NUMERICAL STUDY ON A NATURAL GAS-FUELED ENGINE UNDER LOW TEMPERATURE COMBUSTION MODE

by

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Natural gas, which is also referred to as eco-friendly fuel, is being seen as a potential solution to challenge the decline of crude oil resources and the deteriorating air quality in urban areas. This fuel has been verified to emit less CO, HC, and PM compared to other fuels. A potential approach to reducing NO_x and soot emissions while also achieving low fuel consumption is the low temperature combustion process. In this study, internal combustion engines were simulated under various conditions. The objective was to investigate the effect of different operating variables on the low temperature combustion mode. To begin with, a natural gas powered engine was modeled using complex chemical kinetics software. The outcomes of the simulation were then compared to experimental data, demonstrating a high level of agreement. Subsequently, the impacts of key variables, including the air-fuel ratio, compression ratio, and engine speed, were analyzed using a cycle simulation code. Increasing the compression ratio improves engine performance, and the specific fuel consumption decreases. However, it leads to a significant increase in NO_x emissions until a certain value. Thereafter, it changes the trend. Engine speed indirectly affects performance by increasing fuel consumption and changing ignition timing. A leaner air fuel ration may be used to produce more power and keep the temperature of combustion below a certain value (low-temperature combustion), ensuring low NO_x emissions.

Key words: low temperature, combustion, emissions, natural gas, engine

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Introduction

The internal combustion engine remains the primary power source for various vehicles and transport applications. Despite concerns regarding global warming and the depletion of natural resources, there is currently no viable alternative to these engines, and they are expected to remain dominant for several decades. However, there is a need to develop new combustion systems that can reduce the negative effects of engines on the environment.

Nowadays, research activities have intensified with the purpose of representing a considerably homogeneous combustion of automotive engine fuels with auto ignition. There are two known approaches that have been developed: HCCI refers to homogeneous charge compression ignition in Diesel engines, while CAI refers to controlled auto ignition in spark ignition engines. The main goal of both methods is to operate homogeneously and leanly to reduce fuel consumption and emissions. This latter can be achieved by using low temperature combustion (LTC) mode, which improves emission problems because of its clean burning characteristics [1]. Today's passenger vehicles still frequently have spark-ignited (SI) gasoline engines with direct or indirect injection ports. These engines operate using the Otto process, which involves premixed and stoichiometric combustion. As a consequence, the exhaust gas purification is very efficient with the help of three-way catalytic converters (TWC), and the production of PM is minimal.

The power output of a SI engine running at a stoichiometric air-fuel ratio is determined by the amount of air-fuel mixture present in the cylinder, however, the quality of the mixture remains constant. To vary the quantity of the mixture, the intake pressure is altered, which changes the density of the mixture. This is achieved using a throttle plate located in the intake system upstream of the combustion process. While this solution is reliable and straightforward, it causes significant *pumping losses* that reduce the engine efficiency at partial loads. Alternative methods, such as variable valve timing, electronic throttle control, and other innovative techniques, can enhance fuel economy and reduce pollutant emissions. The most effective after-treatment arrangements for producing cleaner SI engines is a TWC [2, 3]. According to [4], the conversion of the three pollutant species found in exhaust gas into harmless water and CO_2 is only possible within a very limited range of air-fuel proportion, which is slightly under the stoichiometric operating conditions. When the engine runs on a lean fuel mixture, the emission of NO_x is significantly increased [5] because the surplus O₂ in the exhaust gas is utilized to burn unburned HC and CO. In contrast, under rich fuel conditions, HC and CO act as agents to reduce NO_x on the catalyst, resulting in the favorite TWC behavior.

In order to maintain the air-fuel ratio within the narrow range mentioned previously, electronic control systems, sensors, and actuators must be used. The λ sensor, which measures the air-fuel ratio, is an essential component of this control loop. Furthermore, an accurate fuel injection system is required, which is now achieved through the use of *sequential multiport injectors* [6]. These injectors are situated in each intake port and inject fuel sequentially only when the corresponding intake valves are closed. The engine control unit also needs suitable algorithms to operate correctly.

Another critical control system found in commanded ignition engines is the spark angle controller, which can also contribute to improving fuel efficiency. The knock phenomenon limits the efficiency of SI engines by creating unwanted self-ignition that produces high pressure peaks, which can lead to piston and cylinder damage. To avoid knocking in an engine, it is necessary to maintain a safe level of compression ratio (CR) and optimize the ignition timing. Several measures have been introduced in the past [7-9] to increase SI engine efficiency, including direct injection (DI) of fuel, which allows for a more resistant air-fuel mixture against knock combustion, achieved by cooling and increasing its density.

