An Investigation of Compressed Natural Gas Engine for Nitrogen Oxides Reduction

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Abstract: Problem statement: This study describes the use of Reformer Gas (RG) to alter NO\textsubscript{x} emission in a CNG-fueled HCCI engine. Comparison with diesel, natural gas has a very high octane number (\approx 120) and high auto-ignition temperature (\approx 600°C). Composed mostly of methane, natural gas is the only common fuel to manifest relatively pure, single-stage combustion. Other fuels have stronger low-temperature reaction and the required entropy for main stage combustion can be obtained from the low temperature heat release as a result of compression to moderate pressure and temperature. In deviation, the methane molecule resists destruction by free radicals and produces negligible heat release at low temperature. In consequences, in CNG-fueled HCCI engines the activation energy required for auto-ignition must be obtained by extreme levels of charge heating and compression. This causes inherently to a high rate of heat release. HCCI operation with pure CNG fuel was attained but not really practical due to very high NO\textsubscript{x} production. While HCCI operation is usually described as a low NO\textsubscript{x} technique, the knocking behavior when running with pure CNG raised the peak combustion temperature to a value well above normal combustion and the critical Zeldovich NO\textsubscript{x} production threshold, giving very high indicated NO\textsubscript{x} emissions.

Approach: One approach to improving these properties is to convert part of the base CNG fuel to Reformer Gas (RG). In this study, modified COMET engine was operated in HCCI mode using a mixture of CNG fuel and simulated RG (75% H\textsubscript{2} and 25% CO) can be produced on-board from CNG using low current and non-thermal plasma boosted fuel converter.

Results: This study shows that despite of having various RG mass fractions, $\lambda$ was the dominant factor in reducing NO\textsubscript{x} production and increasing RG mass fraction had only a small effect on increasing NO\textsubscript{x}. This disconnect between the overall equivalence ratio and RG fraction shows that the real benefit of the RG blending was to enable lean (high) operation. Higher $\lambda$ also effectively reduced maximum pressure and maximum pressure rate.

Conclusion: Note that due to the low achievable power levels, the NO\textsubscript{x} emissions continue to be high and further combustion enhancements and more controlled combustion would be needed to make the CNG-fuelled HCCI engine practical.

Key words: Homogeneous charge compression ignition, compressed natural gas, reformer gas, air/fuel ratio, overall equivalence, RG mass, RG fraction, HCCI mode, COMET engine, NO\textsubscript{x} production

INTRODUCTION

The internal combustion engine the vital to the current society. Without the transportation performed by the millions of vehicles on the road and at sea we would not have achieved the living standard of modern life. We have two types of internal combustion engines such as spark ignition engine and compression ignition engine. Both have their merits. The SI engine is a preferably simple product and hence has a lower first cost. This engine type in addition made very clean as the Three-Way Catalyst (TWC) is effective for exhaust after treatment. The problem with the a park ignition engine is the poor part load efficiency due to large losses during gas exchange and low combustion and thermo dynamical efficiency. The compression ignition engine is much more fuel efficient and hence the existing choice in applications where fuel cost is more important than initial cost. The problem with the CI engine is the emissions of nitrogen oxides and particulate matter. The treatment to reduce nitrogen oxides and PM is costly and still not generally available on the market. The natural choice of ideal combination would be to find an engine type with the high efficiency

