

# INVESTIGATION OF THE EFFECT OF ADDITIVES TO NATURAL GAS ON HEAVY-DUTY SI ENGINE COMBUSTION CHARACTERISTICS

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# 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. Natural gas is injected in ports and mixes with air before entering the cylinder. For the ignition source, both a spark plug and diesel pilot, which is injected before the top-dead center in the cylinder, are used. The effect of additives such as hydrogen, ethane and nitrogen on the output power and efficiency of the engine and emission levels are examined. 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. Adding ethane and H<sub>2</sub> to the fuel increases the in-cylinder pressure and NOx emissions are increased by ethane, but are virtually eliminated by including nitrogen or hydrogen in the fuel. The results show the higher flame speed of ethane compared to hydrogen, and hydrogen compared to methane. Thus, to reach the MBT condition, the spark time of ethane is the most retarded one and for methane it is the most advanced.

*Keywords*: Natural gas composition; additives; heavy SI engine; combustion characteristics.

# INTRODUCTION

Natural gas is a potential alternative to conventional liquid fuels to use in regular internal combustion engines. The main part of natural gas is methane, but it also contains heavier hydrocarbons and inactive gases. 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 (Richards, McMillian, Gemmen, Rogers, & Cully, 2001). Natural-gas fueling can reduce greenhouse gas (GHG) emissions compared to diesel; adding hydrogen to the natural gas offers even further GHG reductions from transportation applications (McTaggart-Cowan et al., 2007a). 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 spark ignition gas engine (Mat Yasin, Mamat, Sharma, &

Yusop, 2012). One technology for natural-gas fueling 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 (Ghobadian, Najafi, & Nayebi, 2013; Harrington et al., 2002; Sundar Raj & Sendilvelan, 2010). A small amount of diesel fuel is injected late in the compression stroke, prior to the natural-gas injection. The auto-ignition and combustion of this pilot fuel provide the ignition source for the gaseous fuel; the latter then burns in a predominantly non-premixed combustion event(Aziz, Firmansyah, & Shahzad, 2010; Kapilan, Ashok Babu, & Reddy, 2010). Compared to diesel fueling, the main fuel's lower carbon reduces carbon dioxide (CO<sub>2</sub>) emissions; its lower adiabatic flame temperature reduces oxides of nitrogen (NOx) emissions; and its lower soot 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 fueling technologies (McTaggart-Cowan, Reynolds, & Bushe, 2006). Using exhaust gas recirculation (EGR) can achieve substantial further reductions in NOx emissions; however, a lack of oxidizer at high levels of EGR degrades the combustion and increases the emissions of unburned hydrocarbons (Yossefi, Belmont, Ashcroft, & Maskell), carbon monoxide (CO), and PM (McTaggart-Cowan, Munshi, Rogak, Hill, & Bushe, 2007b). At the EGR levels required to achieve low NOx levels, more than 90% of the PM originates from the natural gas (Jones et al., 2005; Mohanamurugan & Sendilvelan, 2011). Natural gas is a mixture of various hydrocarbon molecules. Commercial-grade natural-gas compositions vary from 70% to 95% CH<sub>4</sub>, with the balance composed of heavier hydrocarbons (primarily ethane, C<sub>2</sub>H<sub>6</sub>, and propane, C<sub>3</sub>H<sub>8</sub>), as well as diluents such as molecular nitrogen  $(N_2)$  and  $CO_2$ . There are also trace levels of sulfur compounds, often added as odorants, and other hydrocarbon species. 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, HO<sub>2</sub> and H<sub>2</sub>O<sub>2</sub> radicals enhance the natural-gas ignition process (Hiltner, Agama, Mauss, Johansson, & Christensen, 2003; Khalil & Karim, 2002); at temperatures below 1200 K, it is the methyl peroxy (CH<sub>3</sub>O<sub>2</sub>H) radical that fills this role (Huang & Bushe, 2006). The heavier hydrocarbons also promote the formation of hydrocarbon radicals, including C<sub>2</sub> species such as the ethyl radical (C<sub>2</sub>H<sub>5</sub>) and acetylene  $(C_2H_2)$  (Huang & Bushe, 2006). Ethane and propane also influence the combustion event and pollutant emissions. Enhanced radical formation extends the lean combustion limit (Caillo, Delorme, Denis, Berardi, & Porterie, 2002; El-Sherif, 1998). In premixed-charge spark-ignition engines, ethane addition increases the flame propagation rate (Rahim, Mamat, Taib, & Abdullah, 2012; Yossefi et al., 2000). 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 (Bhaskar, Nagarajan, & Sampath, 2010; Min, Bang, Kim, Chung, & Park, 1998), although these results are not consistent across all reported studies. Fuel quality sensors (Loubar, Rahmouni, Le Corre, & Tazerout, 2005) and closed-loop control engines (Clark et al., 1995) 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 nonpremixed natural-gas combustion. At temperatures >1400 K, fuel additives have little effect as this process is mixing limited (Naber, Siebers, Westbrook, Caton, & DiJulio, 1994). At lower temperatures, the addition of either ethane or propane is found to reduce ignition delay times by as much as 0.7 ms (Naber et al., 1994). 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 of increased NOx emissions with ethane addition to the fuel (Sullivan, Huang, Wang, Bushe, & Rogak, 2005); however, substantially more work is required to understand the effects of the heavier hydrocarbons on the ignition and pollutant formation mechanisms of a naturalgas engine using a non-premixed direct-injection combustion system. 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<sub>2</sub> are unlikely to significantly influence the combustion event (Crookes, 2006; Kalvani Radha, Naga Sarada, Rajagopal, & Nagesh, 2011). However, higher dilution levels may have a greater impact; these influences have been studied in various combustion systems. For a natural gas fueled, premixed-charge engine, adding N<sub>2</sub> to the fuel reduces NOx emissions but impairs efficiency (Crookes, 2006). In a low pressure non-premixed combustion system (an industrial boiler), gaseous-fuel dilution reduces NOx emissions more effectively than does oxidizer dilution; fundamental studies attribute this to more rapid quenching of the NO-forming reactions (Feese & Turns, 1998). In laminar counter-flow diffusion flame studies, N<sub>2</sub> dilution is used to reduce fuel concentrations; no significant effects are observed until the fuel stream contains more than 80% N<sub>2</sub> (by volume) (Fotache, Kreutz, & Law, 1997). 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<sub>2</sub> concentrations. The effects of N<sub>2</sub> addition on a heavy-duty engine fueled with directly injected natural gas have been studied previously (Kamil, Rahman, & Bakar, 2011; McTaggart-Cowan, Rogak, Hill, Munshi, & Bushe, 2007c).

