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0/1 Dimensional Simulation of Combustion Timing Effects on Performance and Emissions in a Methane-Hydrogen Fueled Engine

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Research Article

Abstract

Natural gas has gained attention as a promising alternative fuel to reduce emissions and reliance on petroleum-based fuels. However, its combustion limitations, such as a low lean air-fuel mixture limit and high ignition energy requirements, can be improved by adding hydrogen. This study aims to address these limitations and investigate how adding hydrogen can improve the combustion properties of natural gas. In this study, a 3-cylinder diesel heavy-duty engine with a compression ratio of 17.5:1 was converted to a spark-ignition engine using natural gas with 10% hydrogen by mass. The effects of different start of combustion (SOC) timings (0°, -5°, -10°, -15°, and -20° CA) on engine performance and emissions were analyzed under full-load conditions at 2300 rpm using a 0/1-dimensional combustion simulation program. The best SOC timing was -5° CA, producing the highest brake power (BP) of (78.8 kW) and lowest brake specific fuel consumption(BSFC) of (168.37 g/kWh), improving brake power (BP by 1.18% and reducing (BSFC) by 1.42% compared to the baseline. SOC timings of -5° and -10° CA are operated safely without knocking, with maximum pressure rise rate (MPRR) values of 0.61 MPa/°CA and 0.87 MPa/°CA, respectively, while 15° and -20° CA exceeded the knock limit of 1 MPa/°CA. Advancing SOC to -20° CA increased nitrogen oxides (NO_X) emissions by 1.52 times due to higher in-cylinder temperatures. These results demonstrate that optimizing SOC timing and incorporating hydrogen into methane can enhance engine performance while managing emissions and avoiding knock, contributing to the development of sustainable fuel technologies. Careful calibration of SOC is necessary to avoid damaging components while maximizing performance.

Keywords: Alternative fuels; Engine performance; Hydrogen enriched-CNG fuel; Start of combustion

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1. Introduction

The rising global demand for energy, combined with escalating energy costs and increased emission regulations, has significantly intensified research aimed at enhancing energy efficiency and reducing the environmental impact of fuel consumption. As a result, there is a growing emphasis on developing innovative strategies to lower fuel consumption while minimizing the release of greenhouse gasses into the atmosphere. This ongoing pursuit has led to extensive study of alternative energy sources and cleaner fuel options, driving advancements in sustainable energy solutions and environmentally friendly combustion technologies. [1,2]. The use of gaseous fuels like natural gas, syngas, biogas, and hydrogen in alternative fuel studies has been recognized for their potential to reduce dependency on petroleum-based fuels while lowering engine emissions. These fuels are often seen as cleaner alternatives, contributing to reduced carbon footprints and greenhouse gas (GHG) emissions [3–5]. Natural gas is one of the most notable alternative gaseous fuels. The extraction and distribution technology for natural gas is highly developed, benefiting from decades of infrastructure investment. This has contributed to its widespread availability, particularly with the rise of shale gas and other innovations that have increased its supply and lowered costs globally [6]. Natural gas also has environmental advantages over petroleum-based fuels. It emits approximately 20-30% less carbon dioxide (CO_2) than gasoline when burned, and its combustion results in significantly lower release of hazardous air pollutants, including sulfur dioxide (SO_2) and nitrogen oxides (NO_x) [7]. Natural gas can be a viable alternative fuel for diesel engines, offering better efficiency and reduced CO emissions [4].

While offering significant commercial benefits, natural gas has some drawbacks, as shown in Table 1, including a lower flame speed, a narrow flammability range, higher ignition energy requirements, and a greater quenching distance. However, the incorporation of hydrogen mitigates many of these drawbacks due to its inherent properties. Blending hydrogen with methane (natural gas) presents a viable solution for reducing greenhouse gas emissions in internal combustion engines while maintaining economic feasibility. Since hydrogen is a carbon-free fuel, its addition lowers the overall carbon intensity of combustion, resulting in reduced CO_2 emissions compared to pure methane or conventional fossil fuels. This approach is particularly attractive because it leverages existing natural gas infrastructure, minimizing the need for costly modifications to distribution and refueling systems. Recognizing the environmental and economic benefits of hydrogen-methane blends, the European Union has been updating its legislative framework to facilitate their integration into transportation and industrial sectors. These policy updates aim to encourage investment in hydrogen-enriched fuels and promote their widespread adoption [8]. Adding hydrogen also achieves a higher hydrogen-to-carbon (H/C) ratio, enhances combustion performance, and decreases HC and CO emission levels [9,10]. Several critical challanges are; the storage and transport of hydrogen-methane blends require advanced containment solutions, as hydrogen's high diffusivity and low energy density make handling more complex than conventional fuels. Additionally, safety concerns arise due to hydrogen's flammability and potential leakage risks, necessitating rigorous safety protocols and specialized infrastructure. Addressing these logistical and technical barriers will be essential for the successful deployment of hydrogen-methane fuel mixtures in real-world applications [11].

