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Computational Analysis of HCCI Engine using Bioethanol-Diesel Blends as a Fuel

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ABSTRACT

Bioethanol has long been recognized as a viable alternative fuel for diesel engines, offering significant potential to reduce emissions, particularly carbon monoxide (CO) and nitrogen oxides (NOx), when utilized in homogeneous charge compression ignition (HCCI) engines. Despite this promise, the production and optimization of bioethanol-diesel blends present considerable challenges, necessitating further investigation to address growing diesel fuel demands and stricter environmental regulations. This study explores the feasibility and impact of bioethanol-diesel blends on HCCI engine performance, focusing on combustion and emissions characteristics. Using Chemkin-PRO simulation software, blends with varying bioethanol concentrations (E10, E15, E20, and E30) are analyzed and compared against conventional n-heptane (diesel) fuel. The results demonstrate that increasing the bioethanol content in diesel blends leads to notable reductions in emissions. Specifically, NOx emissions were reduced by 52%, 59%, 69%, and 91% for E10, E15, E20, and E30, respectively. Similarly, CO emissions decreased by 19%, 26%, 30%, and 31% with the same blends. These findings highlight the potential of bioethanol-diesel blends to serve as environmentally sustainable alternatives to conventional diesel fuel, supporting efforts to mitigate emissions in HCCI engine applications.

1. Introduction

Over the past decade, the transportation industry has undergone significant transformation. For instance, there are nearly 100,000 ships of varying sizes, ages, and energy efficiencies operating globally every day for diverse purposes. Shipping, a key sector of transportation, heavily relies on diesel engines due to their superior efficiency compared to gasoline engines. However, the exhaust gases from diesel engines are a major contributor to air pollution at sea [1,2]. These exhaust emissions include sulfur oxides (SOx), carbon monoxide (CO), nitrogen oxides (NOx), unburnt

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hydrocarbons (UHC), water vapor, and smoke. These emissions are concerning because of their negative consequences on ecosystems, and human health [3,4]. Furthermore, global energy consumption surged in the 20th century due to industrialization, leading to challenges like inadequate diesel fuel reserves, exemplified by the 1970 oil crisis [5]. The growing energy demand will continue to strain supply security, as resources are unevenly distributed worldwide. With the global population expected to reach 8 to 10.5 billion by 2050 and rapid economic growth in emerging economies, energy consumption will increase significantly [6]. To address these challenges, it is crucial to use natural resources more efficiently and expand the adoption of renewable energy. Consequently, the shortage and escalating cost of diesel fuel and heightened environmental awareness have spurred scientific efforts to find alternative energy sources.

Biofuels obtained from renewable sources like plants and organic waste present a sustainable strategy to combat the depletion of fossil fuels and the greenhouse gas effect. These biofuels are categorized into different generations based on their feedstock and production methodologies [7-9]. First-generation biofuels are derived from edible crops such as corn, sugarcane, and vegetable oils. In contrast, second-generation biofuels utilize non-edible biomass, including agricultural residues, wood, and municipal waste. Third-generation biofuels, encompassing energy-dedicated crops and algae, represent a more advanced and sustainable innovation.

Other benefits of biofuels include the availability of cheap and plentiful feedstock, economical manufacturing techniques, and scalability for use, especially in developing countries [10]. As shown in Figure 1, biofuels were produced majorly by the USA at 70%, followed by Asia and Europe at 15% each and the rest of the world produced 0.3% [11]. Most biofuels are used for transportation, but they can also be used to generate energy and heat, especially in the USA [12].

Bioethanol has emerged as a promising candidate due to its renewable nature and lower greenhouse gas emissions. When blended with diesel, bioethanol has demonstrated the ability to improve combustion characteristics and reduce harmful emissions [13,14]. In 2022, ethanol fuel accounted for most of the biofuel production (82%) and consumption (75%) in the U.S, as shown in Figure 2.

