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CFD analysis of replacing diesel with CH_4/n-heptane, investigating the effect of fuel injection timing on ignition delay, engine efficiency, and emissions

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ABSTRACT

The engine performance can change after diesel fuel is replaced with a blend of CH_4 and n-heptane at varying percentages. This study investigates the effects of fuel injection timing on the performance, efficiency, and emissions of a dual-fuel diesel engine running on a CH4 and n-heptane mixture. The analysis uses computational fluid dynamics (CFD) and AVL Fire software with advanced chemical kinetics tools, such as Chemkin, to transition from liquid to gaseous fuels.

To accomplish this, the fuel injection timing was adjusted to three settings: 22° before top dead center (BTDC), 18° BTDC, and 14° BTDC. Methane was blended with n-heptane at ratios of 90 %:10 %, 85 %:15 %, and 75 %:25 %. The findings from the numerical simulations demonstrated that prolonging the fuel injection duration in the dual-fuel diesel engine resulted in an escalation in the temperature within the combustion chamber and an augmentation in the maximum cylinder pressure. Additionally, both the ignition delay and the distance from top dead center to the peak ignition pressure were diminished. With the rise in peak cylinder pressure, the output torque experienced a 16 % increase. Conversely, increasing the ratio of liquid fuel in the blend resulted in a shorter ignition delay, which caused a decline in peak cylinder pressure, accompanied by a 17 % drop in output torque and a 70 % decrease in indicator power. The implementation of early fuel injection at elevated engine speeds led to an enhancement in indicator power and an improvement in emissions, culminating in a 31 % reduction in nitrogen oxides (NOx) and a 16 % decrease in soot levels.

1. Introduction

Diesel engines have a significant advantage over gasoline engines in that they produce higher levels of torque and power due to their greater thermal efficiency and higher combustion pressures [1,2]. Due to their high overall efficiency [3], Diesel engines play a pivotal role in the mechanization of agricultural practices, contributing to the augmentation of efficiency and productivity in farming operations [4].

The process of fuel igniting on its own in a diesel engine is affected by the fluid that carries the fuel into the engine [5]. There are three ways to study how things burn: in the lab, using math and science, and computational fluid dynamics (CFD). CFD simulations are seen as a new and affordable way to study how fuels burn in engines [6,7].

Computational Fluid Dynamics (CFD) can evaluate the performance of internal combustion engines in two main ways: open-cycle and closed-cycle approaches [8–10]. Dual-fuel diesel engines are a special type of diesel engine that uses a combination of biodiesel and gaseous fuels as alternative fuels [11]. Alternative fuels offer advantages such as a strong oxygen bond and a simple chemical structure. However, the high activation energy of gaseous fuels presents a challenge to their independent use in CI engines [12].

Gaseous fuels with high activation energies pose a significant challenge to their direct use in compression ignition (CI) engines. These fuels require more thermal energy to ignite properly, which makes achieving consistent and reliable ignition more difficult. Consequently, engines

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Nomenclature

BTDC	Before top dead center
ATDC	After top dead center
GRI 3.0 mesh	Kinetic reaction (3)
K	Kelvin
t	time
V	Fluid flow velocity $\left(\frac{m}{s}\right)$
u	Horizontal component of fluid flow $\left(\frac{m}{s}\right)$
v	Vertical component of fluid flow $\left(\frac{m}{s}\right)$
w	Inside component of fluid flow $\left(\frac{m}{s}\right)$
$\widehat{U}_i$	The local velocity of the fluid in the horizontal direction, $\frac{m}{s}$
$\widehat{U}_j$	The local velocity of the fluid in the vertical direction , $\frac{m}{s}$
g_i	Earth's gravitational acceleration, $\frac{m}{s^2}$
$\widehat{P}$	Local fluid pressure (pa)
$\widehat{H}$	Local enthalpy (J)
$\dot{q}_g$	The rate of heat exchange of the gas mixture (J/s)
$\widehat{T}$	Fluid flow temperature, (K)
Y_i	Entered species
J_i	Species penetration
R_i	Species production rate after reaction
S_i	Source (spices)
LHV	Low heating value (MJ/Kg)
$\dot{m}_{\text{gaseous fuel}}$	Gaseous fuel mass rate, (Kg/h)
$\dot{m}_{\text{Diesel fuel}}$	Mass rate of diesel fuel, (Kg/h)
AFR	Air-fuel ratio