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of the CI engine and the very low emissions of the spark ignition engine with three-way catalyst. One such new concept is named Homogeneous Charge Compression Ignition (HCCI). Homogeneous Charge Compression Ignition engine is a new concept for future power trains which will provide improved fuel efficiency and lower emissions at the same time. It is based on the concept of compression ignition of fuel-air mixtures due to reaching auto ignition temperature. However, there are two critical problems associated with the HCCI engines: control of the autoignition timing and the combustion rate. There are a number of strategies that have been currently investigated to address the above two critical problems, such as a variable compression ratio (Haraldsson et al., 2002; Sjoberg and Dec. 2003; Diaz and Prasad, 2010; Al-Khairi et al., 2011; Risberg et al., 2006) variable intake temperature or hot exhaust gas recirculation study (Christensen et al., 1999). The exhaust gas injection in the intake port changes the intake temperature thereby giving a good control on the combustion phasing inside the HCCI engine. However, EGR consist of many gases giving a good control on the combustion phasing inside the intake port changes the intake temperature thereby giving a good control on the combustion phasing inside these engines. To achieve this, a clear understanding of the in-cylinder combustion characteristics. Experimental quantification of the in-cylinder nitrogen oxide formation is time consuming and technically challenging.

MATERIALS AND METHODS

The Reformer Gas is a mixture of light gases dominated by Hydrogen and Carbon Monoxide and can be produced from Compressed Natural Gas using low current and non-thermal plasma boosted fuel converter. In the COMET engine, HCCI operation on pure Compressed Natural Gas fuel was achieved but not really practical due to very high Nitrogen Oxide production. While HCCI operation is generally characterized as a low Nitrogen Oxides technique, the marginal knocking behavior when running with pure Compressed Natural Gas raised the peak cylinder temperature to a value well above the critical Zeldovich Nitrogen Oxides production mechanism threshold, giving very high indicated Nitrogen Oxides emissions. HCCI operation with leaner mixtures, enabled by Reformer Gas blending, significantly reduced NOx production. The formation of Nitrogen Monoxide and Nitrogen Dioxide can be divided into thermal route, prompt route, N₂O route and fuel-bound nitrogen route (Warnatz et al., 2006). The major NOx formation route in IC engine combustion is the thermal route (Heywood, 1988). The thermal NO route is the major constituent to the NOx emission and can be described with the following three elementary reactions called as extended Zeldovich mechanism Eq. 1-3:

\[
\begin{align*}
O+N₂&\rightarrow NO+N \quad (1) \\
N + O₂&\rightarrow NO+O \quad (2) \\
N+OH&\rightarrow NO+H \quad (3)
\end{align*}
\]

Reaction 1 has very high activation energy and is the rate limiting step. The triple bond of the Nitrogen molecule is strong, the consequence of this causes the reaction rate is slow unless the temperature is high. When assuming quasi-steady state for N concentration, the rate of NO production may be described as Eq. 4:

\[
\frac{d[NO]}{dt} = 2k_1[O][N_2] 
\]

The NOx production may thus be reduced by reducing the concentration of Oxygen or Nitrogen, or reducing the rate coefficient k₁ by reducing the temperature. The rate coefficient k₁ is considered insignificant at temperatures less than 1700 k (Warnatz et al., 2006).

A common European standard for emission legislations were introduced in 1992 with the EURO 1 standard. Since then, the EURO 2, 3 and 4 has been put into force of implementation with ever more stringent requirements (Warnatz et al., 2006). Table 1 shows the Emission standards for heavy duty diesel and gas engines for the Transient Test Cycle (Heywood, 1988).

In the COMET engine, HCCI operation on pure Compressed Natural Gas fuel was achieved but not really practical due to very high Nitrogen Oxide production.

**Experimental setup:** All experiments were conducted on a modified COMET engine to operate in HCCI mode using CNG fuel. Table 2 summarizes the engine specifications for the current experiment. The Schematic diagram of Experimental setup is as shown in Fig. 1.
Table 1: Emission standards for heavy duty diesel and gas engines (motor vehicles over 3500 kg as maximum laden mass) for the transient test cycle (Heywood, 1988)

| Tier     | Date        | Test | CO   | NMHC | CH₄ | NOₓ | PM |
|----------|-------------|------|------|------|-----|-----|----|
| Euro III | 1999.10 EEVs only | ETC  | 3.00 | 0.40 | 0.65 | 2.0 | 0.02 |
|          | 2000.10     | ETC  | 5.45 | 0.78 | 1.60 | 5.0 | 0.16 |
|          |             |      |      |      |      |     | 0.21 |
| Euro IV  | 2005.10     |      | 4.00 | 0.55 | 1.10 | 3.5 | 0.03 |
| Euro V   | 2008.10     |      | 4.00 | 0.55 | 1.10 | 3.5 | 0.03 |