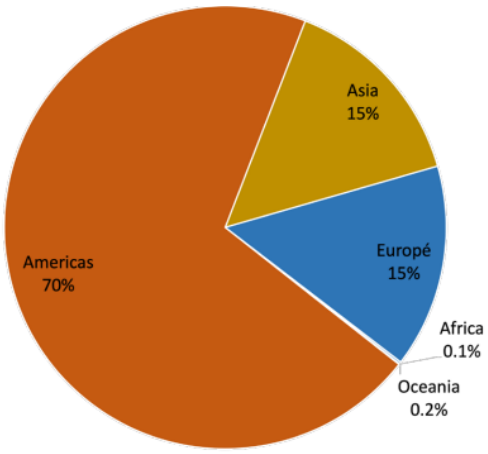

Fig. 1. Liquid biofuels production in continents in 2019. Liquid biofuels are the sum of biogasoline, biodiesel and other liquid biofuels [11]

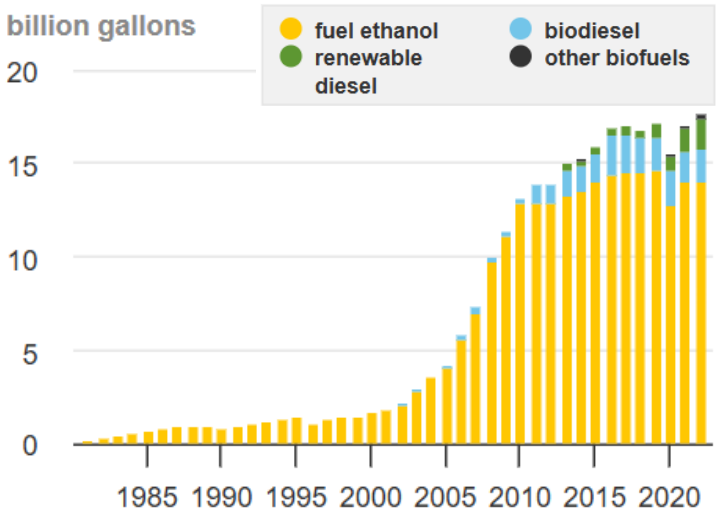

Fig. 2. US biofuels consumption by major type in the year of 1982 until 2022 [15]

Pure ethanol cannot be used directly in diesel engines, but it can be utilized in blends with diesel fuel. Ethanol has various benefits for use as a fuel in diesel engines, including low viscosity, high oxygen content, a high hydrogen-to-carbon (H/C) ratio, low sulfur content, and high evaporative cooling capacity, all of which improve volumetric efficiency [16-18]. The lower viscosity of ethanol compared to diesel improves fuel atomization in the cylinders, facilitating better air-fuel mixing when blended with diesel. Ethanol's high latent heat of evaporation enhances volumetric efficiency by cooling the intake and compression strokes when used in blends with diesel or biodiesel [19].

The homogeneous charge compression ignition (HCCI) engine, known for its high thermal efficiency and low NOx emissions, provides an ideal platform to study the effects of bioethanol-diesel blends [20]. However, the complex interactions between bioethanol and diesel require a deeper understanding, particularly in fuel blending, combustion dynamics, and emission characteristics. In this study, bioethanol blends with diesel are utilized as an alternative fuel, with n-heptane employed to represent diesel fuel in the simulations. N-heptane, with a cetane number of approximately 57, closely matches the cetane number of conventional diesel fuel, making it an appropriate surrogate for simulating diesel combustion processes. Similarly, ethanol represents bioethanol due to its comparable physical and chemical properties. The bioethanol-diesel blends investigated in this study include E10, E15, E20, and E30, corresponding to bioethanol concentrations of 10%, 15%, 20%, and 30%, respectively. To ensure the accuracy of the simulations, the initial engine design data was validated using experimental pressure data from a previous experiment conducted on diesel fuel. This comparison provided a baseline for verifying the reliability of the simulation results before proceeding with the combustion and emissions analyses.