Table 1. Fuel Properties of Hydrogen and Natural Gas [2,9]

Properties	Hydrogen	Natural Gas
Stoichiometric A/F (Air to Fuel) ratio	34.3	17.05
Density (kg/m^3) at standard temperature and pressure	0.085	0.72
Lower heating value (MJ/kg)	120	47.5-60
Flame speed (cm/s)	185-325	20-38
Flammability limit (% volume in air)	4-75	7-21.6
Flame quenching distance (mm)	0.64	2.03
Auto-ignition temperature (°C)	585	595-650

Replacing the diesel injector with a spark plug allows the fuel-air mixture to be introduced into the combustion chamber more uniformly. This prevents the development of rich fuel regions, significantly reducing soot formation to negligible levels [12–16]. Additionally, the high compression ratio of the converted engine, combined with its capability to operate with a leaner mixture, enhances combustion efficiency by generating greater turbulence than a gasoline engine, thereby reducing emissions [17]. In a previous study carried out with the same engine specifications shown in Table 2 and 3, it was found that adding 5% of hydrogen to an engine with compression ratio of 17.5:1, using natural gas as the main fuel improved engine performance while reducing unburned hydrocarbons [10]. McTaggart-Cowan et al. found that hydrogen addition to natural gas fuel mixtures enhances combustion stability, reduces CO, HC, PM, and CO_2 emissions, and improves ignition and flame propagation across all load conditions in heavy-duty engines. While it slightly increases NOx emissions due to higher flame temperatures and altered stoichiometry, hydrogen-enriched fuels, particularly when sourced renewably, offer significant potential for reducing greenhouse gases and pollutants with minimal engine modifications [18]. Verma et al. found that in an engine with an 11:1 compression ratio, using hydrogen-enriched CNG fuel with an H/C ratio of 4.5 (20% hydrogen) demonstrated the best brake thermal efficiency (BTE) and overall performance compared to pure CNG; however, NOx emissions were increased due to increased in-cylinder temperatures [9]. Simio et al. found that a heavy-duty SI engine with an 11:1 compression ratio, fuelled with CNG and two hydrogen-enriched mixtures (15% and 25% hydrogen by volume) under steady-state and transient conditions exhibited reductions in HC, CO, and (CO_2) emissions, along with good engine tolerability to hydrogen, without abnormal combustions, and predictably higher NOx emissions compared to pure CNG with increasing H_2 presence [19]. Bhasker et al. found that a 10% addition of hydrogen to CNG fuel mixture significantly improves the combustion rate and extends the lean misfire limit to an equivalence ratio of 0.42. HC emissions were drastically reduced, by almost 90%, at a compression ratio of 12.5:1 with 10% hydrogen addition. In-cylinder pressure, rate of heat release, and total heat release also increased. These findings highlight the potential of using CNG with small hydrogen additions (5%–10%), resulting in improved performance and reduced emissions [20].

This study initially examined the transition from the diesel combustion regime to the Otto combustion regime in a high compression (17.5:1) tractor engine fueled with natural gas containing 10% hydrogen. Following this transition, the effects of varying start of combustion (SOC) timings on engine performance and emission characteristics were investigated. The analysis was conducted using a 0/1-dimensional combustion program under full-load conditions at 2300 rpm.

2. 0/1 Dimensional Engine Model

The AVL Boost program, shown in the diagram in Figure 1, was utilized to investigate the effects of various start of combustion timings on performance, in-cylinder combustion, and emission characteristics in a spark-ignition engine operating with natural gas and hydrogen in 0D/1D dimensions. All engine components were modelled within the program, and realistic initial and boundary condition values were defined to ensure accuracy [21,22].