may misfire, experience partial combustion, or become unstable when using these gases alone. To address this issue, specialized ignition methods are typically implemented, or the gases are mixed with other fuels to facilitate easier and more stable combustion [13,14].

Many factors affect the quality of combustion in dual-fuel diesel engines [15]. Two key elements are fuel injection time and fuel blend ratio. Research conducted on a single-cylinder diesel engine in a laboratory setting has revealed that advances in methanol fuel injection time, at varying loads, reduce emissions of NOx and carbon dioxide [16,17].

For gas-fueled diesel engines (diesel/gas), the effect of base fuel parameters is critical and directly affects the efficacy of diesel engines that operate on gas fuel. By adjusting the percentage of the primary fuel injection ratio (diesel) to the compressed natural gas replacement fuel percentage, lean mixtures are formed. Based on laboratory tests, dual-fuel diesel engines emit more carbon monoxide pollutants at higher loads than the base fuel mode due to premature flame formation [18–20]. The ignition process in a dual-fuel diesel engine initiates with the initial combination of methane, oxygen, and hydrogen at elevated pressures, typically between 40 and 60 atmospheres [21,22]. The numerical analysis showed that combustion delay is linked to the occurrence of knocking during dual combustion processes [23]. To reduce knocking, it is essential to carefully control the fuel injection timing parameter [24].

Utilizing computational fluid dynamics (CFD) to address combustion challenges in dual-fuel diesel engines seeks to precisely examine the fluid dynamics equations involved in reactive flows [25]. By coupling the kinetics of methane-n-heptane combustion reaction and simulating the field using Kiva software, the behavior of the OM355 EU2 dual-fuel diesel engine has been studied. The findings show that higher base fuel injection rates result in longer ignition delays and a reduction in the pressure curve, which consequently leads to decreased torque and power across different loads [26–28]. The investigation into fuel injection impacts in homogeneous premixed engines through CFD analysis tools has demonstrated that, alongside examining and evaluating the combustion properties of dual-fuel diesel engines [29,30], it is possible to evaluate the performance parameters of the engine under varying load conditions [31,32].

A detailed study of fuel injection timing using CFD in Fire software can provide more information about how a diesel engine with dual fuels ignites [33]. By linking Fire and Chemkin software for advanced analysis of mixing and combustion mechanisms [34–36], the research shows that advancing the injection time in a diesel engine between 10 and 50 degrees before the top dead point improves the thermal efficiency of the engine and reduces the ratio of unburned methane pollutant and carbon monoxide emissions [37,38].

This study presents a novel, comprehensive investigation of the effects of fuel injection timing and mixture ratios on the performance and emissions of a dual-fuel OM355 EU2 diesel engine. The study employs advanced computational fluid dynamics (CFD) analysis integrated with Fire-Chemkin software. Unlike previous studies that often focus on limited parameters or experimental approaches, this work systematically explores three distinct injection timings (22°, 18°, and 14° CA before top dead center) combined with various methane and n-heptane blends. This approach offers unprecedented insights into the complex interactions that drive ignition delay, combustion chamber dynamics, and engine efficiency. The findings reveal significant correlations between injection parameters and critical performance metrics, showcasing substantial increases in output torque and notable reductions in harmful emissions. This innovative approach provides new perspectives for optimizing the operation of dual-fuel engines in agricultural and urban contexts. Ultimately, this research advances the current understanding of diesel engines and presents practical strategies for enhancing their sustainability and efficiency amid evolving energy challenges.