2. Methodology

The Chemkin-PRO software was employed for the simulation of homogeneous charge compression ignition (HCCI) engines. Chemkin-PRO includes a predefined model, the Closed Internal Combustion Engine Simulator, specifically designed to simulate combustion processes within a closed system. The next step involved defining the combustion mechanism, or chemistry set, to represent the fuel behavior during combustion. Since n-heptane is a major component of diesel fuel and shares similar properties, it was used as a surrogate for diesel fuel. The diesel and n-heptane model fuel library were selected to describe the combustion process for both pure diesel and bioethanol-diesel

blends. For the ethanol blends, the same chemistry set was utilized, following the surrogate blending methodology developed by [21]. Chemkin-PRO's extensive library of over 60 fuel components—spanning carbon numbers from 1 to 20 and various chemical classes including linear and branched alkanes, olefins, aromatics, alcohols, esters, and ethers—was integral to accurately representing these fuels. This library allows the formulation of surrogates to represent a wide range of fuels, including gasoline, diesel, renewable fuels, and several additives.

Following the definition of the combustion mechanism, the engine parameters were configured in the Reactor Properties Panel. The engine cycle was modeled to simulate the closed system operation between intake-valve closure (IVC) and exhaust-valve opening. Engine events were expressed in terms of crankshaft rotation angles relative to the top dead center (TDC). For the test engine, the IVC occurred at 160° before TDC (BTDC). The simulation ran for 280 crank angle degrees, with initial conditions for the gas mixture set to a pressure of 107,911 Pa (1.065 atm) and a temperature of 447 K. The detailed specifications of the engine used in the simulation are presented in Table 1.

To account for heat transfer, two approaches were considered: an adiabatic model that assumed no heat loss and a model incorporating heat loss through the cylinder wall. The Woschni correction was applied to improve the estimation of gas velocity inside the cylinder, further enhancing the simulation's accuracy.

Table 1
Geometric properties of the diesel engine

Starting crank angle (°TDC)	-160.0°
Engine crank angle duration	280.0°
Engine speed	1800 rpm
Compression ratio	17.0
Bore	106.0 mm
Stroke	127.0 mm
Connecting rod length	203.0 mm
Equivalence ratio	0.6

Fuel composition was defined based on molar fractions, with the total molar fraction set to 1.0. The molar fractions for each species in the initial fuel mixture for n-heptane (diesel) fuel and other fuels are provided in Table 2. For ethanol-diesel blends, similar methodologies were followed, adjusting the molar fractions accordingly to reflect the blending ratios.

Table 2
Compositions of fuel used in this study

	Molar fractions				
Species	n-Heptane (diesel)	10% ethanol blends (E10)	15% ethanol blends (E15)	20% ethanol blends (E20)	30% ethanol blends (E30)
nC_7H_{16}	0.0308	0.02892	0.02738	0.02610	0.02276
C_2H_5OH (ethanol)	0	0.00428	0.00582	0.00608	0.01044
CO_2	0.0326	0.0338	0.0338	0.03406	0.0338
H_2O	0.0609	0.0621	0.0621	0.06236	0.0621
N_2	0.6861	0.6873	0.6873	0.68756	0.6873
O_2	0.1836	0.1836	0.1836	0.1836	0.1836

3. Results

3.1 Validation Study

For validation purposes, the pressure data from a previous study was utilized and compared with the simulation results obtained in this study. Given that one of the fuels tested in the study is n-heptane (a diesel surrogate), the experimental data was selected for comparison to validate the simulation results [22]. Figure 3 illustrates the comparison between the simulation data and experimental data, showing pressure as a function of crank angle. It can be observed that the simulated pressure does not achieve the same peak as the experiment, with a slight discrepancy observed in the pressure rise and fall timings. However, the difference between the peak pressures of the simulation and the experiment is less than 10%, indicating that the simulation results are in good agreement with the experimental data and can be considered valid for this study.

To evaluate whether the validation is acceptable, a t-Test: Paired Two Samples for Means was conducted to analyze the validation results. This statistical method is used to determine if the null hypothesis—that the means of two populations (in this case, simulation and experimental results) are equal—can be accepted or rejected. Table 3 presents the results of the t-Test analysis comparing the pressure data from the simulation and the experiment. From the table, it was observed that the P-value (P=0.164226) is greater than the significance level (α=0.05). Therefore, the null hypothesis is accepted, indicating no statistically significant difference between the simulated and experimental pressure data. This suggests that the simulation results are in reasonable agreement with the experimental results.