The combustion and heat transfer processes within the program were modelled using the Vibe 2-Zone combustion model and the Woschni 1978 heat transfer approach. Table 2 presents the engine specifications used in the study.

The AVL Boost program offers 0D/1D solutions to problems modelled using gas dynamics equations. In this approach, the calculated temperatures, pressures, and flow rates represent the average values across the pipe cross-sections. To ensure realistic results and minimize losses caused by three-dimensional effects within the engine, correct flow loss coefficients are determined, thereby reducing the margin of error. The program utilizes equations and theories for continuity, momentum, energy, heat transfer, combustion, and emissions to solve the defined conditions, all of which are detailed in the relevant reference resources [21].

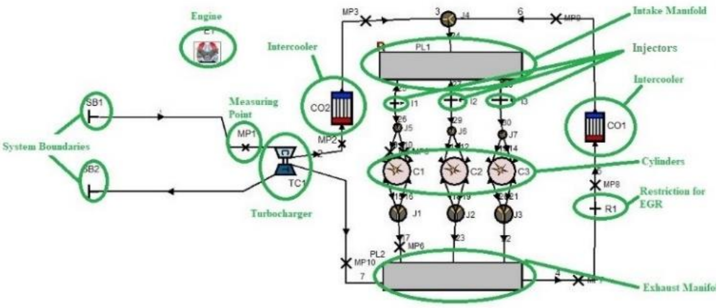

Figure 1. Diagram of the engine components in the AVL Boost program

Table 2. Engine Specifications

Specification	Value
Displaced volume - total (cm^3)	2930
Number of cylinders	3
Bore / Stroke (mm)	104 / 115
Compression ratio (-)	17.5:1
Injection system	Port fuel injection
Valve Time (° CA)	IVO: 28 bTDC IVC: 60 aBDC EVO: 65 bBDC EVC: 33 aTDC

Table 3. Engine Specifications

Parameter	Value
Engine speed (m/s)	2300 @ Full load
Start of combustion (°CA)	0, -5, -10, -15, -20
A/F ratio	26.8
Fuel mass (mg/st) (each cylinder)	64
Methane ratio by mass	90%
Hydrogen addition ratio by mass	10%

In Table 3, the start of combustion (SOC) timing, A/F ratio, fuel mass (miligrams/stroke), and the hydrogen ratio used in the program are given. In the fuel mixture, methane was used to represent natural gas, as methane consists of nearly 95% to 99% of natural gas from regions like Russia and the Middle East. Instead of modifying spark ignition timing, the start of combustion timing was adjusted, disregarding spark characteristics since the focus was on combustion initiation. The fuel consists of a mixture of 90% methane and 10% hydrogen by mass and is injected into each cylinder through a single injector.

3. Results And Discussion

Using AVL Boost program, the diesel combustion model, developed under the diesel combustion regime, was first validated by comparing its results with the experimental case [21]. A spark-ignition model was developed by replacing the diesel injector with a spark plug and installing a natural gas injector on the intake manifold. This new model was studied using both pure natural gas and natural gas-hydrogen mixtures as fuels [10]. The effect of five different start of combustion timings were investigated, starting from the base model which starts at TDC (0 °CA) and four other analysis points from -5 °CA to -20 °CA. The results are also compared with the numerical study of a 1D model of the diesel engine [23] to observe the combined effect of both the hydrogen enriched CNG transition and start of combustion timing.

Figure 2 shows the effect of start of combustion time on BP (Brake Power) and BSFC (Brake Specific Fuel Consumption) values. Since BSFC is basically fuel consumption rate per unit of brake power produced, the relationship between these two parameters is inverse as can be seen at Figure 2. The maximum BP of 78.8 kW and the minimum BSFC of 168.37 g/kWh were attained when combustion starts at -5 °CA. Advanced SOC increases total hydrocarbon (THC) emissions (see figure 8), which indicates more incomplete combustion;Therefore, after -5 °CA, BP decreases and BSFC increases. Comparing with the base model BP was increased by 1.18% and BSFC was decreased by 1.42% at start of combustion timing of -5 °CA. When compared to the diesel model, at SOC timing of 5 °CA, BP was increased by 31.48% and BSFC reduced by 23.79%.