A: For natural gas engines only, B: Not applicable for gas fueled engines at the year 2000 and 2005 stages, C: For engines of less than 0.75 dm³ swept volume per cylinder and a rated power speed of more than 3000 min⁻¹ (Heywood, 1988)

Table 2: Experimental apparatus and fuels

| Engine make | Comet |
|-------------|-------|
| Engine type | Four stroke single cylinder engine |
| Rated power output | 3.5 kW at a speed of 1500 rpm |
| Bore diameter | 30 mm |
| Stroke length | 110 mm |
| Throttle | Fully open |
| Main fuel | CNG |
| Additive fuel | RG |
| CR | 17 |

RESULTS

Table 3-7 shows the results obtained from experiments for different operating conditions.

DISCUSSION

Effect of mixture strength: $\lambda$: As mentioned already, $\lambda$ represents the total air/fuel ratio considering both the CNG and RG as a combined fuel.

In HCCI combustion, the total chemical energy inside the cylinder plays the major role.

Figure 2 indicates that despite of having various RG mass fractions, $\lambda$ was the dominant factor in reducing NOₓ production and increasing RG mass fraction had only a small effect on increasing NOₓ.
Table 3: Effect of Relative air fuel ratio on is NO\textsubscript{x} at constant RG mass fraction

| Relative air fuel ratio, $\lambda$ | Is NO\textsubscript{x} Emission at RG = 60% in (kg/kW-h) | Is NO\textsubscript{x} Emission at RG = 45% in (kg/kW-h) | Is NO\textsubscript{x} Emission at RG = 38% in (kg/kW-h) | Is NO\textsubscript{x} Emission at RG = 30% in (kg/kW-h) |
|----------------------------------|------------------------------------------------------|------------------------------------------------------|------------------------------------------------------|------------------------------------------------------|
| 2.76211                         | 6.07016                                              | 11.87122                                             | 9.03012                                             | 6.31618                                              |
| 2.85822                         | 3.93113                                              | 6.60121                                              | 4.38215                                              | 2.71671                                              |
| 2.92627                         | 2.45150                                              | 4.29141                                              | 2.35140                                              | 2.30114                                              |
| 3.0418                          | 0.80109                                              | 2.41520                                              | 1.15812                                              | 1.10182                                              |
| 3.1519                          | 0.53132                                              | 0.89016                                              | 0.80016                                              | 0.79016                                              |
| 3.24018                         | 0.21630                                              | 0.52178                                              | 0.50178                                              | 0.42718                                              |
| 3.39514                         | 0.18148                                              | 0.035516                                             | 0.030516                                             | 0.025516                                             |

Table 4: Effect of relative air-fuel ratio of maximum pressure and maximum pressure rate at constant RG mass fractions

\[
\begin{array}{ccc}
\text{Relative air fuel ratio, } \lambda & P_{\text{max}} \text{ at } RG = 45\% & \left(\frac{dp}{d\theta}\right)_{\text{max}} \\
\text{In bar} & \text{In bar} & \text{In bar}
\end{array}
\]