2. Materials and methods

2.1. Analyzed engine simulation conditions and parameters

The OM355 EU2 is a diesel engine that is commonly used in urban transport vehicles. The technical specifications of the engine analyzed are shown in Table 1.

The AVL Fire software was utilized to address the ignition issues in the dual-fuel diesel engine. For the initial grid creation, an average grid size of 2.2 mm was chosen. Fig. 1 illustrates the crown design of the OMEGA 1 piston along with the gridded solution field as rendered by the AVL Fire software.

Table 1
Engine Technical Specifications [39,40].

Characteristics	Value
Engine type – number of diesel cylinders	In line-6 cylinders
Injection type	Direct Injection
Engine air intake type	Turbocharger
Cylinder diameter	128 (mm)
Piston stroke length	150 (mm)
Length of the connecting rod	280 (mm)
Number of injector nozzle orifices	4
Diameter of injector orifices	0.31 (mm)
Compression ratio	16:1
Piston crown shape	Omega 1
Maximum engine torque	820 N/m at a speed of 1400 RPM
Maximum output power	179 kW at a speed of 2200 RPM

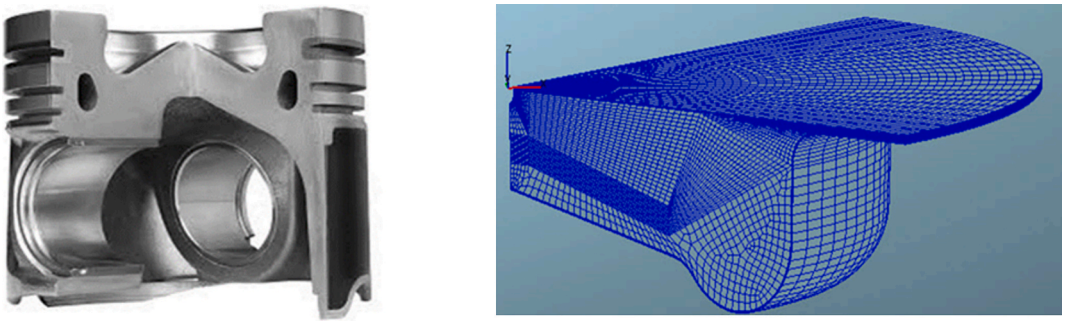

Fig. 1. OMEGA 1. The shape of the piston crown and the gridded solution field.

In most of the research, the simulation of dual-fuel diesel engines has been conducted using the Fire-Chemkin couples. By using the Fire-Chemkin couples, the reaction dynamics in dual-fuel diesel engines have been solved as an initial condition. For this study, the kinetic data of 42 species and 168 reactions from the GRI 3.0 mech mechanism were used. The initial and boundary conditions for the solution domain are presented in Tables 2 and 3.

Methane is considered a gaseous fuel, while n-heptane is a liquid fuel that is sprayed. Methane fuel has a high auto ignition temperature and a low heat value, which prevents flame front formation in compression ignition engines when directly injected. To continue the auto-ignition process in the presence of methane fuel, it is necessary to spray a certain ratio of liquid fuel into the combustion chamber as a primary flame generator. Table 4 shows the auto ignition characteristics of methane and n-heptane fuels.

A two-equation k-epsilon turbulence model was implemented to create optimal conditions within the combustion process, with the Eddy Breakup model selected for combustion analysis. The Dukowicz model was used to study the evaporation and penetration characteristics of the species, while the Kennedy/Hiryasu/Magnussen model, derived from Haywood's relation, was used to evaluate soot emissions. Other pollutants were treated as reactive species and their mass changes from the initial to the final state of the simulation were evaluated separately.

3. Governing equations

The equations formulated to simulate combustion in CI engines include the continuity equation, the momentum equation, the energy equation, the species transport equation, the turbulence equation, the combustion model, the emission equations, the air–fuel ratio equation, and the evaporating spray particle equations. Numerical discretization techniques are used to solve these equations and their interrelationships. The fluid flow dynamics within the solution domain are represented using frameworks based on Cartesian coordinates. When the fluid velocity at the center of the control volume is represented as a vector, the continuity equation can be formulated as follows:

$$-\frac{\partial V}{\partial t}=\frac{\partial(\rho u)}{\partial x}+\frac{\partial(\rho v)}{\partial y}+\frac{\partial(\rho w)}{\partial z} \tag{1}$$

The Naiver-Stokes equation describes the dependence between fluid flow velocity and pressure changes in multiple dimensions.