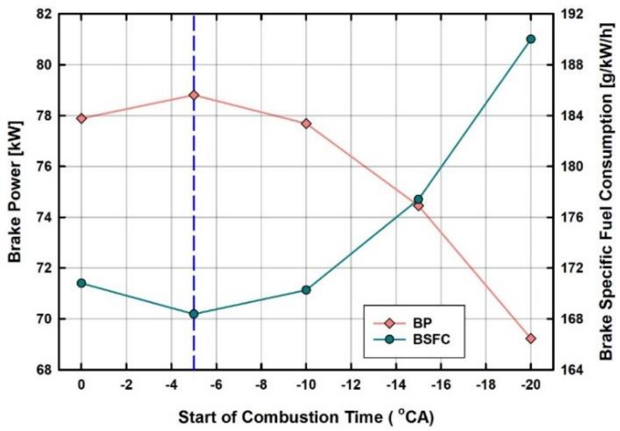

Figure 2. Change of brake specific fuel consumption and brake power with start of combustion time

Figure 3 shows the effect of start of combustion timing on brake mean effective pressure (BMEP), BTE, and MPRR ratios. BTE represents the overall efficiency of converting the fuel's chemical energy into mechanical energy delivered to the engine's shaft. Maximum BTE of 37.5% was achieved when combustion starts at -5 °CA, which is an increase of 1.44% from the base model. When combustion starts earlier, the pressure build-up happens sooner in the compression stroke, leading to higher peak cylinder pressures. Maximum BMEP of 1.40 MPa was achieved at -5 °CA with an increase of 1.18% from the base model. However, if the SOC is too advanced, it can lead to excessive peak pressures (see Figure 5) and reduced efficiency, as in this case after SOC of -5 °CA.

The Maximum Pressure Rise Rate (MPRR) value is an important parameter in engine design and optimization, as it is closely related both to engine knock and noise. A higher MPRR can lead to increased knocking tendencies, which can negatively impact engine performance and durability. According to the literature [24–29], the MPRR value range of 1.0–1.5 MPa/degree is defined as the critical knock threshold. Exceeding this range may result in severe knocking, potentially causing damage to engine components, while staying within the range ensures smoother and more stable combustion. SOC timing of -15 °CA and -20 °CA exceeds the minimum knock limit of 1 MPa/Degree MPRR. Where SOC timing of -5 °CA with 0.61 MPa/Degree of MPRR and SOC timing of -10 °CA with 0.87 MPa/Degree of MPRR can run safely without knocking at full load. Similar to these findings, an experimental study indicated that advancing spark timing with hydrogen-natural gas blends increases the maximum pressure rise rate (MPRR) and the risk of knock due to the high octane number of hydrogen [30]. Comparing the results with the diesel model, an increase of 30.87% in BMEP and a decrase in BTE of 0.7% at SOC timing of -5 °CA was achieved.

Figure 4 illustrates the impact of SOC timing on the development of maximum mean pressure and temperature within the cylinder. As SOC timing was advanced, both in-cylinder pressure and temperature increased. Comparing to the base model, with the optimal SOC timing of -5 °CA, the rate of increase in maximum mean pressure and temperature was 20.14% and 2.19%, respectively. The maximum rate of increase obtained at SOC timing of -20°CA as 70.5% for maximum mean pressure and 12.14% for maximum mean temperature. Also at the same SOC timing, when compared to the diesel model, 87.5% for maximum mean pressure and 40.23% for maximum mean temperature was observed.

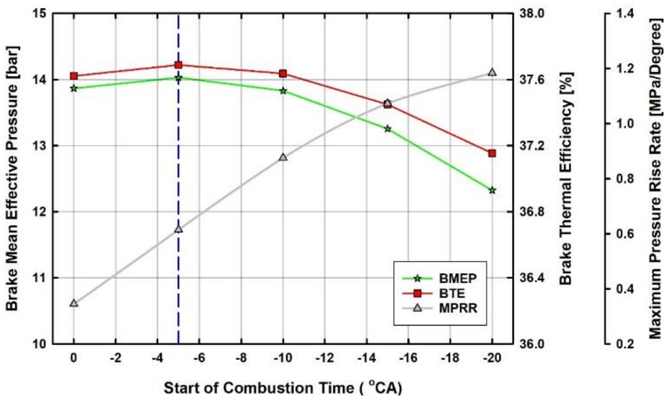

Figure 3. Change of brake mean effective pressure, brake thermal efficiency, and maximum pressure rise rate with start of combustion time