#### **HYDROGEN ADDITION**

The most important effect of blending natural gas and hydrogen for use in homogeneous-charge, spark-ignition engines is extension of the lean combustion limit (Larsen & Wallace, 1997). Combustion bomb studies demonstrate that hydrogen's enhanced diffusivity results in a higher turbulent flame propagation rate for lean mixtures (Kido, Nakahara, Hashimot, & Barat, 2002). The hydrogen also increases the flame's resistance to stretch (Gauducheau, Denet, & Searby, 1998), reducing local extinction events. At a constant air-fuel ratio, NOx emissions are increased due to a higher adiabatic flame temperature while CO and HC emissions are reduced (Sierens & Rosseel, 2000). Flame stability in the presence of EGR is also improved (Allenby, Chang, Megaritis, & Wyszynski, 2001). For non-premixed combustion of hydrogen/methane blends in a co-flowing jet diffusion flame, non-premixed flame stability is enhanced with increasing hydrogen content (Karbasi & Wierzba, 1998). 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 (Choudhuri & Gollahalli, 2003; Naha & Agarawal, 2004). 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 byproducts including CO, HC, and PM, while higher temperatures increase NOx emissions (McTaggart-Cowan, Rogak, Munshi, Hill, & Bushe, 2009).

#### **COMBUSTION MODEL**

The Eddy-Dissipation-Concept (EDC) model was chosen to predict the combustion process. The EDC model is an extension of the eddy-dissipation model to include detailed chemical mechanisms in turbulent flows. It assumes that reaction occurs in small turbulent structures, called the fine scales. The length fraction of the fine scales is modeled as:

$$\xi^* = C_{\xi} \left(\frac{\nu\epsilon}{k^2}\right)^{3/4} \tag{.1}$$

where \* denotes fine-scale quantities,  $C_{\xi}$  is a volume fraction constant and v is kinematic viscosity. The volume fraction of the fine scales is calculated as  $\xi^{*3}$ . Species are assumed to react in the fine structures over a time scale as:

$$\tau^* = C_\tau \left(\frac{\nu}{\epsilon}\right)^{1/2} \tag{2}$$

where  $C_{\tau}$  is a time scale constant. Combustion at the fine scales is assumed to occur as a constant pressure reactor, with initial conditions taken as the current species and temperature in the cell.

### **RESULTS AND DISCUSSION**

The investigated engine is a v-type 12-cylinder, heavy-duty engine. It was modified from a diesel engine by replacing the fuel injector with a spark plug and reshaping the piston head to reduce the compression ratio. The engine specifications are presented in Table 1, and Figure 1 shows the computational domain which was used for calculations.



