

The Influence of Fuel Composition on a Heavy-Duty, Natural Gas Direct Injection Engine

G.P. McTaggart-Cowan^{1*}, S.N. Rogak², S.R. Munshi³, P.G. Hill² and W.K. Bushe²

¹Wolfson School of Mechanical & Manufacturing Engineering, Loughborough University, Loughborough, UK

²Department of Mechanical Engineering, University of British Columbia, Vancouver, Canada

³Westport Power Inc., Vancouver, Canada

Abstract

This work investigates the implications of natural gas composition on the combustion in a heavy-duty natural gas engine and on the associated pollutant emissions. In this engine system, natural gas is injected into the combustion chamber shortly before the end of the compression stroke; a diesel pilot that precedes the natural gas injection provides the ignition source. The effects of adding ethane, propane, hydrogen, and nitrogen to the fuel are reported here. The results indicate that these additives had no significant effect on the engine's power or fuel consumption. Emissions of unburned fuel are reduced for all additives through either enhanced ignition or combustion processes. Black carbon particulate matter emissions are increased by ethane and propane, but are virtually eliminated by including nitrogen or hydrogen in the fuel.

Key Words: *Natural gas composition; hydrogen blended fuel; direct injection engine; pilot ignition; engine emissions*

1. Introduction

Natural gas is a potential alternative to conventional liquid fuels for use in automotive internal combustion engines. While predominantly methane (CH₄), natural gas also contains heavier hydrocarbons and inert diluents. The levels of these species vary substantially with geographical source, time of year, and treatments applied during production or transportation. The addition of unconventional and bio-derived gases to fossil natural gas can have an even greater effect on fuel composition [1]. Natural gas fuelling can reduce greenhouse gas (GHG) emissions compared to diesel; adding hydrogen to the natural gas offers even further GHG reductions from transportation applications [2]. When considering the use of natural gas, it is vital to understand the influences of fuel composition on the combustion system. This work evaluates the implications of natural gas composition on the combustion process and pollutant emissions for a heavy-duty, pilot-ignited, engine fuelled with directly injected natural gas.

1.1 Directly injected natural gas Engine

One technology for natural gas fuelling of heavy-duty engines, developed by Westport Power Inc., uses natural gas injected directly into the combustion chamber late in the compression stroke, retaining the performance and efficiency of an equivalently-sized diesel engine [3]. A small amount of diesel fuel is injected late in the compression stroke, prior to the natural gas injection. The auto-ignition and combustion

* Corresponding author: Wolfson School of Mechanical and Manufacturing Engineering, Loughborough University, Loughborough, LE11 3TU, UK. E-mail: g.mctaggart-cowan@lboro.ac.uk.

of this pilot fuel provides the ignition source for the gaseous fuel; the latter then burns in a predominantly non-premixed combustion event. Compared to diesel fuelling, the main fuel's lower carbon:energy ratio reduces carbon dioxide (CO₂) emissions; its lower adiabatic flame temperature reduces oxides of nitrogen (NO_x) emissions; and, its lower sooting tendency reduces fine particulate matter (PM) emissions. As the natural gas is not premixed in the combustion chamber, emissions of unburned fuel are significantly lower than from many other natural gas fuelling technologies [4]. Using exhaust gas recirculation (EGR) can achieve substantial further reductions in NO_x emissions; however, a lack of oxidizer at high levels of EGR degrades the combustion and increases the emissions of unburned hydrocarbons (HC), carbon monoxide (CO), and PM [5]. At the EGR levels required to achieve low NO_x levels, more than 90% of the PM originates from the natural gas [6].

2. Natural Gas Composition

Natural gas is a mixture of various hydrocarbon molecules. Commercial-grade natural gas compositions vary from 70-95% CH₄, with the balance composed of heavier hydrocarbons (primarily ethane, C₂H₆, and propane, C₃H₈) as well as diluents such as molecular nitrogen (N₂) and CO₂. There are also trace levels of sulphur compounds, often added as odorants, and other hydrocarbon species.

The effect of fuel composition on the combustion process and on the emissions from natural gas fuelled engines has been addressed in both fundamental and applied studies. The majority of research has focused on premixed charge spark ignition engines, which are currently the predominant form of natural gas engines [4]. These results, along with studies of non-premixed flames in laboratory-scale burners, provide insight into the effects of natural gas composition. However, there has been relatively little work on the complex combustion seen in a non-premixed compression-ignition engine, as investigated here.

2.1 Effect of Heavy Hydrocarbons

The principal heavy hydrocarbons found in natural gas are ethane and propane. For premixed auto-ignition combustion, the greatest influences of these species are in the ignition and early combustion phases, where they enhance the ignitability of the mixture; this is primarily a result of increases in the concentration of reactive radicals. At high temperatures, increases in the concentrations of H, OH, HO₂ and H₂O₂ radicals enhanced the natural gas ignition process [7,8]; at temperatures below ~1200 K, it is the methylperoxy (CH₃O₂H) radical that fills this role [9]. The heavier hydrocarbons also promote the formation of hydrocarbon radicals, including C₂ species such as the ethyl radical (C₂H₅) and acetylene (C₂H₂) [9].

Ethane and propane also influence the combustion event and pollutant emissions. Enhanced radical formation extends the lean combustion limit [10,11]. In premixed charge spark-ignition engines, ethane addition increases the flame propagation rate [12]. No significant effects on CO emissions are reported in

most engine studies; however, some researchers report increases in HC emissions with increased ethane and propane concentrations [13], although these results are not consistent across all reported studies. Fuel quality sensors [14] and closed-loop control engines [15] have permitted spark-ignition engines to run successfully on a wide range of fuel compositions.

The presence of heavy hydrocarbons also affects the ignition process in non-premixed natural gas combustion. At temperatures >1400 K, fuel additives have little effect as this process is mixing limited [16]. At lower temperatures, the addition of either ethane or propane is found to reduce ignition delay times by as much as 0.7 ms [16]. However, there is a limit to the effectiveness of improved kinetics, especially at higher temperatures; beyond a certain point mixing limitations dominate the ignition processes. The shorter ignition delay time has also been identified as a potential source for increased NO_x emissions with ethane addition to the fuel [17]; however, substantially more work is required to understand the effects of the heavier hydrocarbons on the ignition and pollutant formation mechanisms of a natural gas engine using a non-premixed direct-injection combustion system.

2.2 Fuel Dilution with Nitrogen

Small quantities of nitrogen may be found in natural gas, often added as a diluent to maintain a specified heating value. Other than reducing the mass- or volume-specific energy content (heating value) of the fuel, small levels of an inert diluent like N_2 are unlikely to significantly influence the combustion event. However, higher dilution levels may have a greater impact; these influences have been studied in various combustion systems. For a natural-gas fuelled, premixed-charge engine, adding N_2 to the fuel reduces NO_x emissions but impairs efficiency [18]. In a low pressure non-premixed combustion system (an industrial boiler), gaseous fuel dilution reduces NO_x emissions more effectively than does oxidizer dilution; fundamental studies attribute this to more rapid quenching of the NO -forming reactions [19]. In laminar counter-flow diffusion flame studies, N_2 dilution is used to reduce fuel concentrations; no significant effects are observed until the fuel stream contains more than 80% N_2 (by volume) [20]. These results indicate that the principal influence of nitrogen addition manifests itself by reducing the heating value of the fuel. There is no evidence of direct participation in the reaction kinetics, even at very high N_2 concentrations.