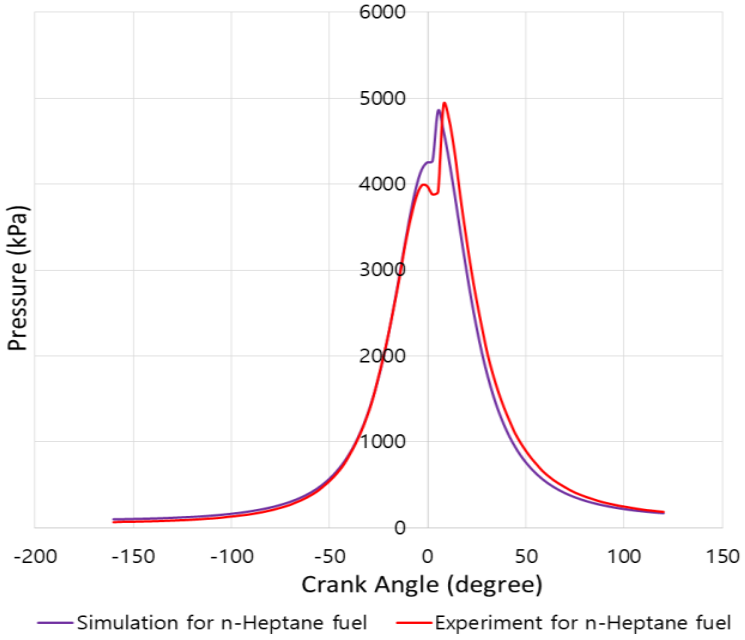

Fig. 3. Comparison of pressure results between simulation and experiment for n-heptane fuel

Table 3
Results of the t-Test: Paired Two Sample for Means comparing the pressure data from simulation and experiment for n-heptane fuel

	Variable 1	Variable 2
Mean	989.981	1012.97
Variance	1642804	1688445
Observations	101	101
Pearson correlation	0.991932	
Hypothesized mean difference	0	
df	100	
t Stat	-1.40128	
P(T<=t) one-tail	0.082113	
t Critical one-tail	1.660234	
P(T<=t) two-tail	0.164226	
t Critical two-tail	1.983972	

3.2 In-cylinder Pressure

The analysis of the in-cylinder peak pressures for different fuel blends run in an HCCI engine at 1800 RPM reveals notable trends influenced by the addition of ethanol to diesel, as shown in Figure 4. Among the tested fuels, n-heptane (diesel) demonstrated the highest peak pressure of 4853 kPa. For the ethanol-diesel blends, the results showed a progressive reduction in peak pressure with increasing ethanol content. The E10 and E15 fuels exhibited no significant variation in peak pressure, with their values closely overlapping that of n-heptane. This indicates that up to 15% ethanol blending does not meaningfully alter the in-cylinder combustion dynamics compared to pure diesel. The similarity in peak pressure suggests that the heating value and latent heat of vaporization for these lower ethanol blends are still close enough to diesel to sustain similar pressure profiles.

In contrast, the E30 fuel exhibited a notably lower peak pressure of 4208 kPa, representing a 13.29% reduction compared to n-heptane. This decline is attributed to the higher ethanol content, which introduces distinct thermodynamic effects. Ethanol has a lower heating value than diesel, reducing the total energy released during combustion [23]. Additionally, ethanol's higher latent heat of vaporization absorbs more heat during the phase change from liquid to vapor, leading to a reduction in the initial temperature and pressure of the air-fuel mixture. These combined effects elongate the ignition delay and reduce the peak pressure achieved during combustion.

The trends observed are consistent with the hypothesis that increasing ethanol content leads to over-dilution of the charge and slower combustion due to ethanol’s thermophysical properties. The longer ignition delay caused by the higher latent heat of vaporization in ethanol-diesel blends plays a critical role in moderating the peak pressures [24].