The new combustion concepts that have been introduced recently consist of homogenizing the air-fuel mixture prior to auto-ignition, so no fuel-rich regions will exist, resulting in a reduction of HC formation. Moreover, high air excess in the combustion chamber will lower overall temperatures, so nitric oxide formation is suppressed as well. To achieve autoignition and improve thermal efficiency, the CR is raised. In addition, load is managed by adjusting the air-fuel ratio. Consequently, the engine functions without the need for a throttle, and the homogeneous charge becomes exceedingly lean during low loads. The LTC results in efficiency enhancements of around 15-20% compared to regular SI engines, putting LTC efficiencies on par with Diesel engines. The LTC methods reduce the post-combustion temperature within the cylinder by *homogenizing* the combustion process, resulting in *flameless* combustion. This is accomplished by compressing a well-mixed combination of fuel, air, and combustion products, which initiates combustion at a lower temperature [10].

Although LTC offers similar efficiency to conventional DI Diesel engines but with fewer drawbacks, such as high NO_x and PM emissions, LTC is particularly important in modern engine concepts, such as HCCI and CAI, where a homogeneous charge is required. This process can produce low combustion temperatures that minimize NO_x formation, even under lean conditions. While modern engine concepts using LTC offer benefits from both SI and CI engines, they also present unique challenges. The objectives of this work are to study possible performance improvements by varying key parameters that can affect combustion temperature and to verify the impact of each parameter on emissions at different engine speeds.

Engine modelling

The difficulties outlined in the previous give emphasis to the crucial role of combustion modeling in advancing technologies such as LTC. Relying exclusively on engine experiments is not practical due to the complex nature of the process and the difficulties in controlling it. Models can assist in developing an indispensable understanding of fundamental phenomena or in bridging the gap between concept and application. There are various LTC modeling approaches that exist and can vary depending on whether the modeling is being done for development or control, which subsequently leads to a difference in the level of complexity and computational effort.

In recent years, there have been several developments in engine modeling that have improved the accuracy and efficiency of the simulations.

- Advanced turbulence models. Turbulence-chemistry interaction models are used to predict the flow and mixing in the engine cylinder. Advanced turbulence models using direct numerical simulation (DNS) and large eddy simulation (LES) have been developed to improve the accuracy of flame structure predictions [11, 12].
- Multi-zone combustion models. Multi-zone combustion models divide the combustion chamber into several sub-zones, each with its own combustion characteristics. This allows for a more accurate prediction of the heat release rate and emissions [1, 13].
- Dynamic boundary conditions. Dynamic boundary conditions allow for a more accurate simulation of the flow in the intake and exhaust systems. This includes the simulation of pressure waves that can impact engine performance [14, 15].
- Artificial intelligence. Machine learning and artifical intelligence techniques are being used to improve engine modeling. This includes the development of neural network-

based models for predicting engine performance and the use of genetic algorithms for optimizing engine designs [16, 17].

 Reduced order models. Reduced order models are simplified versions of 1-D engine models that use fewer computational resources. These models can still provide accurate predictions of engine performance, making them useful for real-time control applications [18].

Recent developments in 1-D internal combustion engine modeling have focused on improving the accuracy and computational efficiency of these models. The 1-D engine models are simplified mathematical representations of the engine that capture the key physical processes that occur during engine operation. They are widely used in industry and academia to simulate engine performance and optimize engine design. Most classical engine models use a single or multi-zone approach to simulate the gases inside the engine cylinder. However, this method has a drawback in that it can only analyze the evolution occurring within the engine cylinder. One way to address this issue is to merge the cylinder models with an engine-cycle simulation code that can estimate the ideal values at intake valve closure. Such codes are typically 1-D and provide calculations for the entire engine components, from air intake to exhaust pipe, including modeling of gas exchange processes as they calculate outcomes for the whole engine cycle.

Ogink [19] developed a single-zone model that can predict combustion phasing, such as the exact timing of auto-ignition and heat release rate in compression ignition and gasoline HCCI applications. In a similar manner, Milovanovic *et al.* [20] studied the gas exchange process under the influence of variable valve timing (VVT) strategies in an HCCI engine. In order to conduct the simulation, the researchers merged the 1-D fluid dynamics code with the AURORA chemical kinetics program. Taghavifar and Mazari [21] use 1-D Diesel engine cycle modeling and chemical species prediction integrated with MOPSO optimization for improved NO_x control and pressure boost. The results of engine cycle modeling are validated with experimental data, and they found a robust concordance. Narayanaswamy and Rutland [22] explore the early injection processes, employing the commercial 1-D engine cycle code GT-Power combined with an external in-cylinder model that includes multi-zone chemistry calculations).