The effects of N_2 addition on a heavy-duty engine fuelled with directly injected natural gas have been studied previously [21]. The key findings from this work indicated that diluting the natural gas (while increasing the injection mass to retain the same total fuel energy) resulted in a slower initial combustion but faster and more stable late-stage combustion. This is attributed to the higher kinetic energy of the gas jet and resulting improvement in mixing. The current work compares these effects with those of other fuel additives.

2.3 Hydrogen Addition

The most important effect of blending natural gas and hydrogen for use in homogenous-charge, spark-ignition engines is extension of the lean combustion limit [22]. Combustion bomb studies demonstrate that hydrogen's enhanced diffusivity results in a higher turbulent flame propagation rate for lean mixtures [23]. The hydrogen also increases the flame's resistance to stretch [24], reducing local extinction events. At a constant air-fuel ratio, NO_x emissions are increased due to a higher adiabatic flame temperature while CO and HC emissions are reduced [25]. Flame stability in the presence of EGR is also improved [26].

For non-premixed combustion of hydrogen/methane blends, for a co-flowing jet diffusion flame, non-premixed flame stability is enhanced with increasing hydrogen content [27]. In a non-premixed steady flow burner, hydrogen addition reduces prompt NO formation due to a reduction in CH, but increases thermal NO due to higher flame temperatures and higher H, O, and OH radical concentrations [28,29]. In a direct-injection natural gas engine, replacing the natural gas with a hydrogen/methane blend increases the ignitability of the gaseous fuel and improves combustion stability, leading to significant reductions in emissions of combustion by-products including CO, HC, and PM, while higher temperatures increase NO_x emissions [30]. The current work compares these effects with those of other fuel additives.

3. Experimental Apparatus and Procedures

A single-cylinder research engine equipped with a prototype fuelling system was used to investigate the effects of gaseous fuel composition on a pilot-ignited, directly injected natural gas engine. The engine used is a Cummins ISX series modified for single cylinder operation (Table 1); the experimental facility has been described in detail previously [31,32]. The diesel and natural gas injection processes are controlled electronically using a single multi-fuel injector. The engine is also equipped with a custom air-exchange system to ensure that the charge conditions are independent of variations in fuel composition and injection timing. A cooled high-pressure EGR loop controls intake charge dilution.

Table 1: Engine and Injector Specifications

Engine	Cummins single cylinder 4-stroke, 4-valve
Fuelling	Direct injection; diesel pilot, gaseous main fuel
Displacement (/cylinder)	2.5 L
Compression Ratio	17:1
Bore/Stroke/Connecting Rod Length	137/169/261 mm
Injector	Westport Innovations Inc. dual-fuel concentric needle
<i>Injection control</i>	Separate diesel and NG solenoids
<i>Injector holes</i>	7 pilot, 9 gas
<i>Injection angle</i>	18° below fire deck

The engine facility is fully instrumented, with measurements of air and fuel flow (both diesel pilot and natural gas) as well as exhaust gas composition. The gaseous fuel flow measurement uses a coriolis-force mass flow sensor, and hence is insensitive to changes in gaseous fuel composition. The combustion

process is monitored using a high-speed water-cooled in-cylinder pressure transducer in conjunction with a $\frac{1}{2}^\circ$ crank-angle encoder to identify the piston location. The net heat-release rate (HRR) can be calculated from this information [33]:

$$\frac{dQ_{net}}{d\theta} = \frac{\gamma}{\gamma-1} p \frac{dV}{d\theta} + \frac{1}{\gamma-1} V \frac{dp}{d\theta}, \quad (1)$$

where θ is the crank angle (CA), p is the in-cylinder pressure at a given crank angle, V is the cylinder volume at that point and γ is the specific heat ratio (c_p/c_v – assumed constant). The net heat release rate (HRR) represents the rate of energy release from the combustion processes less wall heat transfer and crevice flow losses. The start-of-combustion for the gaseous fuel and the peak combustion intensity are identified from the HRR. Integrating the HRR as a function of CA (integrated heat release, IHR) provides a representation of the total energy released up to a specified CA. The mid-point of the energy release (50% IHR) is used to represent combustion timing, while the time between the 10% IHR and 90% IHR points is used to represent the duration of the gaseous fuel combustion. These parameters are based on the average heat-release rate from 50 consecutive cycles.

Exhaust emissions equipment includes a raw exhaust emissions bench equipped with NO_x, O₂, CO, CO₂, total HC and CH₄ analyzers. A separate CO₂ analyzer measures the intake CO₂ concentration; when combined with the exhaust CO₂ measurement, the EGR fraction can be determined. PM emissions are measured using a custom built micro-dilution system, where the raw sample is diluted with clean dry air at a volume ratio of 15:1. Total mass is measured with a tapered element oscillating microbalance (TEOM). The TEOM results were validated with gravimetric filter mass measurements (probability of association using chi-squared analysis > 99.9%). The black carbon (BC) concentration is measured using an AethalometerTM (Magee scientific) where PM is collected on a quartz filter; the attenuation of monochromatic light shone through the filter indicates the BC content of the collected PM. More information on the experimental apparatus and the emissions measurement equipment is available elsewhere [32].

3.1 Fuels

The additives to natural gas investigated in this work were propane, ethane, hydrogen and nitrogen; pure methane was also used as a comparison to the natural gas. The nitrogen, ethane and propane fuel blends were prepared using bottled gas (purity >99.9%) combined with commercially-distributed natural gas in large-volume storage tanks. The blends were left in the storage tanks for at least 48 hours to ensure that they were fully mixed before being supplied to the high-pressure gas compression system for supply to the engine. To avoid condensation of the heavy hydrocarbons, all concentrations were kept below the saturation partial pressure at all times. Random samples of the fuels were taken from the supply line to the

engine during the testing with each fuel, and the results were analyzed by gas chromatography. The Hydrogen blends and pure methane were supplied as bottled gases with compositions certified by the supplier (Praxair Inc.). The principal constituents of the fuels used in these tests are shown in Table 2. All other measured constituents (including butane, pentane, hexane, and heptane) were < 0.1%.