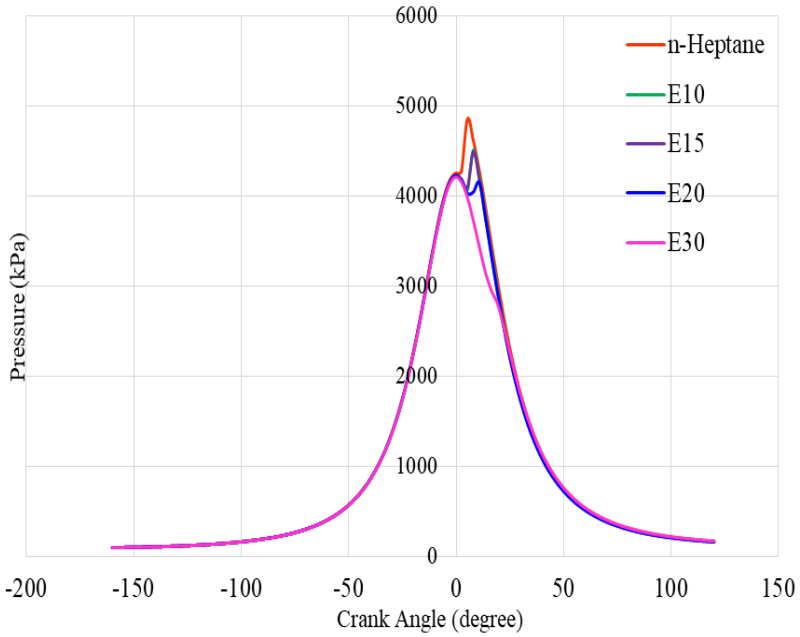

Fig. 4. The in-cylinder pressure for various fuels

3.3 In-cylinder Temperature

Figure 5 illustrates the in-cylinder temperature distribution for different fuel types under identical working conditions and at the same crank angle. E30 has the lowest peak temperature, while n-heptane achieves the highest temperature. The elevated latent heat of vaporization of ethanol absorbs substantial thermal energy during vaporization, cooling the air-fuel mixture. This effect is consistent with Gay-Lussac's Law, which establishes a direct relationship between gas pressure and temperature [25]. The cooling effect reduces cylinder pressure for ethanol-diesel blends, thereby lowering the combustion temperature.