A 1-D cycle simulation code is used in the present work. It can predict mass flow, pressure, and temperature in various components. The code conducts both transient and steady-state simulations that are appropriate for analyzing engine control. The properties of each component, fuel, and simulation considerations are defined for the parametric study. In the simulation, every component is divided into numerous subcomponents. These smaller components have very infinitesimal volumes, and their fluid scalar properties such as pressure, density, temperature, and internal energy are assumed to remain constant. Additionally, the vector properties, including fluid velocity and mass flux, can be transmitted across the boundaries of each subcomponent; the simultaneous solution of eqs. (1)-(3) gives information on the change in scalar characteristics.

$$\frac{\mathrm{d}m}{\mathrm{d}t} = \sum_{\mathrm{boundaries}} m_{\mathrm{flux}} \tag{1}$$

$$\frac{\mathrm{d}(m_{\mathrm{flux}})}{\mathrm{d}t} = \frac{\mathrm{d}pA + \sum_{\mathrm{boundaries}} (m_{\mathrm{flux}}u) - 4C_f \frac{\rho u^2}{2} \frac{\mathrm{d}xA}{D} - C_p \left(\frac{1}{2}\rho u^2\right)A}{\mathrm{d}x}$$
(2)

$$\frac{\mathrm{d}(me)}{\mathrm{d}t} = p \frac{\mathrm{d}V}{\mathrm{d}t} + \sum_{\mathrm{boundaries}} m_{\mathrm{flux}} H - h_g A(T_{\mathrm{gas}} - T_{\mathrm{wall}})$$
(3)

Results and discussions

It is possible to assess the influence of various operational settings and component modifications on the outcome using the engine simulation. This allows for more efficient testing of several combinations to enhance fuel efficiency and expand the operating range, as opposed to conducting real experiments on an engine test bench.

Table 1 presents the specifications for the natural gas fueled engine utilized in this study. Initially, the simulated parameters were evaluated, and they were subject to comparison with a 2-zone model and experimental data [23] to ensure the fidelity of the simulation results.

Table	1. Engine specifications	

Manufacturer	Lister- Petter
Engine type	four-stroke, SI
Number of cylinders	1
Bore/stroke	95.5/88.7 mm
Displacement	635 cm ³
Compression ratio	12.9
Connecting rod length	165.3

A simulation of an SI engine was conducted at a speed of 1500 rpm. As shown in fig. 1, the cycle simulation model faithfully reproduces the experimental measurements and can give a perfect accordance over the complete cycle, which is not possible with the two-zone model.

The results indicate that there is a positive correlation between an increasing CR and higher torque output, fig. 2. This is because raising the CR of the engine also leads to an enhancement in brake thermal efficiency, which supports the analysis of the ideal cycle. As a result, the final output, which is torque, is expected to be higher. As well, many studies suggest that cylinder-gas properties are altered as the CR increases. This change results in higher peak burned gas pressures and temperatures, which cause faster combustion a well as an increase in the surface/volume ratio near TDC. As a result, increasing the CR reduces the overall heat flux to the cooling system, or, in other words, decreases heat transfer to the coolant. This implies that the engine performance is improved since the same amount of input produces a lesser total heat loss.

Figure 3 shows the engine power outputs, the maximum is achieved at approximately 3800 rpm and then slightly decreases for all values of CR. While engine speed does not directly affect engine performance, it does increase fuel consumption and cause changes in ignition timing, both of which can impact performance. Early combustion in the combustion chamber may lead to engine knocking due to the fuel self-igniting from high temperatures within the cylinder before being ignited by the spark plug.



Figure 1. Validation of simulated model

Figure 2. Variation of torque for various CR

Regarding fuel consumption, fig. 4 illustrates the gas flow rate to the engine under varying CR. It indicates that the fuel consumption is almost the same at low and medium rpm, then increases at high rpm with the limit values (CR = 9 and CR = 12) of the CR.



Figure 3. Variation of power for various CR



However, when examining specific fuel consumption, as shown in fig. 5, it appears that fuel consumption decreases with an increase in CR up to a value then it changes the trend. As was expected, the specific fuel consumption trend aligns with the theoretical trend of fuel consumption. In general, the specific fuel consumption tends to decrease when the engine speed increases until it reaches a minimum, and thereafter it begins to increase again at high speeds. The reason for this is that at high speeds, there are greater friction losses, which lead to an increase in fuel consumption. On the other hand, when the engine runs at low speeds, the longer time per cycle leads to more heat loss, which causes an increase in fuel consumption.

Figure 6 shows the result of NO_x emissions for different CR with varying engine speeds. The quantity of NO_x increases significantly when increasing the engine speed, which is due to the elevated temperature levels resulting from reduced cooling and increased hot residual gas, leading to favorable NO_x formation conditions. However, the results indicate that the amount of NO_x fluctuated up and down at different engine speeds even for the same CR, which could be due to other factors such as the varying equivalent ratio.