Table 2: Fuel Compositions (molar percentage)

	Natural Gas	Low N ₂	High N ₂	Low ethane	High ethane	Low propane	High propane	Low H ₂	High H ₂	CH ₄
N ₂	1.47	18.89	38.88	1.09	1.19	2.02	2.82	0.34	0.0	0.0
H ₂	0	0.0	0.0	0.0	0.0	0.0	0.0	14.7	35.1	0.0
CH ₄	96.6	78.2	59.4	91.43	89.39	93.5	91.3	84.0	64.9	100
CO ₂	0.44	0.28	0.24	0.40	0.34	0.41	0.38	0.05	0.0	0.0
C ₂ H ₆	1.41	2.31	1.17	6.60	8.62	1.59	1.5	0.75	0.0	0.0
C ₃ H ₈	0.32	0.25	0.22	0.32	0.28	2.23	3.73	0.19	0.0	0.0
MW [†] (kg/kmol)	16.7	18.83	21.04	17.37	17.63	17.34	17.85	14.14	11.09	16.04
LHV [‡] (MJ/kg)	48.1	35.5	23.8	48.3	48.2	47.5	46.9	51.2	54.4	50.0
T _{adiabatic} ^{**} (K)	2485	2440	2400	2530	2550	2495	2510	2500	2520	2485
H:C ratio	3.94	3.93	3.94	3.88	3.86	3.91	3.88	4.32	4.61	4.00
MN ^{††}	103	103	116	85	80	86	82	85	64	100
Wobbe ^{‡‡}	44.6	34.9	24.7	45.6	45.9	44.8	44.8	43.7	41.3	45.5
C _p /C _v	1.308	1.314	1.337	1.299	1.296	1.301	1.296	1.32	1.338	1.311

* assessment conducted by Praxair Inc. All other compositions determined by gas chromatography.

† molecular weight (MW)

‡ lower heating value (LHV) of gaseous fuel

** adiabatic flame temperature calculated for a stoichiometric mixture

†† methane number (MN), calculated based on measured composition, representative of knocking tendency [34]

‡‡ Wobbe index (MJ/m³), HHV / $\sqrt{\text{specific gravity}}$ [14]

Table 2 also provides key characteristics (calculated based on the fuel composition) of the blended fuels. These include the molecular weight (MW), lower heating value (LHV), hydrogen to carbon (H:C) ratio, and the adiabatic flame temperature. The flame temperature is calculated based on a stoichiometric mixture: one of the confounding effects of varying the fuel composition is that it can influence both the adiabatic flame temperature and the mixture fraction in the reaction zone of a non-premixed combustion event.

3.2 Experimental Conditions

A mid-load operating condition (shown in Table 3), representative of mid-load steady-state cruising for a heavy-duty engine, was selected to compare the effects of the various fuels. An EGR level of 30% was used to achieve relatively low NO_x emissions without degrading the combustion event.

Table 3: Engine operating conditions

Speed (RPM)	1200
Gross Indicated Power (kW) [% load]	35 [75%]
Gross Ind. Mean Effective Pressure (bar)	13.5
Gaseous Fuel Pressure (MPa)	21
EGR (mass %)	30
Intake Oxygen Mass Fraction	0.19
Combustion Timings (50% IHR)	0,5,10,15°ATDC

Varying the combustion timing relative to the engine crank angle (based on the mid-point of the combustion – 50% IHR) provides a range of combustion conditions while maintaining constant charge composition and overall equivalence ratio. For this work, the combustion timing was controlled by varying the timing of the start of the pilot fuel injection process. The timing of the gas start-of-injection (GSOI) was fixed at 1.0 ms after the end of the diesel injection. The 50% IHR was used as the control variable representing the combustion timing; the start-of-injection timing was adjusted for the different fuel blends to maintain the 50%IHR at the specified value. For all timings, the engine’s power output was held constant by varying the mass flow-rate of the gaseous fuel. The pilot quantity was fixed at 5% of the total fuel on an energy basis; this amounted to approximately 6 mg diesel / cycle for all the conditions tested. The pilot diesel and gaseous fuel rail pressures were constant at 21 MPa for all the tests.

3.3 Experimental Methodology

Due to the time and cost involved in preparing the individual fuel blends, the tests could not be fully randomized. As a result, the experiments were conducted as blocks, with each fuel blend representing a specific block. The order of testing of the various fuel additives was randomized. For the ethane, propane, and nitrogen tests, sufficient fuel was prepared in advance to conduct at least 3 replications of each test condition. The presented results represent an average of these values. Natural gas tests were conducted at the beginning, middle, and end of the test plan: at least six test points per operating condition were collected. Experimental uncertainty, Table 4, for each fuel parameter is estimated based on the standard deviation of the data collected at each test point; as such, it includes errors due to variability in both measurement equipment and in engine operating condition. The larger uncertainty in the PM measurements is a result of the added complexity of the measurement system for these species combined with greater inter-test variability in emissions levels.

Table 4: Average experimental variability

GID	± 4%
GISFC	± 1%
Maximum HRR	± 4%
Burn Duration	± 2%
CO	± 9%
NO _x	± 6%
HC	± 4%
PM (total mass)	± 15%
PM (black carbon)	± 20%

Due to the cost of supplying bottled hydrogen/methane blends and pure methane, it was only possible to conduct a single test at each test point. A replication of the intermediate timing point (50% IHR at 10° ATDC) was also conducted for all cases, to ensure repeatability of the results.

4. Results

To aid comparison and interpretation, the emissions and performance results for each of the fuels tested are presented relative to the equivalent baseline natural gas condition. That is, the values presented are the results for one fuel at a specific timing, divided by the average value with natural gas fuelling at the same timing ($\text{Relative Result}_{\text{fuel } x, \text{ timing } y} = \text{Measured}_{\text{fuel } x, \text{ timing } y} / \text{Measured}_{\text{NG}, \text{ timing } y}$). These results are then presented in bar-charts, subdivided by fuel blend. For each fuel, four bars representing the four combustion timings are presented. Further details and interpretation of the hydrogen and nitrogen results are available elsewhere ([30] and [21], respectively).

4.1 Combustion Process

Varying the fuel composition has a significant influence on the combustion event. These influences are summarized in Figure 1, where the gaseous-fuel ignition delay (GID), maximum heat release rate, fuel consumption and burn duration are presented. The GID is the time from the actual start-of-injection of the gaseous fuel to the first clear indication of gaseous fuel combustion. The injector mechanical delay, which has been measured at 0.75 ms independent of fuel composition or cylinder pressure, is not included in this delay. The start of combustion is identified from the heat release rate as the inflection point where rapid heat release starts to occur after the pilot fuel has ignited. As such, it is likely not the same as the first appearance of a flame kernel on the gaseous jet: however, it does provide a reliable indication of the commencement of the main gaseous fuel combustion event.

Figure 1 indicates that, compared to natural gas fuelling, the GID is reduced by all the fuel additives; the only increase is with pure methane. Hydrogen addition to the fuel results in an increase in ignitability for the gaseous fuel, and a corresponding reduction in ignition delay [30]. The effects of ethane and propane are similar to those of hydrogen; the fuel is more ignitable, leading to reduced ignition delays; this agrees with previous work on homogeneous charge engines [7,16]. The absence of these species in the pure methane case leads to the observed increase in GID. Nitrogen addition tends to increase the momentum of the gaseous jet, reducing its ignition delay by changes in mixing and spatial location [21]. This view is corroborated by the correlation between methane number (MN) and GID, where a 1% change in MN leads to a 0.75% change in GID (both relative to natural gas fuelling for a given timing) for all the fuels excluding N_2 . When N_2 is included, there is no consistent relationship between MN and GID.* It is interesting to note that despite significantly changing the in-cylinder conditions encountered during the ignition event, the effects of fuel composition were relatively consistent across all combustion timings.

