Knock Occurrence Prediction and Performance Optimization of a Natural Gas S.I. Engine

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Abstract
Natural gas is used as alternative fuel in spark ignition engines in many countries to satisfy air quality standards. Gas engines can be operated in stoichiometric and lean burn condition with different combustion and emission details. In this study a natural gas spark-ignition engine at stoichiometric condition was optimized to avoid knock occurrence. Compression ratio and engine speed were optimized to obtain the lowest fuel consumption accompanied with high power and low emission. A quasi-dimensional two-zone combustion model was developed to simulate combustion and a knocking model was incorporated with main model to predict any auto-ignition that might occur. The model was validated by comparing with available experimental results. Performance parameters and exhaust emissions were also computed by using this model. It was found that using cooled EGR especially at high compression ratios has a key role in reducing NO emission.

1. Introduction
Natural gas has been used as alternative fuel in spark ignition engines form the early 1980s [1]. The main motivations in using natural gas are: 1. NG engines are able to operate at high compression ratios without knock occurrence; 2. Engines running on natural gas emit significantly lower emissions compared to engines running on conventional fuels. Even if natural gas cannot prove itself as an intrinsically better fuel than conventional fuels in terms of engine emissions, natural gas vehicles that operate on CNG fuel are expected to find widespread use because the sources of natural gas are far bigger than those of oil, and natural gas will be available at a competitive cost for a long time [2].

One of the natural gas engine combustion technologies is the lean burn combustion technique [3]. This technology led to high engine efficiency accompanied with longer durability and lower cost. Today after almost a quarter century of continuous lean burn engine development and investment, most of the conventional gas engines operate with lean burn mode.

Most of the research conducted in the lean-burn strategy basically focused on extending the maximum burning lean limit in order to reduce NOx emissions to satisfy the increasing emission restrictions. That usually was achieved by designing fast-burning combustion chambers and/or employing the stratified charge concept, usually by using either a combustion pre-chamber or direct fuel injection. Recently, laser ignition systems have been developed in order to ignite extremely lean fuel air mixtures, which require high ignition energy.

In order for the engine under the lean burn mode to produce lower NOx emissions, it has to operate with a leaner mixture. It means that operating near the misfire is inevitable limit to produce lower NOx emissions. At this condition of the engine the HC and CO emissions increase and the engine efficiency decreases [4, 5].

Another method to control NOx emissions is to retard the spark timing, which also leads to a decrease in engine efficiency and an increase in HC emissions. Therefore, it would be difficult for the conventional gas engine operating on lean burn mode to meet the stringent future emission standards especially for NOx emissions [6].

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The current emission reduction technologies used for the NOx emission after-treatment in lean burn engines such as the selective catalytic reduction (SCR) devices are expensive and add some complexity to the engine use.

The alternative technique that has been used for four decades is the use of a three way catalyst (TWC) to reduce NOx, HC, and CO emissions [7]. It is much less expensive than the SCR devices used in lean burn engines. However, in order for the TWC to operate efficiently, the engine must operate at near stoichiometric condition. When the engine operates near the stoichiometric mixture, the in-cylinder temperature increases, and consequently, the thermal stresses and the knocking tendency increase. This would lead to some restrictions on the use of turbocharging, high compression ratio, and maximum brake torque (MBT) spark advance timing. As a result, the engine would operate less efficiently than a similar lean burn engine.

In order to overcome to these restrictions, the in-cylinder temperature should be reduced. One of the methods is to recycle some of the exhaust gases back into the cylinder intake that is called exhaust gas recirculation (EGR). Using EGR will lead to a decrease in the in-cylinder temperature and a decrease in knocking tendency. In addition, adding EGR to the inlet mixture will reduce the oxygen partial pressure in the inlet mixture, and consequently the in-cylinder NOx production will decrease [7].

In this study a quasi-dimensional two-zone combustion model was incorporated to simulate the in-cylinder conditions of NG engine.

2. Engine thermodynamic cycle modeling

Ferguson [8] method was used to model thermodynamic cycle in which the following assumptions are considered for simplification:

1. The cylinder charge is spatially homogeneous during compression and expansion processes. It means that the thermodynamic properties vary only with time.
2. For the combustion process, two zones (unburned and the burned zones) are used. The two zones have equal pressure and different temperatures and are separated from each other by the flame front.
3. The flame front thickness is negligible and heat transfer between two zones equals to zero.
4. Heat transfers by convection and radiation from each zone to combustion chamber walls.
5. The cylinder wall temperature is assumed to be constant (420 K).
6. Burned gases consist of 10 species (O$_2$, N$_2$, CO, H$_2$O, CO$_2$, O, H, NO, OH and H$_2$) in chemical equilibrium during combustion and expansion processes.
7. All gases are considered to be ideal gases during the engine thermodynamic cycle.
8. During cycle some mass leaks from rings and crevices. The blow-by coefficient is assumed to be 0.8.
9. The combustion chamber wall area in contact with burned gases is proportional to the square root of burned mass fraction. It means burned gases take greater volume.