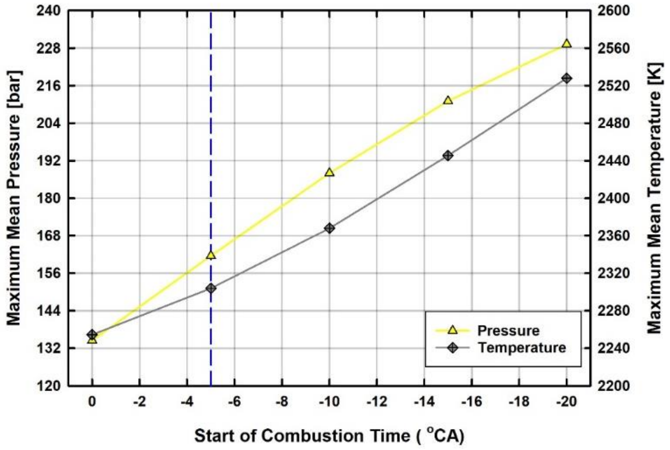

Figure 4. Change of maximum mean pressure and temperature with start of combustion time

As the mean temperature in the cylinder increases, cooling requirements of cylinder heads, pistons, valves, exhaust manifolds, and turbocharger housings will also increase; most internal combustion engine pistons are constructed from aluminum alloys, and their maximum operating temperature should not exceed 66% of the alloy's melting point, which is approximately 600°C [31]. The temperature values in Figure 4 can also be defined as the safe zone since they provide these values after cooling.

Additionally, peak cylinder pressure (PCP) limitations must be taken into account for SOC time of -15 and -20 °CA. Traditional designs were limited to PCPs of approximately 200 bar due to material constraints, but advancements in materials and manufacturing have pushed this limit higher. Studies, have demonstrated that cylinder heads are capable of operating at 250 bar using alloyed gray cast iron and compacted graphite iron, highlighting enhanced durability and fatigue resistance [32,33]. Materials such as martensitic steels and nickel-based superalloys have been explored to address the increased mechanical and thermal loads at elevated PCPs, indicating that future heavy-duty diesel engines could achieve PCPs exceeding 250 bar while maintaining reliability and affordability [32]. Exceeding these limits can lead to thermal fatigue and mechanical failure. As in our case shown in Figure 4, SOC timing of -15 and -20 °CA exceeds 200 bar and therefore mechanical strength have to be considered.

Figure 5 presents the in-cylinder pressure variation over crank angle degrees at different SOC timings. An advanced SOC induces a rapid increase in both temperature and pressure, thereby increasing the maximum in-cylinder pressure and moving its occurrence to an earlier crank angle [34]. Maximum in-cylinder pressure was obtained as 229.26 bar at -20 °CA. For the optimal SOC timing of -5 °CA, 161.54 bar of in-cylinder pressure were obtained. With the advancing SOC time, in-cylinder pressure values increased due to increased time available for the fuel-air mixture to undergo combustion, resulting in higher peak pressures.

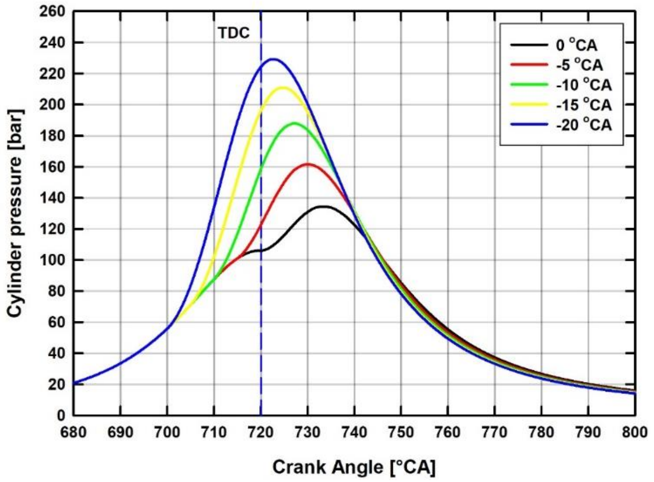

Figure 5. Change of in-cylinder pressure with start of combustion time

In Figure 6, the variation of the in-cylinder rate of heat release values over crank angle degrees at different SOC timings are given. At SOC timing of 5 °CA the maximum heat release rate (HRR) value obtained as 173.38 J/deg with a decrease of 1.47% compared to the base model. It was observed that advancing the start of combustion results in lower maximum HRR values. The maximum HRR value at SOC time at -20 °CA is 2.88% lower compared to the base model. To achieve higher thermal efficiencies, the crank angle at where 50% of the heat is released should be just after TDC [29].

