HCNG. Such a study requires physical measurement enhancements, as well as a more sophisticated heat release code.

Additionally, individual cycle pressure data (as well as averaged) should be saved so that error analysis and intimate cycle-to-cycle analysis can be performed, if desired (Randolph, 1990).

### 6.7.1 Requirements for Spark-Ignited Heat Release Model

In a spark-ignited engine SOC occurs at the time when the spark is fired. Additionally, it is important to treat the burned and unburned gases separately (two-zone model). Conte and Boulouchos did so in their 2006 works on flame speed and flame front propagation of reformer gas. Furthermore, the two-zone heat release model, which accounts for the burned and unburned
gases separately, and employs an equilibrium solver to provide the thermodynamic properties of the burned constituents has been available since 1966 (at least), when Krieger and Borman published their two-zone model (Krieger and Borman, 1966). While it is complex to integrate the necessary models/solvers, it is disappointing that utilization of the two-zone model is not used more widely in the experimental spark-ignited engine combustion literature.

The author of the present work attempted to employ a two-zone model for the present work, but more debugging and testing is required before the code can be utilized with confidence. A summary of the model is explained below.

The initial construct for the system of five ODE’s was employed in Matlab (borrowed matrix form of equations and concept of iterating on the constant from the Woschni function for heat transfer from Guezennec and Hamama, along with an equilibrium solver (via Cantera), and the following assumptions observed (Guezennec and Hamama, 1999):

- Cylinder volume comprises unburned gases (air, fuel, residuals or combustion products) and burned gases (uniform mixture of combustion products)
- Both burned and unburned gases at the same uniform pressure, at a given crank angle degree
- Both unburned and burned gases follow ideal gas law behavior
- Both unburned and burned gases are at thermodynamic equilibrium
- Heat transfer is convective only, between gases and cylinder walls
- Residual fraction is neglected (assume 100% fresh charge)
- Chemical equilibrium solver was employed at each crank angle degree to discern the composition of the burned gases, in order to adequately compute the specific heat for the burned gas mixture at each time step (crank angle degree).
- The constant in the Woschni function for heat loss is iterated to match the asymptotic burn rate to the combustion efficiency; in this way, the heat loss is “tuned”
Figure 6-5 summarizes the simplified flow chart for the two-zone heat release code that was constructed for the present work, but not employed due to bugs that have yet to be resolved.

Figure 6-5 Flow diagram representing the functionality of the two-zone model initiated (but not employed) for the present work.

6.8 Emissions data analysis

The emissions results were outside of the primary scope of the present work, and hence were reported but not discussed thoroughly. Further exploration of the emissions data is possible if there is interest. Furthermore, it is typical for studies of HCNG and CNG to show that hydrogen addition increases NOx at lean conditions, where the present work shows increased NOx at lean conditions but not until $\Phi < 0.8$. This should be investigated, specifically due to concerns related to the fuel composition and potential for inaccuracies of the equivalence ratio computation.
6.9 Engine optimized for CNG combustion

As noted in Chapter 5, the engine geometry of the Ricardo Hydra engine is sub-optimal from a CNG standpoint. Literature surveys about the optimized engine geometry for CNG as well as engine data from proper CNG engines should be investigated. Natural gas can tolerate a compression ratio of up to 13, perhaps (Thring and Overington, 1982). The engine geometry, such as S/B and subsequent S/V and displacement volume could then be optimized differently, perhaps, than the engine in the present study. How does hydrogen addition influence the combustion process of natural gas in and engine designed specifically for CNG?
References


Appendix A  Additional Data

Figure A-1 Volumetric efficiency as a function of equivalence ratio for 2000 RPM, fixed spark timing
(○) HCNG-q, (□) CNG-q in the quiescent intake port configuration

Figure A-2 Combustion efficiency as a function of equivalence ratio for 2000 RPM, fixed spark timing
(○) HCNG-q, (□) CNG-q in the quiescent intake port configuration
Figure A-3 Thermal conversion efficiency (BTE divided by the combustion efficiency) as a function of equivalence ratio for 2000 RPM, fixed spark timing (○) HCNG-q, (□) CNG-q in the quiescent intake port configuration

Figure A-4 Volumetric efficiency as a function of equivalence ratio for 2000 RPM MBT timing (○) HCNG-q, (□) CNG-q in the quiescent intake port configuration
Figure A-5 Combustion efficiency as a function of equivalence ratio for 2000 RPM MBT timing (○) HCNG-q, (□) CNG-q in the quiescent intake port configuration

Figure A-6 Thermal conversion efficiency (BTE divided by the combustion efficiency) as a function of equivalence ratio for 2000 RPM MBT timing (○) HCNG-q, (□) CNG-q in the quiescent intake port configuration
Figure A-7 Volumetric efficiency as a function of equivalence ratio for 2000 RPM at fixed spark timing for (◊) HCNG-s, (▼) CNG-s, with intake-induced swirl.