2.1. The burning rate

Wiebe function was used to determine the burning rate. This function shows burned mass fraction:

$$x_b = 1 - \exp\left(-a \left(\frac{\theta - \theta_s}{\Delta \theta}\right)^{m+1}\right)$$

(1)

Where $\theta_s$ is the crank angle at the start of combustion, $\Delta \theta$ is the total combustion duration (from $X_b = 0$ to $X_b = 1$) and $a$ and $m$ are adjustable parameters which fix the shape of the curve. The curves of actual burned mass fraction have been fitted with $a=5$, and $m=2$ as suggested by Heywood.

2.2. Combustion duration

To compute combustion duration in this model the following correlation was used [9]:

$$\Delta \theta = 544.26 \phi^2 - 942.71 \phi + 451.19$$

(2)

Where $\phi$ is equivalence ratio. This equation gives combustion duration in terms of equivalence ratio and does not require any knowledge about flame shape and propagation details.
2.3. Heat Transfer

Annand [8] model was used to calculate heat transfer. This model considers heat transfer as convection and radiation mechanisms. The radiation mechanism only occurs in combustion process where the temperature of burned gas is very high.

2.4. NO formation model

The extended Zeldovich mechanism was used to determine the rate of NO concentration during combustion and expansion processes as follows:

\[
\frac{d[NO]}{dt} = \frac{2R_1 \left[1 - \left(\frac{[NO]}{[NO]_e}\right)^2\right]}{1 + \left(\frac{[NO]}{[NO]_e}\right) \left(\frac{R_1}{R_2 + R_3}\right)}
\]

Where:

\[R_1 = K_1 \left[O\right]_e \left[N_2\right]_e\]

\[R_2 = K_2 \left[NO\right]_e \left[O\right]_e\]

\[R_3 = K_3 \left[NO\right]_e \left[H\right]_e\]

Where subscript e refers to equilibrium value. The rate constants (K), in units of m³/kmol.s, were calculated from Ref. [7].

2.5. Knocking model

Engine knock is an abnormal combustion phenomenon which can cause engine damage. The most accepted theory that explains engine knock is the auto-ignition theory. The auto-ignition theory states that when the fuel–air mixture in the end gas region ahead of the flame front is compressed to high values of pressure and temperature, the fuel oxidation process can occur in parts or in the entire end gas region. This releases the chemical energy in the end gas region at extremely high rates resulting in high local pressures. The non-uniform pressure distribution inside the combustion chamber causes pressure waves or shock waves to propagate across the chamber causing noise which is known as knock. There are two types of auto-ignition models that are used to simulate engine knocking. These are the detailed chemical kinetic models and the empirical delay time models. The chemical kinetic models describe the chemical mechanisms which govern the hydrocarbon oxidation process in the end gas region during the auto-ignition time. The auto-ignition chemical kinetic process is complex and it may be described with thousands of elementary reaction steps and species. The lack of knowledge of the elementary reaction steps and rate coefficients in addition to the long computational time required to analyze thousands of equations makes empirical delay time models more practical for engine designers [10]. The empirical delay time models usually correlate a delay time equation, which is usually in the form of Arrhenius equation using experimental data to determine a simple empirical correlation for the ignition delay time. The ignition delay time represents the time required for the unburned mixture to establish necessary radicals to start the auto-ignition process. In the current study, an empirical delay time knocking model was incorporated to the combustion model in order to predict engine knocking and the crank angle at which knocking might occur.

This model was developed based on the auto-ignition model developed by Soylu [11] for natural gas engines. He modeled the ignition delay time by using an equation, which was in the form of Arrhenius equation:

\[
\tau = x_1 P^{x_2} \exp(x_3 E_u / T_u)
\]

Where \(P\) is the cylinder pressure, \(T_u\) is the unburned mixture temperature, \(E_u\) is the temperature coefficient \((E_u = 7000)\), whereas \(x_1, x_2,\) and \(x_3\) are experimentally determined constants. This method is known as the knock Integral method, and has the following form:

\[
\int \frac{dt}{\tau} = 1
\]

The integration is performed from the intake valve closing time to the knocking time. The substitution of Eq.(7) to Eq.(8) leads to the following equation:
\[ \int dt/x_1 p^{x_2(t)} \exp(x_3 7000/T_{\text{IVC}}) = 1 \] (9)

The lower limit of above integrand is IVC and the upper limit is when knock occurs. The value of constants are:

\[ x_1 = 0.985 \] (10)
\[ x_2 = -0.887 \] (11)
\[ x_3 = (-0.575 + 10.058 PR - 54.053 PR^2) \phi + 1.456 - 8.703 PR + 43.615 PR^2 \] (12)

Were PR is the propane ratio in natural gas fuel.

3. Results and discussion

The presented model was used to predict the performance of a single cylinder Ricardo E6 engine. Table 1 shows the engine specifications.