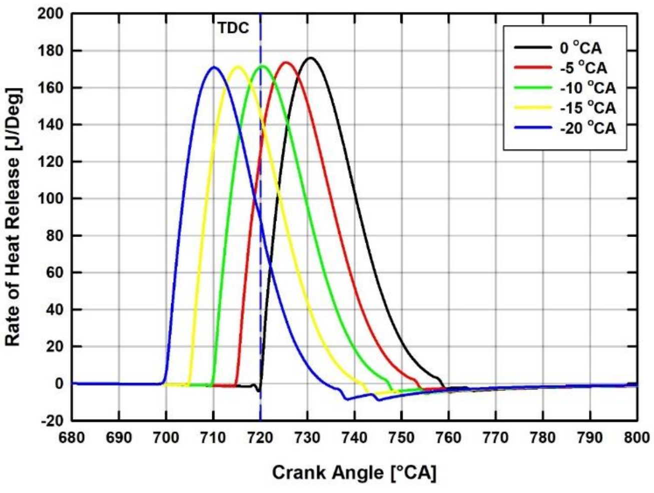

Figure 6. Change of in-cylinder heat release rate with start of combustion time

In Figure 7, the effects of different SOC timings to in-cylinder temperature variation over crank angle degrees values are shown. When the HRR and in-cylinder temperature values were analysed together, it was observed that the earlier onset of HRR caused by advanced combustion led to earlier and higher peak temperatures. At SOC timing of -20 °CA maximum temperature was observed as 2527 K at 727 °CA which is still on the safe zone.

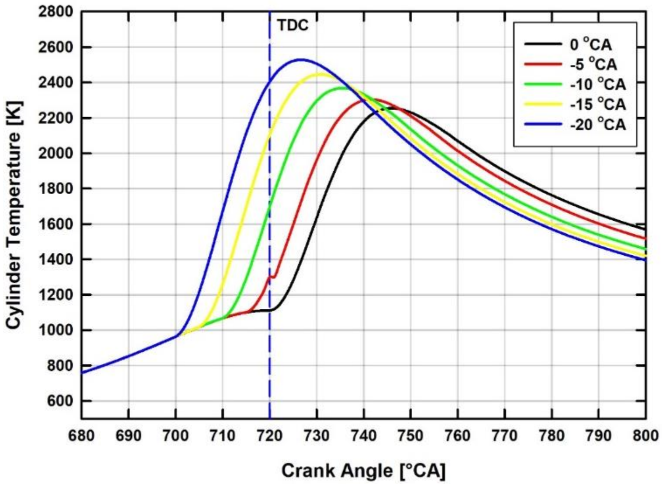

Figure 7. Change of in-cylinder temperature with start of combustion time

Figure 8 presents the effects of varying SOC timings on in-cylinder emission values. The emission values are normalized relative to the baseline model, where the SOC timing of 0 corresponds to TDC.

As advanced SOC leads to higher in-cylinder temperatures and since NO_X formation is highly temperature-dependent, the elevated peak temperatures enhance thermal NO_X production. It was observed that NO_X values increased by up to 1.52 times with the increase in in-cylinder temperature with advanced SOC.