Figure A-8 Combustion efficiency as a function of equivalence ratio for 2000 RPM at fixed spark timing for (◊) HCNG-s, (▼) CNG-s, with intake-induced swirl.
Figure A-9 Thermal conversion efficiency (BTE divided by the combustion efficiency) as a function of equivalence ratio as a function of equivalence ratio for 2000 RPM at fixed spark timing for (◊) HCNG-s, (▽) CNG-s, with intake-induced swirl.

Figure A-10 Volumetric efficiency as a function of equivalence ratio as a function of equivalence ratio for 2000 RPM at MBT timing for (◊) HCNG-s, (▽) CNG-s, with intake-induced swirl.
Figure A-11 Combustion efficiency as a function of equivalence ratio for 2000 RPM at MBT timing for (◊) HCNG-s, (▼) CNG-s, with intake-induced swirl

Figure A-12 Thermal conversion efficiency (BTE divided by the combustion efficiency) as a function of equivalence ratio for 2000 RPM at MBT timing for (◊) HCNG-s, (▼) CNG-s, with intake-induced swirl
Figure A-13 Volumetric efficiency as a function of equivalence ratio 2750 RPM at MBT timing for (○) HCNG-q, (□) CNG-q, (△) CNG-s

Figure A-14 Combustion efficiency as a function of equivalence ratio 2750 RPM at MBT timing for (○) HCNG-q, (□) CNG-q, (△) CNG-s
Figure A-15 Thermal conversion efficiency (BTE divided by the combustion efficiency) as a function of equivalence ratio 2750 RPM at MBT timing for (○) HCNG-q, (□) CNG-q, (▽) CNG-s
Appendix B  Heat Release Code

% Program written by Jamie Clark, September 2007
% Updated by Mel Fox September 25, 2007
% Updated by Mel Fox January 23, 2010 & February 14, 2010

% Program reads Pressure, Volume and CAD Data from pressure traces
% Data used to compute heat release characteristics
% Inputs used to calc these outputs, to be used as inputs to Hydra DAQ:
%   k-factor of the fuel mixture (for proper flowrate calc from MFC)
%   LHV of the fuel mixture
%   mass fraction of each component in the fuel
%   H/C ratio of the fuel mixture
% HR data matrix comes from the process.m file

% engine properties
cyl = 1;  % number of cylinders in the engine
bore = .086;  % m
stroke = .086;  % m
cr = 10.44;  % compression ratio
conrod = .143;  % m (connecting rod length)
crankrad = .043;  % m

% unit conversions
% see initHR.m for the variables/consts commented out below
% umassair = massair * 60 / 1000;  %mass airflow conversion to kg/min
%mair = umassair/cyl/(speed/2);  % mass flow of air in kg
% Tin = intakeAir + 273.15;  %convert intake temp C to Kelvin
% Tin = 298;  %in K
R = 8.314;  %universal gas constant J/mol-K
Rr = 8.314/(29*1000);  %R specific for air - kJ/kgK
rps = speed / 60;  %engine speed in radians
sp = 2*stroke*rps;  %mean piston speed
f = conrod/crankrad;  % for heat transfer
start = round((ST + 360)*10);  %find CAD where spark was fired.%use ST data, add value at TDC, multiply by 10 to convert to resolution of pressure measurement, and round it to get rid of the decimal
%increment of CAD
ENRG = mfuel*lhvmix*1000;  %fuel in cylinder per cycle (J)

% Heat Transfer Calcs
C1 = 2.28;  %constant c1 from Heywood
w = C1 * sp;  % average flow velocity inside the cylinder for compression and expansion - can add "+ C2*Vd*Ttr/prVr*(Pcyl-Pmotored)"
Twall = 450;  %assumed wall temperature in Kelvin

% Engine Volume calculations
Vd = pi*bore^2*stroke/4;  %swept volume, displaced volume (m3)
Vc = Vd/(cr-1);  %clearance volume (m3)
for i = 1:7200;
    radCA(i) = HR(i,1)*pi/180; % convert crank angle position to radians
    % cylVol already computed, loaded to cylVol matrix
end

Pres(2) = HR(2,3)*100000; % pressure in Pa

for i = 3:7198;
    Pres(i) = ((IntPres(i-1) + IntPres(i) + IntPres(i+1))/3); % smoothed pressure trace
    Pres(i) = Pres(i)*100000; % convert bar to Pa
end

for i = 5:7195;
    dp(i) = (-Pres(i+2)+8*Pres(i+1)-8*Pres(i-1)+Pres(i-2))/(12*delCA); % calculate dp (Pa/deg)
end