* The plots of correlations are available as 'extra information' from the journal web-site.

The maximum HRR (also shown in Figure 1) follows equivalent trends to the GID. There is a linear relationship between these two parameters, where a change of 1% in GID results in an equivalent (1%) change in maximum HRR (correlation coefficient 0.83, see Figure A2); only the high-N₂ case differs significantly from this correlation, due to the significant reduction in the heating value of the fuel. This relationship is a result of the maximum HRR being reached during the early, premixed, phase of the combustion event. A shorter ignition delay will tend to result in less fuel having premixed, and as a result less is available to burn in the premixed combustion, reducing the peak HRR. These effects are clearly seen in Figure 2, which represents the HRR at a selected intermediate timing (50% IHR at 10°ATDC) for the 'high' levels of all fuels.

Nitrogen fuelling results in a lower, longer heat release rate, as shown in Figure 2. This suggests that the combustion rate is limited by the rate at which the fuel is being introduced into the combustion chamber. The slower combustion is also demonstrated by the burn duration (represented by the crank-angle time from 10% IHR to 90% IHR) in Figure 1. Using the 10% IHR as the lower bound for the combustion duration ensures that this parameter represents only the gaseous combustion, and avoids the pilot fuel combustion, which only contributed 5% of the total energy. With the hydrocarbon additives, the burn durations are increased compared to natural gas; this is a result of the shorter GID leading to a reduced premixed combustion, and hence a longer non-premixed combustion event. This effect was particularly noticeable at the earliest combustion timings.

The efficiency of the overall combustion process is represented in Figure 1 by the gross indicated specific fuel consumption (GISFC). This parameter represents the mass of fuel, on an energy-equivalent mass of diesel basis, per unit of gross indicated power produced. The various fuel blends have a remarkably small influence on fuel conversion efficiency. This is most likely a result of the combustion timing being adjusted to ensure that the mid-point of the heat-release occurred at the same timing for all fuels. Only the N₂ case shows a significant change in efficiency. Approximately half this improvement is due to the increase in mass of the injected fuel, which will increase the work done during the expansion stroke. Improved late-cycle combustion also contributes to the improved efficiency and reduces unburned hydrocarbon emissions, as shown in Figure 3 [21].

4.2 Gaseous Emissions

Varying the fuel composition has a significant impact on emissions, as shown in Figure 3. The increase in adiabatic flame temperature with the addition of ethane, propane, or hydrogen to the fuel (as shown in Table 2) results in higher NO_x emissions, as these are generated predominantly through the strongly temperature-dependent thermal NO mechanism [35]. The current results support this, with a 1%

change in T_{ad} resulting in a 5% change in NO_x emissions. The calculated adiabatic flame temperature is not the only factor influencing NO_x emissions; changes in the fuel composition may also influence the mixture fraction at which reactions occur. This affects the reaction zone temperature, the temperature of the post-reaction gases and the time before these gases mix with cooler charge, all of which strongly influence NO_x emission levels. As a result, the changes in NO_x emissions depend strongly on combustion timing, with (in general) smaller increases in NO_x with more advanced timings.

All the fuel additives reduce hydrocarbon emissions. These emissions are predominantly unburned methane (total HC and CH_4 emissions were experimentally indistinguishable). The mechanisms for the reduction in HC emissions are thought to vary for the different fuel additives. For H_2 , higher radical concentrations and a wider flammability range result in more complete consumption of the fuel [30]. Conversely, the N_2 addition results in improved late-cycle mixing, helping to consume more of the fuel not reacted in the initial combustion event [21]. The fact that the reductions in HC emissions with the ethane and propane are largest at the latest combustion timings suggests that these fuels may be helping to delay the onset of bulk quenching. Bulk quenching occurs as the in-cylinder temperature and pressure fall during the expansion stroke. If the combustion is late, then more of the fuel will not have reacted prior to the reactions being extinguished by this fall in temperature. The shorter ignition delay time could also result in less gaseous fuel having mixed beyond a combustible range prior to ignition occurring, reducing emissions. However, as the reduction in GID was relatively consistent across all timings, it is likely that this reduction in over-mixing is having a smaller effect than the reduced bulk quenching effect. Identifying the principal sources of unburned hydrocarbon emissions is an area of ongoing research.

CO is another combustion by-product that is sensitive to fuel composition, as shown in Figure 3. The fact that the effect of fuel composition on CO emissions is very different from that on HC emissions suggests that there are different formation routes for these harmful products. This agrees with the interpretation that the HC emissions are primarily unreacted fuel, while the CO is a by-product of partial combustion. At early combustion timings, CO emissions are increased, while at late timings, they are reduced for virtually all the fuel blends. For N_2 dilution, the increase in CO is thought to be a result of interaction between the gaseous jet (which will have higher momentum, and hence greater penetration, due to the larger mass of fuel injected) and the piston bowl [21]. For the heavy hydrocarbon additives, it is likely an effect of changes to the reaction zone chemistry; however, the specific nature of these effects is unclear. The reduction in CO emissions at the latest timing is consistent with the delay in the onset of bulk quenching, as discussed above, due either to improved mixing (N_2) or to increased reaction zone radical

concentrations (ethane, propane, H₂). The potential importance of this latter effect is reinforced by the increase in CO when the engine was fueled with pure methane.

4.3 Particulate Matter Emissions

The effect of fuel composition on the total particulate matter mass is shown in Figure 3. Carbon isotope tracer studies have demonstrated that the bulk of the PM formed under these conditions originates from the gaseous fuel [6]. The influence of fuel composition varies strongly with combustion timing. With N₂ dilution, the increase at early timings has been attributed to reaction zone impingement, while the relatively small reduction at late timings is a result of the emissions being primarily volatiles [21]. The consistent reductions with hydrogen addition have been attributed to increased reactive radical concentrations reducing the initial formation of PM and enhancing post-formation oxidation [30]. The increase in PM with ethane and propane is most likely a result of enhanced PM precursor formation in the reaction zone. Species such as C₂H₂ and C₂H₅, which are key participants in the formation of carbonaceous PM, are important intermediates in the chemical reaction path for natural gas with ethane or propane additives [9]. The fact that the increases in PM emissions are smaller at the earliest timing may be a result of the greater time for oxidation to occur during the expansion stroke, after the end of the main combustion. Interestingly, the changes in the PM emissions trend with changes in specific heat ratio (C_p/C_v) of the fuel, with a 1% change in specific heat ratio resulting in a 50% change in PM (see Figure A3). It is at this point unclear why PM trends with specific heat ratio; it is unlikely that this correlation would hold with oxygenated fuels or different diluents (such as CO₂).