Table 2
Initial conditions for the solver domain [18].

Characteristic	Value
Injection start time	16° BTDC
Air valve closing	120° BTDC
Exhaust valve opening	116° ATDC
Initial pressure	1.2 bar
The initial temperature	360 K
The initial temperature of liquid fuel	353 K

Table 3
Initial and boundary conditions of the computational domain.

Characteristic	Value
Wall- temperature	590 K
Mesh movement-Temperature	600 K
Wall-temperature	580 K(Heat flux = 0)

Table 4
Auto ignition characteristics of methane and n-heptane fuels [41].

Flammability properties	Methane	n-Heptane
Low heating value	50.02 (MJ/kg)	42.8 (MJ/kg)
Flame Formation Range (%)	5 to 15	0.7 to 5
Auto ignition Temperature	813 K	477 to 533 K
Density	0.65 kg/ m^3	881 to 883 kg/m^3

$$\widehat{\rho}\frac{D\widehat{U_i}}{Dt}=\widehat{\rho}\frac{\partial\widehat{U_i}}{\partial t}+\widehat{\rho}\widehat{U_i}\frac{\partial\widehat{U_i}}{\partial x_j}=\widehat{\rho}g_i+\frac{\partial\widehat{\sigma_{ij}}}{\partial x_j}$$
$$=\widehat{\rho}g_i-\frac{\partial\widehat{P}}{\partial x_i}+\frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial\vartheta_i}{\partial x_j}+\frac{\partial\vartheta_j}{\partial x_i}-\frac{2}{3}\frac{\partial\vartheta_K}{\partial x_K}\delta_{ij}\right)\right] \tag{2}$$

where $\widehat{U}_i$ is the local fluid flow velocity, $\widehat{\rho}$ is the fluid density, g_i is the gravitational acceleration, $\widehat{P}$ is the fluid pressure, μ is the kinematic viscosity, ϑ_i, ϑ_j and δ_{ij} are elements of the stress tensor and the heat exchange between the fluid flow and the wall of the solution field, respectively [42]. The enthalpy equation quantifies the heat generated by combustion, the heat exchange at the walls, and the rate of heat release, all of which affect the performance metrics of the engine. The energy equation can be expressed in polynomial form:

$$\widehat{\rho}\frac{D\widehat{H}}{Dt}=\widehat{\rho}\left(\frac{\partial\widehat{H}}{\partial t}+\widehat{U_j}\frac{\partial\widehat{H}}{\partial x_j}\right)=\widehat{\rho}\dot{q}_g+\frac{\partial\widehat{P}}{\partial t}+\frac{\partial}{\partial x_i}\left(\widehat{\tau_{ij}}\,\widehat{U_j}\right)+\frac{\partial}{\partial x_i}\left(\lambda\frac{\partial\widehat{T}}{\partial x_j}\right) \tag{3}$$

where $\widehat{H}$ is the local enthalpy of the fluid flow, $\dot{q}_g$ is the exchange heat rate in the gas mixture, $\widehat{\tau}_{ij}$ is the shear stress between the fluid flow lines, λ is the fuel ratio, and $\widehat{T}$ is the fluid temperature.

With respect to species transfer, the specific amounts of all species, as well as their mixing, penetration, and evaporation behavior in the two fluid phases are detailed. To characterize the reaction kinetics in dual-fuel diesel engines, the behavior of each species at each stage of the reaction is evaluated, guided by the species transfer relationships [43].

$$\frac{\partial}{\partial t}(\rho Y_i)+\nabla(\rho\vec{v}Y_i)=-\nabla\vec{J_i}+R_i+S_i \tag{4}$$

where Y_i denotes the introduced species, ϑ symbolizes the viscosity of the fluid flow, J_i determines the penetration of the species, R_i represents the production rate of the species after the reaction, and S_i is the origin of the species produced during the previous reaction and introduced into

the new equation.