Figure 1. Computational domain

In Figure 2, the numerical and experimental results (Ma et al., 2007) for cylinder pressure are compared. The simulation model is validated by comparing the predicted cylinder pressure and experimental cylinder pressure under the condition of full load, 1200 r/min for fuel blends of 30% hydrogen fractions. As shown in Figure 2, the predicted results of the numerical model have acceptable agreement with the experimental results.

	Parameter	Value
	Engine type	12-cylinder, spark ignition
	Displacement volume	(L) 38.151
	Compression ratio	10.5
	Bore (mm)	150
	Stroke (mm)	180
	Intake valve timing	IVO: 77° BTDC
	C	IVC: 46° ABDC
	Exhaust valve timing	EVO: 77° BBDC
	C	EVC: 75° ATDC
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Figure 2. In-cylinder pressure, predicted and experimental (Ma et al., 2007)

Crank Angle (Degree)

In Figure 3, it is obvious that the spark time has a significant effect on the maximum pressure. As can be seen from the figure, when the spark time for the mixture blend of 30% ethane and 70% methane is at 330 deg, the peak pressure will be around 92 bar. As the spark is retarded about 10 and 8 degrees, the peak pressure, as expected, will reduce by about 6 bar in each step respectively. Also, it can be seen that the spark time is adjusted to take place in a crank angle to cause the maximum pressure occurring at 370 deg with different blends to have approximately the same peak pressure. Varying the fuel composition has a significant impact on emissions. The increase in adiabatic flame temperature with the addition of ethane, propane, or hydrogen to the fuel results in higher NOx emissions, as these are generated predominantly through the strongly temperature-dependent thermal NO mechanism (Hill & McTaggart-Cowan, 2005). 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 NOx emission levels. NOx has a direct relation to temperature and because, in more advanced sparks, peak temperature and pressure are higher, the NOx will therefore also have a higher peak where we have higher temperature.



Figure 3. Effect of fuel composition on in-cylinder pressure.



Figure 4. Effect of fuel composition on NO emission

As can be seen from Figure 4, the effect of the composition and time of the spark is more obvious near the TDC, but near 490 deg, after reducing the temperature, all the different cases shown in the Figure will have approximately the same frozen

mass of NOx. In Figure 5, the effect of fuel dilution by  $N_2$  on NO emission is shown. As shown, by adding the  $N_2$  species to the mixture, the amount of NO emission first increases and then decreases. When  $N_2$  is added to the mixture for dilution, the maximum temperature of combustion, because of lean burn, will be reduced. On the other hand, adding  $N_2$  will give a greater chance of a reaction between  $N_2$  and  $O_2$  to produce NO. As seen in this figure, there is a critical amount for dilution (lambda=1.2), where the excess amount of  $N_2$  overcomes to temperature decrease, which is the result of dilution, and so at this point NO emission is at its highest level.



Figure 5. Effect of fuel dilution with  $N_2$  on NO emission (fuel comp. 30%  $H_2$ + 70%  $CH_4$ )



Figure 6. Effect of fuel composition on CO emission

CO is another combustion by-product that is sensitive to fuel composition, as shown in Figure 6. At early combustion timings, CO emissions are increased, while at

late timings, they are reduced for virtually all the fuel blends. For the heavy hydrocarbon additives, this is probably an effect of changes to the reaction zone chemistry; this means that when heavy hydrocarbon  $(C_2H_6)$  is added to CH<sub>4</sub>, because of more carbon atoms, the amount of CO production will be increased (for the same spark timing). Meanwhile, when retarding the spark timing, the amount of CO will be reduced as a result of the increased combustion delay. The reduction in CO emissions at the latest timing is consistent with the delay in the onset of bulk quenching, due either to improved mixing (N<sub>2</sub>) or to increased reaction zone radical concentrations (ethane, propane, and H<sub>2</sub>). The potential importance of this latter effect is reinforced by the increase in CO when the engine was fueled with pure methane.

### CONCLUSIONS

In this work the effects of varying the fuel composition in a natural-gas heavy-duty engine by adding ethane, propane, hydrogen or nitrogen to the gaseous fuel are investigated. The main findings of this study are:

- i) Adding ethane, propane and  $H_2$  to the fuel increases the in-cylinder pressure and NOx emission. These effects depend mostly on combustion timing.
- ii) There is a critical amount of fuel dilution with  $N_2$  with respect to NOx emission, where the excess of  $N_2$  overcomes to decrease of the adiabatic temperature of the flame up to lambda=1.2.
- iii) The results show the higher flame speed of ethane compared to hydrogen and hydrogen compared to methane. So, if we want to reach the MBT condition, the spark time of ethane is the most retarded and for methane it is the most advanced, with hydrogen lying somewhere between. In this case, the peak pressures will be approximately the same. Neglecting the MBT condition, the more we advance the spark (348 deg, 340 deg, 330 deg), the higher will be the peak pressure (80 bar, 86 bar, 92 bar).

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