The increase in PM with ethane and propane is primarily due to increased black carbon (BC) emissions. The relative increase in these emissions is shown in Figure 4, along with the relative contribution of the BC to the total PM mass. As the latter figure shows, the fraction of the total PM formed of BC does not differ significantly with ethane or propane additives. As total PM mass increases with the heavier hydrocarbons, this result indicates that ethane and propane are increasing both BC and volatile PM mass emissions. High levels of both N₂ and H₂ virtually eliminate the BC emissions, although the total PM emissions are non-zero; the balance of the emissions can be attributed to volatile species (such as condensed lubricating oil or diesel fuel).

5. Implications for Engine Operation

There are various options for accommodating the potential impacts of fuel composition variability on an engine fuelled with directly injected natural gas, as investigated here. The variations in composition do not significantly influence the performance of the engine; as a result, the engine will operate reliably over a wide range of compositions. On the other hand, emissions, especially of PM, are sensitive to composition.

Relatively high levels of ethane and propane in the fuel significantly increase PM emissions. However, the levels tested here are above those normally found in liquefied natural gas (LNG), which is currently the most promising fuel phase for heavy-duty natural gas on-road transportation engines.

Interestingly, the Wobbe index, widely used as a measure of natural gas composition, did not predict the effects of fuel composition on performance or emissions of this combustion system (there was no significant correlation between Wobbe index and any of the parameters presented in this work). However, the specific heat value of the fuel is a useful indicator of PM and BC emissions, while a calculation of the adiabatic flame temperature will give a preliminary estimate of the effects of fuel composition on NO_x.

If the potential concentration of heavy hydrocarbons in the fuel is known, then the engine control system could adjust its operation to offset these PM emissions: methods could include increasing fuel injection pressure [5], adjusting injection timing or varying EGR levels. Ideally, a real-time analysis of fuel composition would provide 'closed-loop' control: however, it is more realistic to expect that the engine management system would be adjusted based on the expected fuel composition in a target market. This arrangement could be combined with a fuel quality requirement to ensure that the engine and fuel met emissions regulations. In locales with serious air-quality concerns, provision of a 'cleaner' fuel would have a direct result of further reducing emissions.

As an alternative, the impacts of heavier hydrocarbons on emissions could be offset by including hydrogen or nitrogen in the fuel. The addition of nitrogen to the fuel generates substantial benefits; however, the high levels tested here would result in too large a reduction in vehicle range to be a practical transportation fuel. There is greater potential for the application of fuel dilution (either with N₂ or another inert species) in stationary power generation, especially if a suitable diluent is readily available. The addition of hydrogen to the fuel significantly improves the combustion process, and has the added benefit of reducing tailpipe CO₂ emissions. If the hydrogen is generated from low-CO₂ sources, then the net GHG emissions from the engine could be reduced [2]. Savings in emissions of both local and global air pollutants through fuel optimization are additional to the reductions already achieved by replacing the bulk of the diesel fuel with natural gas in this engine system.

6. Conclusions

This work investigated the effects of varying the fuel composition in a directly injected natural gas engine at a fixed speed and load condition, by adding ethane, propane, hydrogen or nitrogen to the gaseous fuel. The principal findings from this study are:

- 1) The influences of the range of fuel compositions investigated here on the combustion event itself are relatively small. Reductions in ignition delay at constant combustion phasing lead to lower peak heat release rates. However, these changes are not large enough to significantly impair engine operation. Effects on fuel consumption were minimal, except for a reduction with large amounts of inert diluent in the fuel.
- 2) Enhancing the combustion event, either through improved mixing (N_2) or increased gaseous fuel reactivity (H_2 , ethane, propane) can significantly reduce unburned fuel emissions. These effects are effectively independent of combustion timing.
- 3) Adding ethane or propane to the fuel increases PM total mass, with both BC and volatile emissions increasing. Conversely, the addition of N_2 or H_2 to the fuel virtually eliminates BC emissions. These effects depend significantly on combustion timing.
- 4) In general, variations in NO_x emissions follow changes in adiabatic flame temperature. These effects also vary with injection timing, suggesting that reaction zone stoichiometry and post combustion mixing are also influenced by fuel composition.
- 5) In cases of large divergences in fuel composition from 'average' levels, the effects on pollutant emissions are sufficiently large that it may be necessary to account for fuel quality in the engine management system. Offsetting the presence of heavy hydrocarbons with hydrogen could significantly reduce emissions without impairing engine performance.

Acknowledgements

The authors gratefully acknowledge financial and technical support for this research from Westport Power Inc. Financial support was provided by the Natural Sciences and Engineering Research Council of Canada. Particular thanks to H. Jones and R. Parry at the University of British Columbia for their invaluable assistance in conducting the research.

References

- [1] Richards, G.A., M.M. McMillian, R.S. Gemmen, W.A. Rogers and S.R. Cully. Issues for Low-Emission, Fuel-Flexible Power Systems. *Progress in Energy and Combustion Science*. **27**. 2001. 141-169.
- [2] McTaggart-Cowan, G.P., S.R. Munshi, S.N. Rogak, P.G. Hill and W.K. Bushe. Hydrogen-Methane Blend Fuelling of a Heavy-Duty Direct-Injection Engine. *Proceedings of the ASME International Mechanical Engineering Conference and Exposition*, v.6. Article number IMECE2007-41373. 2007. 521-530.
- [3] Harrington, J., S. Munshi, C. Nedelcu, P. Ouellette, J. Thompson and S. Whitfield. Direct Injection of Natural Gas in a Heavy-Duty Diesel Engine. *SAE Technical Paper 2002-01-1630*. 2002.

- [4] McTaggart-Cowan, G.P., C.C.O. Reynolds and W.K. Bushe. Natural Gas Fuelling for Heavy-Duty On-Road Use: Current Trends and Future Direction. *International Journal of Environmental Studies*. **63**(4). 2006. 421-440.
- [5] McTaggart-Cowan, G.P., H.L. Jones, S.N. Rogak, W.K. Bushe, P.G. Hill and S.R. Munshi. The Effects of High Pressure Injection on a Compression Ignition, Direct Injection of Natural Gas Engine. *ASME Journal of Engineering for Gas Turbines and Power*. **129**. 2007. 579-588
- [6] Jones, H.L., G.P. McTaggart-Cowan, S.N. Rogak, W.K. Bushe, S.R. Munshi and B.A. Buchholz. Source Apportionment of Particulate matter from a Direct Injection Pilot-Ignited Natural Gas Fuelled Heavy Duty DI Engine. SAE Technical Paper 2005-01-2149. 2005.
- [7] Khalil, E.B. and G.A. Karim. A Kinetic Investigation of the Role of Changes in the Composition of Natural Gas in Engine Applications. *ASME Journal of Engineering for Gas Turbines and Power*. **124**. 2002. 404-411.
- [8] Hiltner, J., R. Agama, F. Mauss, B. Johansson and M. Christensen. Homogeneous Charge Compression Ignition Operation with Natural Gas: Fuel Composition Implications. *ASME Journal of Engineering for Gas Turbines and Power*. **125**. 2003. 837-844.
- [9] Huang, J. and W.K. Bushe. Experimental and Kinetic Study of Autoignition in Methane/Ethane/Air and Methane/Propane/Air mixtures under Engine-Relevant Conditions. *Combustion and Flame*. **144**. 2006. 74-88.
- [10] El-Sherif, A.S. Effects of Natural Gas Composition on the Nitrogen Oxide, Flame Structure, and Burning Velocity under Laminar Premixed Flame Conditions. *Fuel*. **77**(14). 1998. 1539-1547.
- [11] Caillol, C. T. Delorme, P. Denis, G. Berardi and B. Porterie. A Combustion Model for Analyzing the Effects of Natural Gas Composition on the Operation of a Spark Ignition Engine. SAE Technical Paper 2002-01-2236. 2002.
- [12] Yossefi, D., M.R. Belmont, S.J. Ashcroft and A.J. Maskell. A comparison of the relative effects of fuel composition and ignition energy on the early stages of combustion in a natural gas spark ignition engine using simulation. *Proc. IMechE Part D, Journal of Automobile Engineering*. 214. 2000. 383-394.
- [13] Min, B.H., K.H. Bang, H.Y. Kim, J.T. Chung and S. Park. Effects of Gas Composition on the Performance and Hydrocarbon Emissions for CNG Engines. SAE Technical Paper 981918. 1998.
- [14] Loubar, K., C. Rahmouni, O. Le Corre and M. Tazerout. Combustion Properties Determination of Natural Gas Using Thermal Conductivity and CO₂ Content. SAE Technical Paper 2005-01-3774. 2005.
- [15] Clark, N.N., G.E. Mott, C.M. Atkinson, R.J. deJong, F.J. Atkinson, T. Latvakosky and M.L. Traver. Effect of Fuel Composition on the Operation of a Lean Burn Natural Gas Engine. SAE Technical Paper 952560. 1995.