Figure 7 shows the quantity of HC emitted in the engine exhaust gas. It appears that an increase in CR results in a corresponding increase in HC emissions. The HC emissions are caused by unburned HC and include crevices such as spaces between the cylinder wall above the piston ring and the piston. During compression and combustion, the unburned mixture is enforced into the crevices and appears later during the expansion or exhaust strokes. This is a principal source of HC production from four-stroke engines. Hence, an increase in the CR leads to an increase in pressure inside the engine, which could force more unburned mixture into the crevices. Regarding the amount of HC with respect to engine speed, it initially decreases and then starts to rise again for all values of the CR. This behavior may be due to oxidation at the tailpipe since, at higher engine speeds, the temperature levels of the exhaust gas are higher, resulting in increased HC emissions into the exhaust gas.

Figure 8 illustrates the influence of the CR on the third primary exhaust gas emitted. It is well known that the air-fuel ratio is the main significant factor influencing the concentration of CO in emissions. The value of the concentration follows the same trend according to the speed but does not change significantly by varying the CR except for a low CR, which marks a maximum around 1.6%.

Figure 9 illustrates how the concentration of NO_x changes based on the air-fuel ratio (AFR). A leaner AFR can produce higher levels of NO_x . While fig. 10 depicts the gas temperature at a given moment in time based on the air-fuel ratio and CA, a leaner AFR can cause the engine to run hot. Engines typically produce the most power when running at stoichiometric conditions (AFR close to 14.7), which means that there is just enough air to burn all of the fuel completely. However, in some engines, particularly high-performance ones, a leaner AFR may be used to produce more power.

It should be observed that when the air-fuel ratio goes up, the ignition timing is slightly delayed due to chemical kinetics. Additionally, during real engine operations, a higher AFR could lead to uneffective mixing between air and fuel, resulting in ignition delays. Figure 11 shows the NO_x concentration at a given moment in time for air-fuel ratios ranging from 13 to 16. We can see that there is an increase in NO_x with the increase in AFR, the latter giving higher temperatures, fig. 10, hence a favorable condition for the formation of NO_x.

2.00



Figure 9. The NO_x emissions as function of AFR

CA [°C]



Figure 11. Instantaneous NO_x concentration



3000

4000

5000

CA [°C]

2000

= 10



Figure 10. Instantaneous gas temperature

Conclusions

The aim of the investigation was to predict the process of LTC in order to boost engine efficiency and decrease pollution. The findings demonstrated that in an LTC engine, ignition occurs through spark modes at various fuel and air mixtures. By modifying the predetermined parameters to optimize LTC, it is feasible to achieve enhanced efficiency and reduced pollution for the engine.

In this study, a simulation was conducted on a sample SI engine, and the predicted results

were compared to experimental data to confirm the accuracy of the simulation. Once the simulation was validated, the impact of key engine-operating parameters, in this case the CR and the air-fuel ratio, on LTC performance and emissions was analyzed. The results of the tests led to the following conclusions.

Natural gas, also known as green fuel, is being considered as a solution to address the depletion of crude oil resources and the worsening urban air quality. This gas has already been proven to have lower emissions of CO and HC compared to other fuels. To improve en-

2000

gine performance and further reduce emissions, certain parameters affecting operating cylinder pressure and temperature need to be thoroughly analyzed and optimized.

The model for simulating cycles in engines used in this study overcomes some of the limitations of an in-cylinder model while still enabling accurate predictions of ignition and emissions through the use of detailed chemical kinetics. This approach treats the engine components as uniform areas where intricate chemical processes can be applied in an efficient manner.

As the engine speed rises, the specific fuel consumption decreases until it reaches a minimum and then starts to increase at high speeds. This is because at high speeds, there is an increase in friction losses, which leads to an increase in fuel consumption. On the other hand, at low engine speeds, the longer time per cycle results in more heat loss, which causes an increase in fuel consumption.

When the air-fuel ratio goes up, the ignition timing is slowed down a bit, primarily because of chemical reactions. A decrease in pressure also delays ignition. A higher air-fuel ratio could lead to less mixing of air and fuel, which can delay ignition and cause higher temperature peaks.

In order to achieve more accurate results for engine components where flow exhibits significant 3-D effects, it is suggested to combine chemical kinetics and cycle simulation models with phenomenological models using CFD simulation. This coupling would allow for better accounting of flow and geometry effects such as turbulence and mixing, which can ultimately lead to reduced emissions and improved efficiency in the combustion process. Therefore, it is recommended to use the LTC mode in the future.

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