### Table 1. Engine specification

| Specification               | Value          |
|-----------------------------|----------------|
| Displacement Volume         | 508 cm³        |
| Bore                        | 76.21 mm       |
| Connecting rod length       | 241.3 mm       |
| Stroke                      | 111.11 mm      |
| Compression ratio           | 4.5:1 – 20:1   |
| IVC                         | 34 degree abdc |
| EVO                         | 43 degree bbdc |

3.1. Model Validation

Figure 1 shows the Pressure diagram in terms of crank angle. Comparing between simulation and test results shows that there is a good agreement between the predicted and experimental in-cylinder pressure variations.

![In-cylinder pressure variations - comparison between modeling and test result](image)

3.2. Intake mixture condition to avoid knock occurrence and obtain low emission and high performance

In order to simulate turbocharging behavior, all investigations were made at inlet pressure of 210 KPa. In this condition knock occurrence is very probable because of high values of in-cylinder pressure. Therefore EGR was added to a stoichiometric fuel–air mixture.
Figure 2 shows the percentage of EGR used at different compression ratio and speed conditions. The minimum value of EGR in the inlet mixture was kept at 20% in order to obtain low NO emission.

However, knocking was predicted at higher compression ratio and speed conditions when EGR was equal to 20%. Therefore, EGR was increased to minimum percentage of dilution that could prevent knocking at higher compression ratios as shown in figure 2.

![Figure 2](image_url)

Figure 2. The percentage of EGR used at inlet Pressure of 210 KPa at different compression ratio and speed conditions.

3.3. Variations of brake at different compression ratio and speed conditions

Figure 3 shows the effect of engine compression ratio variations on brake power at inlet pressure of 210 KPa and different speed conditions. The modest increase in engine brake power which occurred at lower compression ratio and lower EGR dilution rate was due to the increase of the expansion work with the increase of compression ratio. However, the increased mass of EGR which was added at constant inlet pressure in order to avoid engine knocking replaced some part of the fresh mixture and led to a decrease in engine brake power at higher compression ratio.

![Figure 3](image_url)

Figure 3. The effect of engine compression ratio and speed variations on engine brake power at inlet pressure of 210 KPa.

3.4. NO emission

In-cylinder temperature affect the in-cylinder mechanical and thermal stresses in addition to NO emission. The variation of the in-cylinder temperature was studied at different compression ratios and EGR dilution rates. At a lower
speed of 1000 rpm, the maximum burned gas temperature increased with the increase of compression ratio as shown in figure 4.

Figure 4. The variation of in-cylinder temperature with crank angle during combustion at engine speed of 1000 rpm, inlet pressure of 210 KPa and different compression ratio values.

Figure 5 shows the NO emission variation with engine compression ratio at different engine speeds with inlet mixture pressure of 210 KPa. The increase of the maximum cylinder gas temperature led to an increase in NO emission by about 24% as shown in figure 5.

Figure 5. NO emission variations with engine compression ratio and speed at inlet Pressure of 210 KPa, and different EGR dilution rates.

At a higher speed of 3000 rpm, the maximum burned gas temperature decreased due to the increase of EGR dilution as shown in figure 6. This decrease in the maximum burned gas temperature decreased the NO emission by about 28% as shown in figure 5. This indicates the strong dependence of NO emission on the maximum burned gas temperature. It also indicates the potential of EGR on reducing the maximum burned gas temperature and consequently NO emission at high compression ratios. Generally, the trend of NO emission change followed the maximum burned gas temperature change at any speed.
3.5. Fuel consumption

Figure 7 shows the change of brake specific fuel consumption with engine compression ratio. The excessive EGR dilution rate which was used at 3000 rpm and higher compression ratio, in order to prevent engine knocking, slowed down the burning rate significantly and led to a significant increase in fuel consumption as most of the fuel was burned away from the top dead centre. The value of the compression ratio at which the minimum fuel consumption occurs varies with engine speed as shown in figure 7.

4. Conclusions

A quasi-dimensional two-zone combustion model was developed in order to optimize a natural gas SI engine employing a stoichiometric mixture with EGR dilution at high inlet pressure condition to obtain the lowest fuel consumption accompanied with high power and low emissions. The effect of compression ratio on engine performance was studied. The following conclusions have been obtained:
• The use of cooled EGR with a dilution rate ranged from 20% to 30% depending on engine speed suppressed engine knocking and allowed using high inlet pressure condition (200 kPa) in a relatively high compression ratio values (up to 13).

• The use of high compression ratio condition (up to 13) at high speed of 3000 rpm demanded using excessive EGR dilution (up to 30%) to avoid knocking. The excessive dilution slowed the burning rate significantly and led to a significant increase in fuel consumption.

• The value of the compression ratio at which the minimum fuel consumption occurs varies with engine speed and the value of EGR dilution which is used at the corresponding optimum compression ratio varies from about 21% to 23% at inlet conditions of 200 kPa and 333 K.

• A minimum fuel consumption of about 200 g/kWh was achieved at engine speed of 1500 rpm, inlet conditions of 200 kPa and 333 K, and a compression ratio of about 12.

• Cooled EGR has the potential on reducing the maximum burned gas temperature and consequently NO emission at high compression ratio conditions.

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