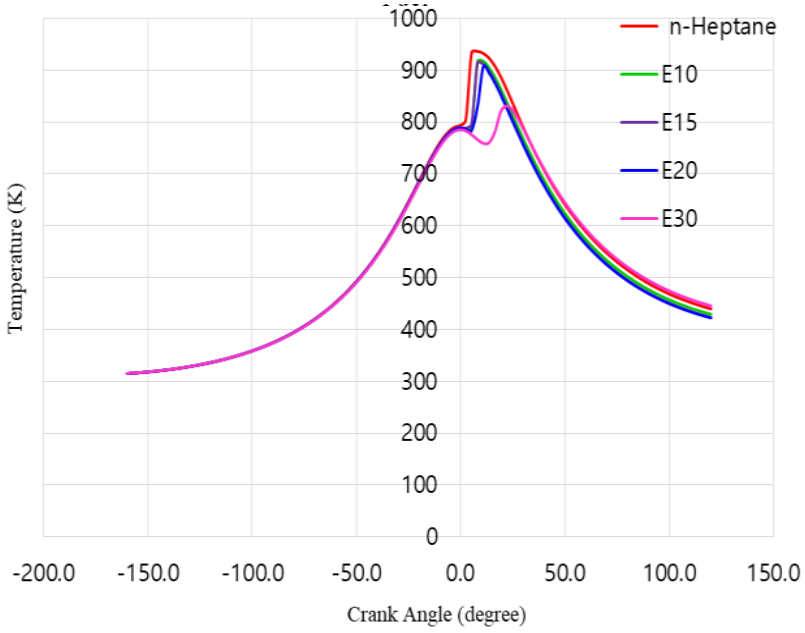

Fig. 5. The in-cylinder temperature for various fuels

3.4 Heat Release Rate

Figure 6 highlights the variation in the heat release rate (HRR) with the crank angle for n-heptane and bioethanol-diesel blends (E10, E15, E20, and E30). The HRR represents the rate at which heat is released during combustion, providing insights into combustion efficiency and the dynamics of fuel-air interactions. The maximum HRR is observed for the E20 blend, reaching a peak of 80.0 J/degree at 8˚ ATDC. The HRR trends in descending order are E20 > E30 > E15 > E10 > n-heptane, indicating that ethanol-diesel blends consistently outperform pure diesel in terms of HRR. This can be attributed to improved fuel-air mixing and more complete combustion facilitated by ethanol's oxygen content.

The second-highest HRR is recorded for E30, followed by E15 and E10. Despite E30's higher ethanol content, its HRR is slightly lower than E20, likely due to the dominating effect of ethanol's higher latent heat of vaporization. The increased heat absorption during vaporization reduces the available thermal energy, moderating the HRR compared to E20. In the case of n-heptane, the HRR is the lowest among all fuels, reflecting the absence of ethanol's oxygenating and mixing-enhancing effects.

Ethanol-diesel blends exhibit longer ignition delays compared to n-heptane, especially at higher ethanol concentrations. The ignition delay is the period between the start of fuel injection and the onset of combustion. For bioethanol-diesel blends, the longer delay period allows more fuel to accumulate in the combustion chamber. This accumulation contributes to a rapid and higher HRR once ignition occurs, as observed with E20 and E30. The prolonged ignition delay is influenced by ethanol's higher latent heat of vaporization, which lowers the initial temperature of the air-fuel mixture. Additionally, ethanol's lower cetane number compared to diesel reduces its readiness to auto-ignite, further contributing to the delay [26].

Ethanol's hydroxyl group provides additional oxygen atoms, promoting efficient combustion and better heat release [27,28]. The enhanced mixing of ethanol-diesel blends ensures more homogeneous combustion, reducing UHC and improving overall energy release. However, the reduced HRR of E30 compared to E20 suggests that there is an optimal ethanol concentration (likely near 20%) where the benefits of ethanol's oxygen content and mixing efficiency outweigh the cooling effects of its latent heat of vaporization.