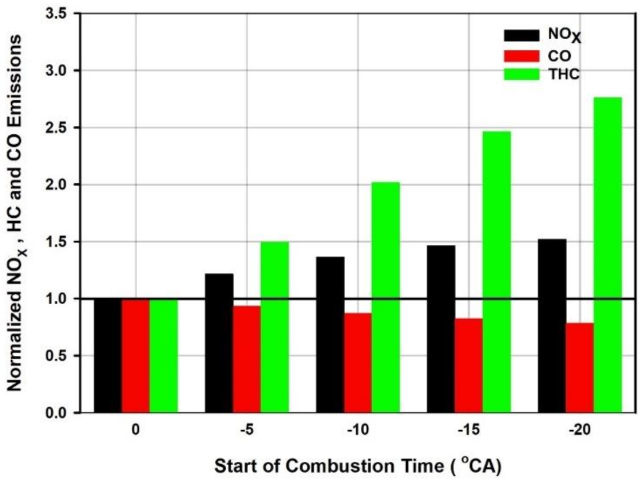

Figure 8. Change of in-cylinder normalized emissions with start of combustion time

In the experimental study by Hu and Huang, it was reported that HC emissions result from the incomplete combustion of the air-fuel mixture trapped in the upper crevice between the piston and cylinder wall. Additionally, the study findings revealed that advanced ignition timing increases HC emissions in natural gas and hydrogen-fueled engines, producing higher HC emissions compared to delayed ignition timing [35]. In the Vibe 2-Zone model used in the study, calculations are made as burned and unburned zones. While the high temperature in the burned zone reduces emission levels by promoting the oxidation of carbon monoxide (CO), lean mixture and lack of turbulence in the unburned zone may lead to an increase in hydrocarbon (HC) emissions. Late start of combustion (SOC) reduces HC emissions by providing homogenization of the unburned zone. This homogenization process is essentially possible with longer mixing time, turbulence effect, effective vaporization of the fuel and molecular diffusion mechanisms. The homogenized mixture provides more efficient oxidation of hydrocarbons and thus decreases HC emissions. In this study, it was found that advanced SOC significantly increases THC emissions, with an observed maximum rise of up to 2.76 times due to less time for thorough mixing of the air-fuel mixture.

However, the decrease in temperature in the cylinder during late SOC limits the conversion of CO to carbon dioxide (CO_2). This situation causes an increase in CO emissions due to the low temperature in the burned zone. Thus, late SOC has opposite effects on HC and CO emissions. With an advanced SOC timing of -20° CA, CO emissions were reduced by up to 0.78 times due to the increased oxidation efficiency.

4. CONCLUSION

The effects of advancing the SOC timing on engine performance, in-cylinder combustion characteristics and emission values in a converted engine using methane-hydrogen as fuel with spark ignition and a high compression ratio are:

- Considering the MPRR value as the knock threshold while using a fuel mixture of natural gas with 10% hydrogen, SOC timings of -5 and -10 °CA were found to be safe from knocking. However, knocking occurred when the start of combustion was further advanced to -15 °CA. This indicates that while moderate SOC advancement can be beneficial, excessive advancement leads to detonation and instability, which must be carefully managed in practical applications.
- Advancing the start of combustion by -5 °CA has improved engine performance values like BP, BSFC, BTE, and BMEP. These improvements highlight the potential of optimized SOC timing in achieving better fuel economy, higher power output, and improved thermal efficiency, making it a viable strategy.
- For SOC time of -15 and -20 °CA, temperature and pressure limitations have to be considered. At these advanced timings, the risk of exceeding material limits increases, potentially leading to mechanical failures, increased wear, and reduced engine lifespan.
- Advanced SOC, enhances NO_X and HC production while reducing CO emissions.

Finally, it was observed that in a converted engine using methane-hydrogen as fuel with spark ignition and a high compression ratio, advancing the start of combustion timing by up to 5 °CA improved engine performance while the emission values vary. However, excessive advancement resulted in sudden peak pressures, which negatively affected performance and increased the risk of knocking. This underscores the importance of precise SOC optimization to achieve a balance between performance gains and emission control while ensuring engine durability and stability.

Future research recommendations include; optimizing SOC timing for different hydrogen blends, analyzing detailed knock, thermal and mechanical stress limits to enhance engine durability. Additionally, studies on combustion stability, emissions control, alternative fuels, and transient performance will further refine SOC strategies for improved efficiency and lower emissions in methane-hydrogen-fueled engines.

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Conflict of Interest Statement

The authors declare that there is no conflict of interest in the study.

CRediT Author Statement

Fatih Aktas: Conceptualization, Visualization, Investigation, Methodology, Data curation, Software, Review & Editing.

Yasarata Korkmaz: Visualization, Methodology, Software, Writing - Review & Editing.

Gonca Kethudaoglu: Conceptualization, Visualization, Methodology, Software, Writing - Review & Editing.

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