- [16] Naber, J.D., D.L. Siebers, C.K. Westbrook, J.A. Caton and S. S. DiJulio. Natural Gas Autoignition Under Diesel Conditions: Experiments and Chemical Kinetic Modeling. SAE Technical paper 942034. 1994.
- [17] Sullivan, G.D., J. Huang, T.X. Wang, W. K. Bushe and S.N. Rogak. Emissions Variability in Gaseous Fuel Direct Injection Compression Ignition Combustion. SAE Technical Paper 2005-01-0917. 2005.
- [18] Crookes, R.J. Comparative Bio-Fuel Performance in Internal Combustion Engines. Biomass & Bioenergy. **30**. 2006. pp. 461-468.
- [19] Feese, J.J. and S.R. Turns. Nitric Oxide Emissions from Laminar Diffusion Flames: Effects of Air-Side versus Fuel-Side Diluent Addition. Combustion and Flame. **113**. 1998. 66-78.
- [20] Fotache, C.G., T.G. Kreutz and C.K. Law. Ignition of Counterflowing Methane versus Heater Air under Reduced and Elevated Pressures. Combustion and Flame. **108**. 1997. 442-470.
- [21] McTaggart-Cowan, G.P., S.N. Rogak, P.G. Hill, S.R. Munshi and W.K. Bushe. The effects of fuel dilution in a natural-gas direct-injection engine. Proc. IMechE Part D: J. Automobile Engineering. **222** (D3). 2007. 441-453.
- [22] Larsen, J.F. and J.S. Wallace. Comparison of Emissions and Efficiency of a Turbocharged Lean-Burn Natural Gas and Hythane-Fueled Engine. ASME Journal of Engineering for Gas Turbines and Power, **119**. 1997. 218-226.
- [23] Kido, H., M. Nakahara, J. Hashimoto and D. Barat. Turbulent burning velocities of two-component fuel mixtures of methane, propane, and hydrogen. JSME International Journal, Series B. **45**. 2002. 355-362.
- [24] Gauducheau, J.L., B. Denet and G. Searby A numerical study of lean CH₄/H₂/air premixed flames at high pressure. Combustion Science and Technology. **137**. 1998. 81-99.
- [25] Sierens, R. and E. Rosseel. Variable Composition Hydrogen/Natural Gas Mixtures for increased Engine Efficiency and Decreased Emissions. ASME Journal of Engineering for Gas Turbines and Power. **122**. 2000. 135-140.
- [26] Allenby, S., W-C. Chang, A. Megaritis and M.L. Wyszynski. Hydrogen Enrichment: A Way to Maintain Combustion Stability in a Natural Gas Fuelled Engine with Exhaust Gas Recirculation, the Potential of Fuel Reforming. Proceedings of the Institution of Mechanical Engineers, Part D. **215** 2001. 405-418.
- [27] Karbasi, M. and I. Wierzbza The Effects of Hydrogen Addition on the Stability Limits of Methane Jet Diffusion Flames. Int. J. Hydrogen Energy, **23**(2). 1998. 123-129.
- [28] Naha, S. and S.K. Agarawal. Fuel Effects on NO_x Emissions in Partially Premixed Flames. Combustion and Flame, **139**. 2004. 90-105.
- [29] Choudhuri, A.R. and S.R. Gollahalli. Characteristics of hydrogen-hydrocarbon composite fuel turbulent jet flames. Int. Journal of Hydrogen Energy. **28**. 2003. pp. 445-454.

- [30] McTaggart-Cowan, G.P., S.N. Rogak, S.R. Munshi, P.G. Hill and W.K. Bushe. Combustion in a Heavy-Duty Direct-Injection Engine using Hydrogen-Methane Blend Fuels. *International Journal of Engine Research*. **10**(1). 2009. pp. 1-13.
- [31] McTaggart-Cowan, G.P., W.K. Bushe, P.G. Hill and S.R. Munshi. A Supercharged Heavy-Duty Diesel Single-Cylinder Research Engine for High-Pressure Direct Injection of Natural Gas. *International Journal of Engine Research*. **4**(4). 2004. pp. 315-330.
- [32] McTaggart-Cowan, G.P. Pollutant Formation in a Gaseous-Fuelled, Direct Injection engine. PhD Thesis. The University of British Columbia. 2006.
- [33] Heywood, J.B. *Internal Combustion Engine Fundamentals*. McGraw-Hill. 1988.
- [34] Kubesh, J., S.R. King, W.E. Liss. Effect of Gas Composition on Octane Number of Natural Gas Fuels. SAE Technical Paper 922359. 1992.
- [35] Hill, P.G. and G.P. McTaggart-Cowan Nitrogen Oxide Production in a Diesel Engine Fueled by Natural Gas. SAE Technical Paper 2005-01-1727. 2005.