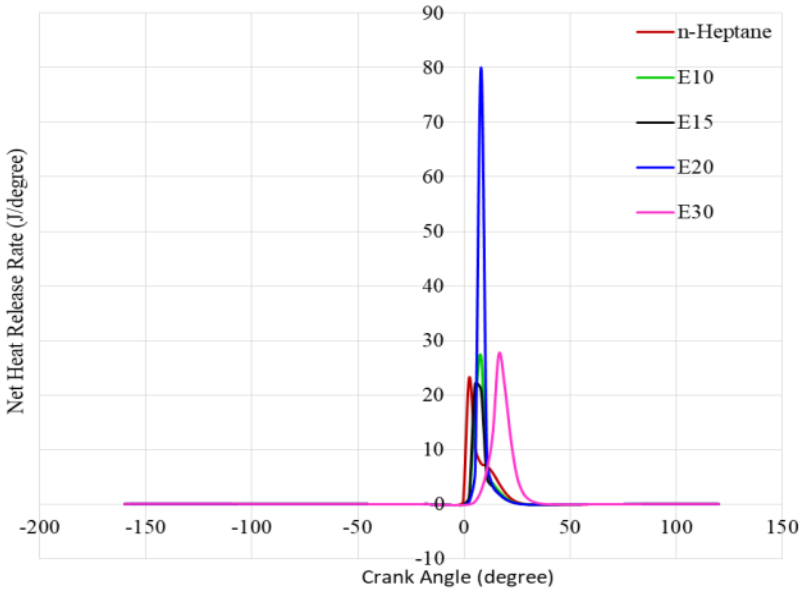

Fig. 6. The heat release rate for various fuels

3.5 Emission Profiles

The emission reductions associated with ethanol-blended fuels, as shown in Figures 7 and 8 for E10, E15, E20, and E30, provide significant insights into their potential environmental benefits. The results reveal a clear trend of reducing emissions of NOx and CO as the ethanol content increases. Specifically, the reduction in NOx emissions ranges from 52.44% for E10 to a remarkable 91.81% for E30. This substantial reduction is primarily attributed to ethanol's ability to lower combustion temperatures. By reducing peak flame temperatures during combustion, ethanol blends prevent the formation of excessive NOx. CO emissions also show a progressive decrease across the ethanol blends, from 19.63% for E10 to 31.22% for E30. This reduction is indicative of the enhanced combustion efficiency that ethanol offers due to its oxygen content. The oxygenates in ethanol help facilitate more complete combustion, leading to fewer UHC and thus reducing CO formation. Compared to n-heptane, which tends to produce higher CO emissions due to incomplete combustion, ethanol blends perform significantly better in terms of CO reductions. While lower ethanol blends, such as E10, exhibit a 3.56% reduction in HC emissions, higher ethanol blends, particularly E30, show a slight increase in HC emissions, with a -2.02% change. The trend suggests that the benefits of ethanol in reducing HC emissions diminish as the ethanol content increases, likely due to issues with combustion efficiency at higher ethanol concentrations. At higher ethanol levels, the mixture may experience incomplete combustion or issues related to vaporization, which can contribute to increased HC emissions.