| Relative air fuel ratio, $\lambda$ | $P_{\text{max}}$ at RG = 45% in bar | $\left(\frac{dp}{d\theta}\right)_{\text{max}}$ at RG = 45% in bar | $P_{\text{max}}$ at RG = 30% in bar | $\left(\frac{dp}{d\theta}\right)_{\text{max}}$ at RG = 30% in bar |
|----------------------------------|--------------------------------------|---------------------------------------------------------------|--------------------------------------|---------------------------------------------------------------|
| 2.76211                         | 77.72815                              | 77.952230                                                     | 76.91253                             | 75.42233                                                     |
| 2.85182                         | 77.52110                              | 77.298180                                                     | 73.97526                             | 73.01128                                                     |
| 2.92267                         | 77.53713                              | 75.531730                                                     | 67.40224                             | 69.32167                                                     |
| 3.04298                         | 73.11115                              | 73.101990                                                     | 60.80383                             | 62.62180                                                     |
| 3.1529                          | 70.69422                              | 71.501820                                                     | 53.02418                             | 55.28114                                                     |
| 3.24108                         | 68.56329                              | 70.042254                                                     | 37.20418                             | 39.02114                                                     |
| 3.39514                         | 65.85129                              | 68.662740                                                     | 23.68018                             | 25.42114                                                     |

Table 5: is NO\textsubscript{x} increase with an increasing RG mass fraction of constant relative air fuel ratio

| RG% at $\lambda=2.5$ in (kg/kW-h) | is NO\textsubscript{x} Emission at $\lambda=2.5$ in (kg/kW-h) | is NO\textsubscript{x} Emission at $\lambda=2.6$ in (kg/kW-h) | is NO\textsubscript{x} Emission at $\lambda=2.7$ in (kg/kW-h) | is NO\textsubscript{x} Emission at $\lambda=2.8$ in (kg/kW-h) |
|----------------------------------|------------------------------------------------------|------------------------------------------------------|------------------------------------------------------|------------------------------------------------------|
| 16                               | 7.6887                                               | 30                                                   | 8.58019                                              | 30                                                   |
| 23                               | 11.8026                                              | 38                                                   | 9.11722                                              | 38                                                   |
| 30                               | 16.15721                                             | 41                                                   | 10.38528                                             | 41                                                   |
| 39                               | 15.6622                                              | 45                                                   | 11.95628                                             | 45                                                   |
| 46                               | 19.53233                                             | 52                                                   | 13.40229                                             | 52                                                   |

Higher $\lambda$ effectively reduced the maximum pressure and maximum pressure rate. The input energy in a lean mixture is lower, so a lower combustion temperature, lower maximum pressure ($P_{\text{max}}$) and the lower maximum pressure rate ($\left(\frac{dp}{d\theta}\right)_{\text{max}}$) were expected as shown in Fig. 3. $P_{\text{max}}$ was mostly dominated by $\lambda$ rather than RG mass fractions. At very lean conditions, the influence of RG mass fraction on $P_{\text{max}}$ increased, presumably by ensuring combustion of the most dilute zones in the combustion chamber. $\left(\frac{dp}{d\theta}\right)_{\text{max}}$ is a strong
function of both $\lambda$ and RG mass fraction as indicated in Fig. 3.

**Effect of RG mass fraction:** RG addition was found to be an effective means of expanding the lean boundary of the HCCI operating window. As mentioned earlier, the operating region of CNG for this engine is not a practical operating window. For the knock boundary, a limit of \(\left(\frac{dP}{d\theta}\right)_{\text{max}} = 20\text{ bar CAD}\) was chosen to represent a medium knocking condition, while in other experimental HCCI studies, \(10\text{ bar CAD}\) is usually considered as a boundary (Iida et al., 2001).

Also, the lean operating limit measured in this study is not a misfiring boundary and was defined as the maximum usable $\lambda$ without a drop in engine speed. Increasing the fuel’s RG mass fraction expanded the operating window significantly on the lean side, while the pure CNG-fueled HCCI engine could operate at $\lambda = 2$, blending a fuel with 60% RG increased the lean operation range to $\lambda = 3.5$. Hence, the mechanism of all the positive $\lambda$ effect on operating parameters such as decreasing maximum pressure, maximum pressure rate and is NO\textsubscript{x} as indicated in Fig. 4. Note that due to the low achievable power levels, the specific NO\textsubscript{x} levels continue to be high and further combustion enhancements would be needed to make the CNG-fueled HCCI engine practical. RG addition has a secondary impact on NO\textsubscript{x} emissions. Looking at any of the constant $\lambda$ lines in Fig. 4 indicates that displacing CNG with RG at a constant air/fuel ratio actually increases NO\textsubscript{x}.