Figures

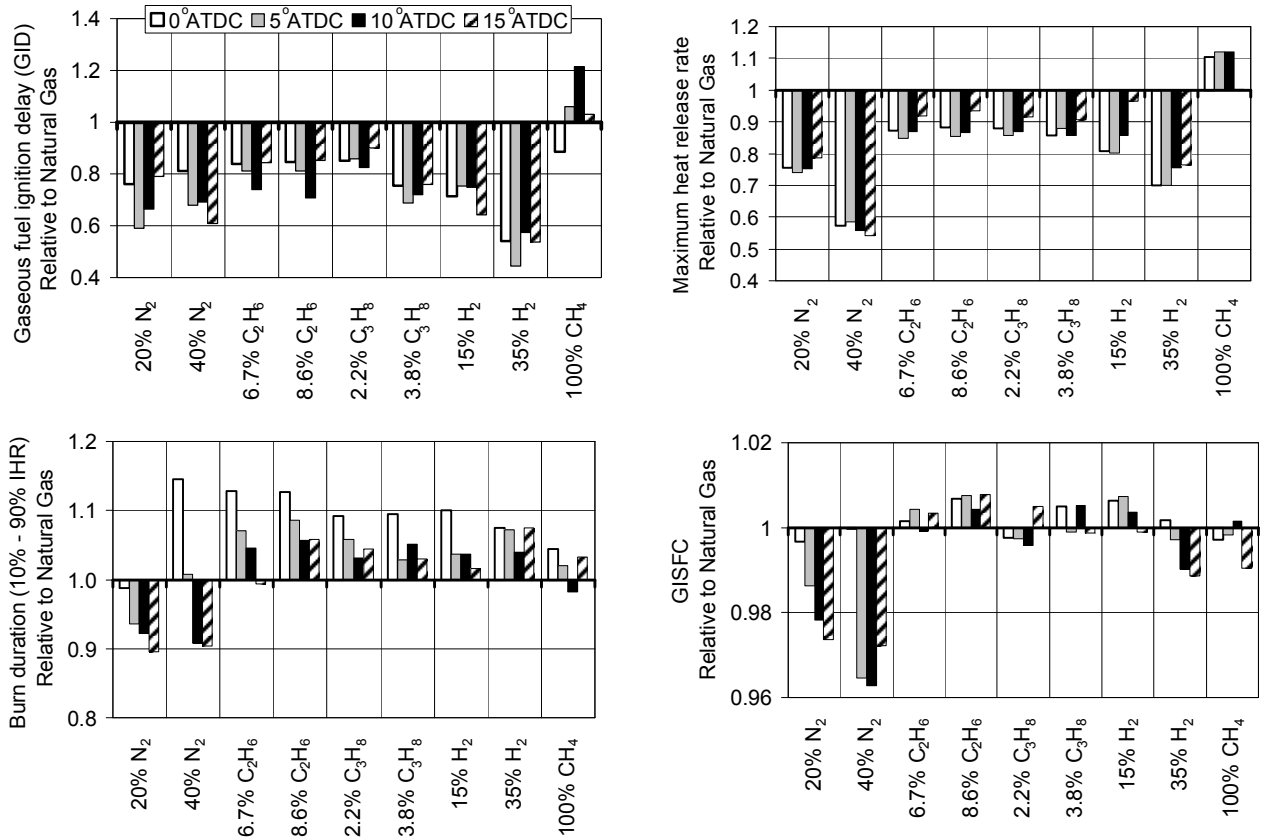


Figure 1: Effect of fuel composition on combustion event, relative to equivalent natural-gas fuelled timing condition. All four timings are shown for each fuel composition (L-R: 50% IHR at 0°, 5°, 10°, and 15°ATDC).

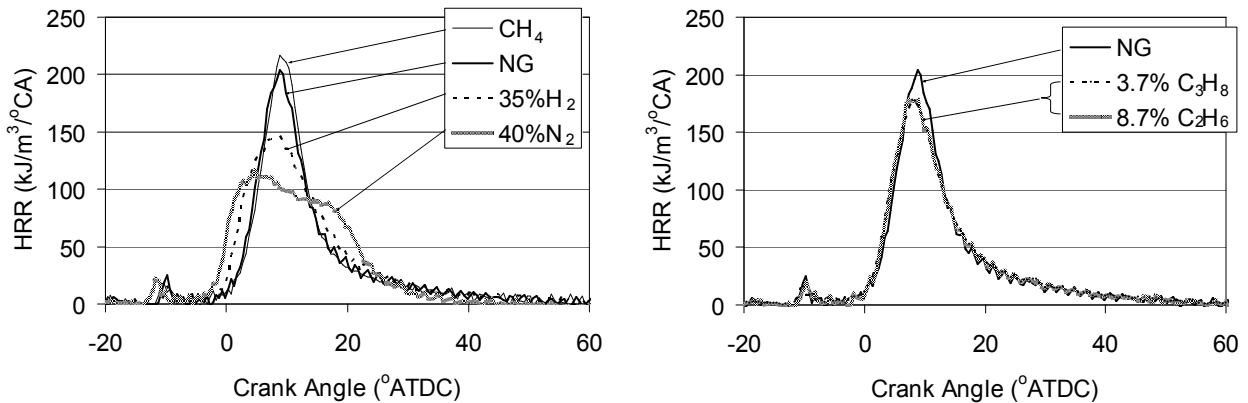


Figure 2: Effect of fuel composition on heat release rate. Timing for 50% IHR at 10°ATDC.