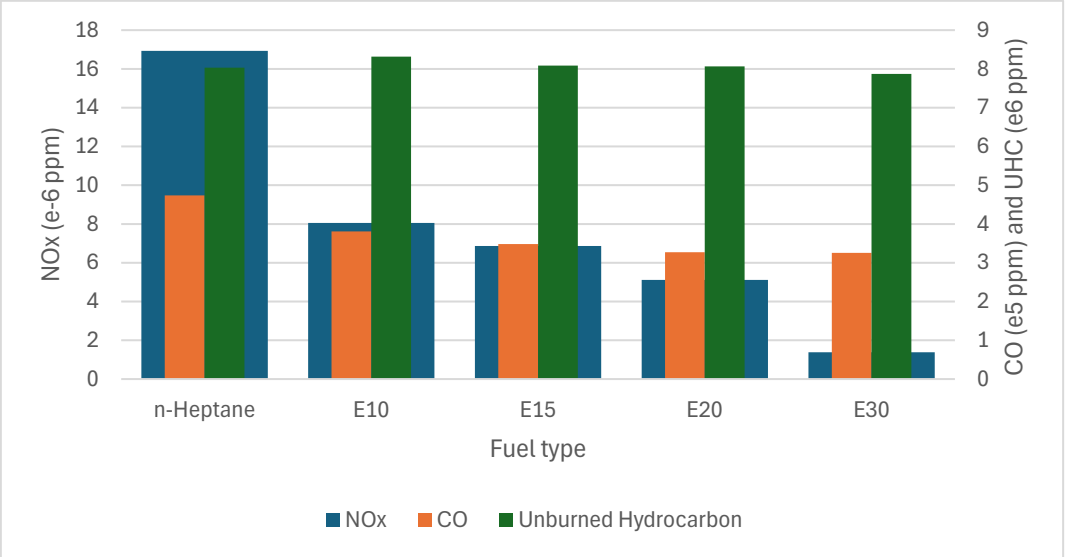

Fig. 7. NOx, CO and UHC emissions for various fuels

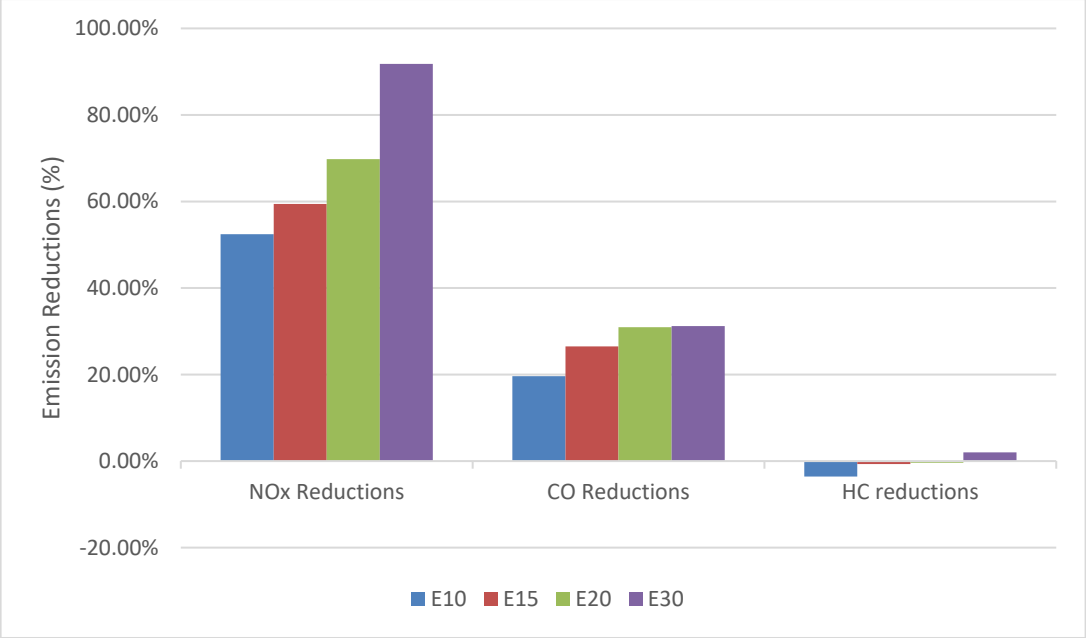

Fig. 8. Emission reductions in the diesel engine using various fuels, compared to n-heptane

4. Conclusions

In summary, ethanol-diesel blends exhibit longer ignition delays, particularly at higher ethanol concentrations, due to the higher latent heat of vaporization of ethanol. This delay leads to a higher fuel accumulation in the cylinder, contributing to a higher HRR at the start of combustion for blends like E20 and E30. The E20 blend achieved the highest HRR, followed by E30, suggesting that ethanol's properties contribute to improved fuel-air mixing and more complete combustion. However, E30 showed a slight reduction in HRR due to the cooling effects of ethanol, which moderates the overall combustion process.

Adding ethanol to diesel results in a substantial reduction in NOx emissions, with the highest reduction observed in the E30 blend (91.81% compared to n-heptane). This reduction is primarily due to ethanol's cooling effect, which lowers peak combustion temperatures and reduces the formation of NOx, which is highly temperature-dependent. The oxygen content in ethanol also promotes more complete combustion, further mitigating NOx formation by minimizing the formation of high-temperature zones within the cylinder.

CO emissions decrease with increasing ethanol content in the fuel blends, with the highest reduction observed in E30, which shows a 31.22% decrease compared to n-heptane. The reduction in CO emissions is a result of better fuel-air mixing and the oxygenating effect of ethanol, which leads to more efficient combustion. Ethanol's ability to enhance combustion efficiency helps to reduce incomplete combustion, a key contributor to CO formation.

There is a slight increase in UHC emissions for the ethanol blends, particularly in E10, E15, and E20, which shows a slight increase in UHC (up to 3.56%) compared to n-heptane. However, the UHC emissions slightly decrease in the E30 blend (-2.02%), indicating that the higher ethanol content may improve combustion efficiency in some cases, leading to lower UHC emissions. This could be due to the further oxygenation and better mixing of the air-fuel mixture, particularly at higher ethanol levels.

While higher ethanol content in the blend, such as E30, provides significant environmental benefits through reductions in NOx and CO emissions, it also introduces trade-offs, such as a reduction in HRR and potential performance losses due to the cooling effect. The optimal ethanol

blend appears to be around E20, where NOx emissions are significantly reduced without compromising HRR and combustion efficiency to the same extent as in E30.

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