The observed trends of engine and combustion parameters resulting from RG additions in a CNG fueled HCCI engine can be further investigated using the cylinder pressure traces collected in this study. Figure 5 and 6 shows that RG increased the maximum cylinder pressure and maximum cylinder pressure rate substantially. With NO\textsubscript{x}, $\lambda$ has the dominant effect. Hence, expanding the operating region towards leaner mixture can reduce $P_{\text{max}}$ and \(\left(\frac{dP}{d\theta}\right)_{\text{max}}\), while, for a given $\lambda$ increasing RG mass fraction increased the $P_{\text{max}}$ and \(\left(\frac{dP}{d\theta}\right)_{\text{max}}\). If we considered a reasonably acceptable noise level of \(\left(\frac{dP}{d\theta}\right)_{\text{max}} = 10\text{ bar CAD}\), the only operating points would be at $\lambda = 2.8$ with RG mass fraction less than 35%. Also, increasing the RG mass fraction advanced $P_{\text{max}}$ and \(\left(\frac{dP}{d\theta}\right)_{\text{max}}\) timings earlier in the combustion cycle.

Fig. 3: Effect of relative air fuel ratio on is NO\textsubscript{x} at constant RG mass fraction lines. Effect of relative air fuel ratio of maximum pressure and maximum pressure rate at constant RG mass fraction lines

Fig. 4: is NO\textsubscript{x} increase with increasing RG mass fraction at constant Effect of relative air fuel ratio on is NO\textsubscript{x} at constant RG mass fraction lines
The effect of RG addition on combustion onset is a complicated thermal/chemical phenomenon that cannot be explained just by looking at engine operating parameters. The base fuel characteristics play an important role. For example, in another study on an HCCI engine fueled with normal heptanes (Machrafi et al., 2008) showed that increasing RG fraction actually retarded combustion timing. In that case, adding RG, which is a higher octane component than the base fuel, retarded ignition. In contrast, RG added to a CNG-fueled engine is a lower octane component than the base fuel and it advanced ignition timing. In this case, the combustion timing change could be a result of added H$_2$O$_2$ production before the main stage of methane auto-ignition.

The tendency of RG to shift the allowable operating range towards leaner mixtures advances the peak pressure timing. Also, despite the elimination of audible knock, the advance in peak cylinder pressure timing generally resulted in higher peak pressures in RG addition, (Fig. 6) Overall, both the peak pressure timing and peak pressure were highly correlated with RG fraction and $\lambda$.

**CONCLUSION**

A CNG-fueled COMET engine was modified to operate at high compression ratios and high intake temperature enabling to attain HCCI combustion. With CNG fuel the operating range was very limited between both boundaries marked by heavy knock and misfire. The attainable engine speed range was low. Overall, the COMET engine appeared to be poorly suited for HCCI combustion with natural gas fuel. As a result, HCCI operation on pure CNG was considered unsuccessful because of high indicated specific NO$_x$, high cyclic variation and low efficiency. A Partial Reformar Gas replacement was found to be beneficial for expanding the operating range of fuel rich side, reducing knock severity and reducing indicated specific NO$_x$ emission, maximum peak cylinder pressure and rate of pressure rise with respect to crank angle which could not be achieved on pure CNG fueling. However, considering the situation of constant relative air fuel ratio the peak cylinder pressure, rate of pressure rise with respect to crank angle and NO$_x$ levels were increased substantially while replacing Compressed Natural Gas with Reformar Gas. This implies that the best quantity of RG is the minimum necessary to enable and enhance operation at the desirable operating point.

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