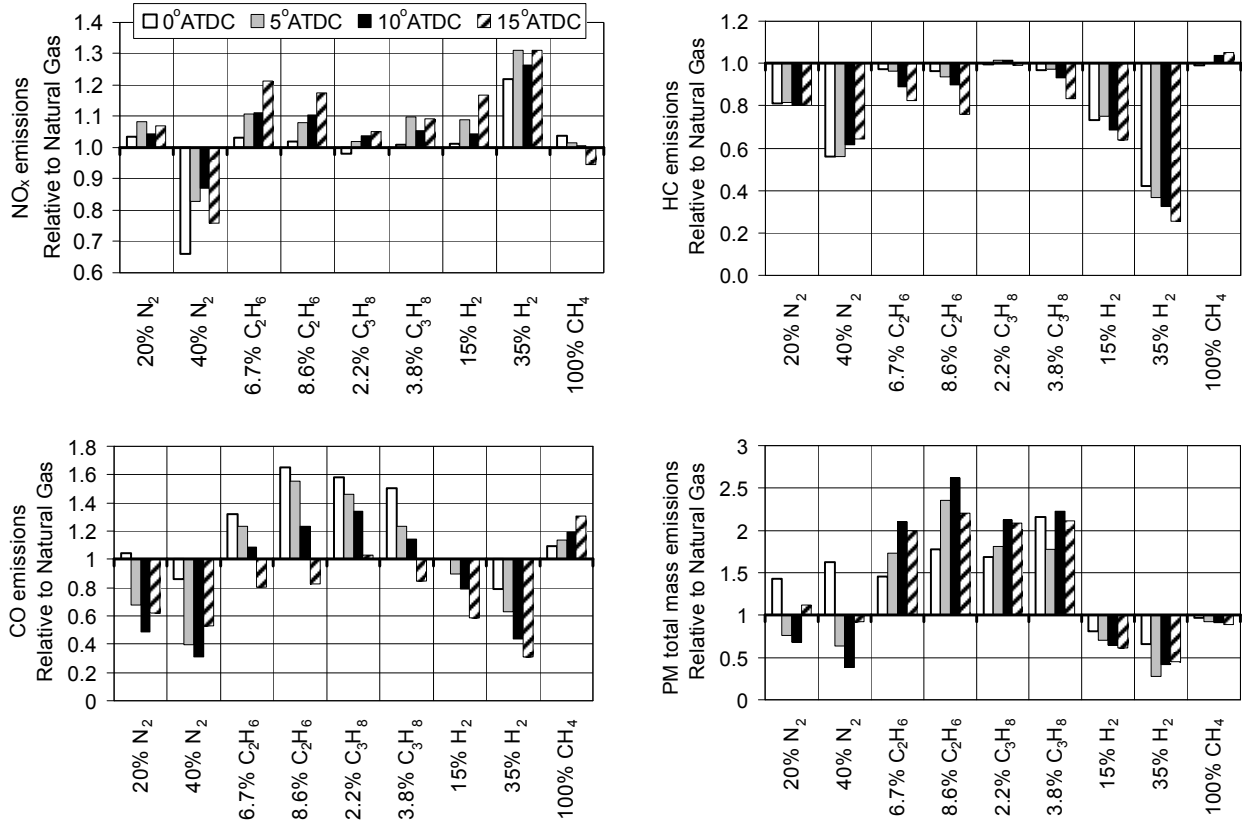


Figure 3: Effect of fuel composition on emissions, relative to equivalent natural-gas fuelled timing condition. All four timings are shown for each fuel composition (L-R: 50% IHR at 0°, 5°, 10°, and 15°ATDC).

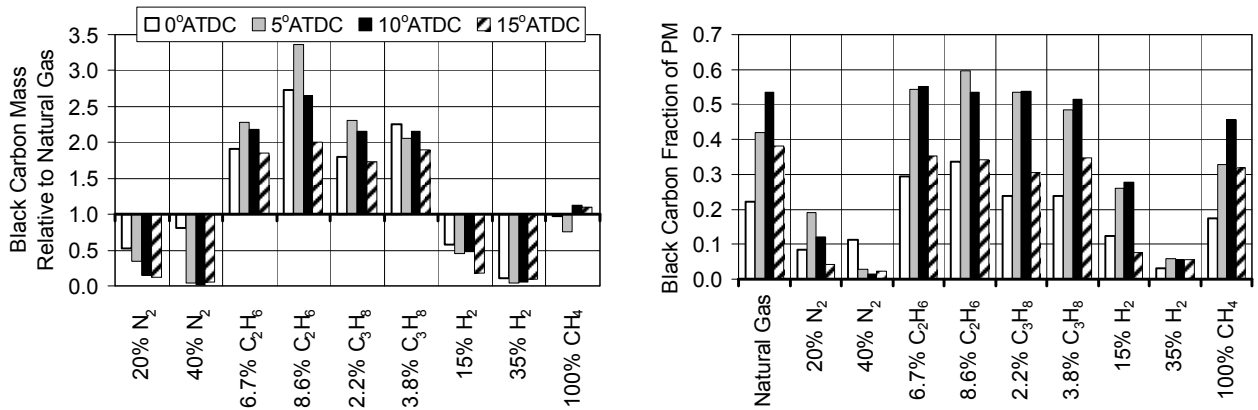


Figure 4: Effect of fuel composition on black carbon (soot) particulate matter emissions. All four timings are shown for each fuel composition (L-R: 50% IHR at 0°, 5°, 10°, and 15°ATDC).

APPENDIX 1

Extra Information Plots

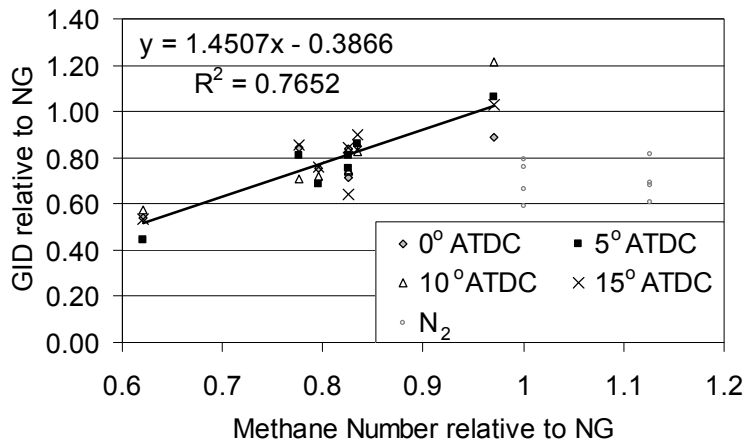


Figure A1: Relationship between GID and fuel methane number (both relative to natural gas). N₂ data points are shown separately, and are excluded from the regression fit.

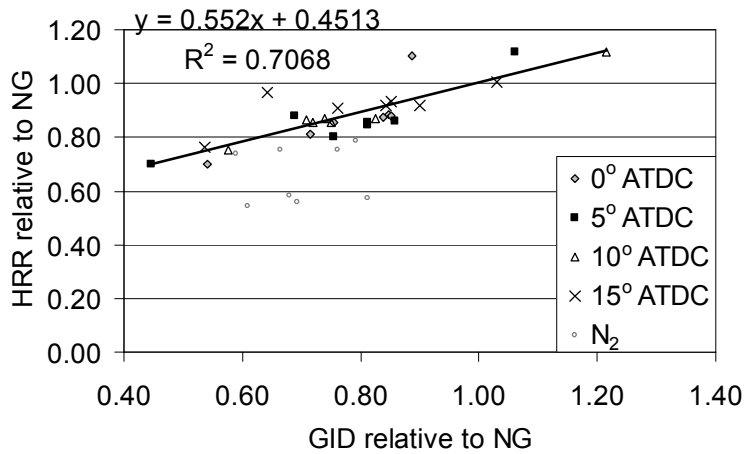


Figure A2: Relationship between change in HRR and change in GID. N₂ data points are shown separately, and are excluded from the regression fit through the remaining data.

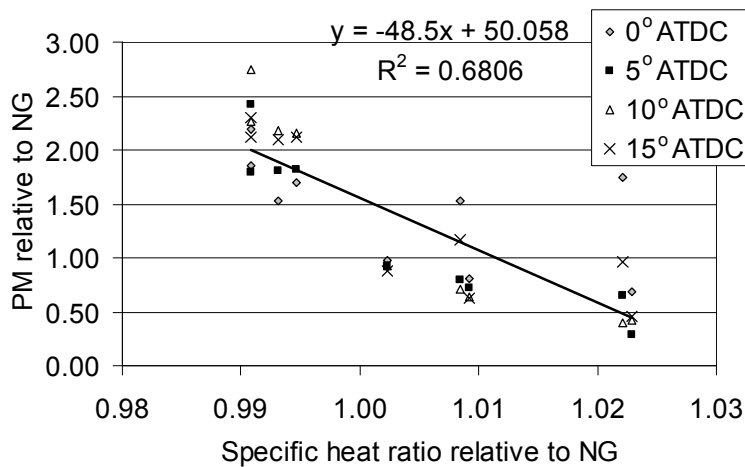


Figure A3: Relationship between PM and fuel specific heat ratio, both relative to natural gas. All data points included in regression.