% initialize dq, T and Q
for i = 5:7195;
    dq(i)= 0.0;
    Q(i)= 0.0;
    T(i)= Tin;
    T2(i) = Tin;
    t(i) = Tin;
    Qtot = 0;
    done10 = 0;
    done50 = 0;
    done75 = 0;
    done90 = 0;
    done105 = 0;
    pair(i) = 0;
    Re(i) = 0;
    mu(i) = 0;
    Aw(i) = 0;
    hc(i) = 0;
    dQwall(i) = 0;
    W(i)= 0;
    dQw(i) = 0;
    mb(i)=0;
    startmfb=0;
    unitconv = 0.012;
end

% assume initial conditions
gamma = 2; % initialized gamma
Cv = 0.897; % initialize Cv

% energy and temperature computations
for i = start:7195;
    % Calculate Heat Release
dq(i) = (gamma/(gamma-1))*Pres(i)*dv(i)+(1/(gamma-1))*cylVol(i)*dp(i);

% solve Instantaneous Heat release J/deg
Q(i) = dq(i)* delCA + Q(i-1);                  %Cumulative heat Release in J

% first temperature calculation (T(K))
dt(i) = 1/(((mair + mfuel)*Cv)*((dq(i)/1000)-kPres(i)*dv(i))); %T in K. 1000 converts J to kJ. calculate change in temperature
T(i) = dt(i) * delCA + T(i-1);               %intergrate temp

% second temperature calculation
dt2(i) = 1/((mair +((Q(i)/1000)/lhvmix))*Cv)*(dq(i)/1000 - kPres(i) * dv(i));
T2(i) = dt2(i) * delCA + T2(i-1);

% third Temperature Calculation
tg(i) = (Pres(i) * cylVol(i)) / ((R/unitconv) * (mair + mfuel));  % ideal gas law temperature calculation, gives highest #

% Woschni heat transfer
Aw(i) = (pi * bore ^ 2 / 2) + ((pi * bore * stroke / 2) * (f + 1 - cos(radCA(i)) + (f ^ 2 - (sin(radCA(i))) ^ 2 ^ 0.5));    % area of wall exposed unit of m2
hc(i) = 3.26 * bore^-0.2 * (Pres(i)/1000)^0.8 * tg(i)^-0.55 * w^0.8; % heat transfer coefficient in W/m2K pressure in kPa

dQw(i) = hc(i) * Aw(i) * (T(i) - Twall) ;       %J/s

dQwall(i) = dQw(i) * (1/(360*rps));   % convert Watt to J/deg
Qwall(i) = dQwall(i) * delCA + Qwall(i-1);  % cumulative heat transfer

% recalculate gamma
if T(i) > 1000
    gamma = 1.485 - 0.00025527 * T(i) + 1.3911e-7 * T(i)^2 - 3.6506e-11 * T(i)^3 + 3.6966e-15 * T(i)^4;
else
    gamma = 1.3966 + 6.0455e-5 * T(i) - 1.5686e-7 * T(i)^2 - 5.6788e-11 * T(i)^3 + 9.2994e-14 * T(i)^4;
end

dQgross(i) = dq(i) + dQwall(i);  %J/deg    % calculate gross HR

dmb(i) = dQgross(i)/(lhvmix*1000);  % fuel burn rate kg/deg
Qgross(i) = Q(i) + Qwall(i);                 % Integrate to get total heat release

% calculate MFB
perQ(i) = Q(i)/ENRG*100;             %percent of energy released compared to available fuel, at a given CAD
perQgross(i) = Qgross(i)/ENRG*100;  %percent of energy released compared to available fuel, at a given CAD including heat loss to wall

% determine CA and Pressure at SOC, 10, 50 and 90% mfb
CA = start;
P = kPres(i);

%initialize end of loop
done5 = 0;
done10 = 0;
done50 = 0;
done75 = 0;
done90 = 0;
for i = start:7195;  
    %"done" is used to secure the value of CAmfb, and allow the loop to continue on to select new values
        if (perQgross(i) >=5) && (done5 == 0);
            CAmfb5 = i/10;
            Pmfb5 = kPres(i);
            done5 = 1;
        elseif (perQgross(i) >=10) && (done10 == 0);
            CAmfb10 = i/10;
            Pmfb10 = kPres(i);
            done10 = 1;
        elseif (perQgross(i) >= 50) && (done50 == 0);
            CAmfb50 = i/10;
            Pmfb50 = kPres(i);
            done50 = 1;
        elseif (perQgross(i) >= 75) && (done75 == 0);
            CAmfb75 = i/10;
            Pmfb75 = kPres(i);
            done75 = 1;
        elseif (perQgross(i) >= 90) && (done90 == 0);
            CAmfb90 = i/10;
            Pmfb90 = kPres(i);
            done90 = 1;
        end
    end
# VITA
## Melanie Corrigan

### Education
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<td>Wayne State University</td>
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### Work Experience
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