Calculating the air–fuel ratio in CI engines is essential to determine if the fuel mixture is lean or rich. In turbocharged diesel engines, the typical range of stoichiometric air–fuel ratios is 20:1 to 25:1. For this study, a stoichiometric air–fuel ratio of 23:1 was used [44].

$$AFR = \dot{m}_{gaseousfuel} . LHV_{gaseousfuel} \Big/ \dot{m}_{Diesel\ fuel} . LHV_{Diesel\ fuel} + \dot{m}_{gaseous\ fuel} . LHV_{gaseous\ fuel} \quad (5)$$

where $\dot{m}_{\text{gaseous fuel}}$ and $\dot{m}_{\text{Diesel fuel}}$ are the mass flow rate of gaseous fuel and injection fuel, respectively. The flow rate ratio of gaseous fuel to liquid fuel determines the volume percentage of the fuels.

4. Differences in simulation approach

Several fundamental differences in the modeling approach are involved when transitioning from liquid fuels, such as diesel, to gaseous fuels, such as methane (CH_4) and n-heptane, in AVL Fire.

Modeling fuel injection and combustion differs significantly between liquid and gaseous fuels. For liquid fuels, detailed spray and atomization models simulate droplet breakup, vaporization, and mixing. These models require complex physics and property data, such as viscosity and droplet size. Gaseous fuels, on the other hand, are introduced as a mass flow or mixture intake, which removes the need for spray and atomization and simplifies injection. Thermodynamically, liquids involve phase changes and vaporization, which complicates the process. Gases, on the other hand, undergo direct mixing, which simplifies the models. Liquids require detailed property characterization, whereas gases are mainly described by ideal or real gas laws. Liquid fuels often require complex spray and liquid-phase reaction models, whereas gaseous fuels use premixed or diffusion combustion models, which are faster and less computationally intensive.

4.1. Integration with Chemkin software

Transitioning from liquid to gaseous fuels often requires coupling AVL Fire with advanced chemical kinetics tools, such as Chemkin. This combination allows for the comprehensive simulation of complex gas-phase reactions, especially those involving hydrocarbons like n-heptane. This leads to more precise estimations of emissions and combustion behavior.

However, when modeling solely liquid fuels, AVL Fire's built-in combustion modules are typically sufficient for capturing the necessary reaction processes. In these cases, integrating external chemical kinetics software like Chemkin is unnecessary.

5. Variables

The study variables in this research included three fuel injection timings: 22° Before Top Dead Center (BTDC), 18° BTDC, and 14° BTDC. Using the OM355 EU2 diesel engine startup catalog, two index speeds of 1400 and 2200 rpm were selected. In addition, the volumetric percentage of methane fuel was examined at three levels: 90 %, 85 %, and 75 %.

6. Detailed modeling techniques

6.1. Combustion mechanisms and reaction kinetics

This research uses a comprehensive chemical kinetic framework, specifically the GRI 3.This framework uses the GRI 3.0 mechanism, which includes 42 species and 168 reactions. It accurately simulates various stages of combustion, including ignition delay, heat release, and flame development. The framework solves species transfer equations that account for production rates, penetration, and source terms. It also employs specialized soot modeling techniques, such as the Kennedy/Hiryasu/Magnussen approach based on Haywood's correlation. The framework incorporates the auto-ignition properties of methane and n-heptane. These properties include ignition temperature, calorific value, and flammability limits. This ensures a precise representation of the combustion process.

6.2. Modeling of flame propagation and combustion

This work analyzes the detailed combustion process using the Eddy Breakup model, which accounts for turbulence-chemistry interactions during flame formation. The Dukowicz model simulates spray evaporation and penetration behaviors. Flame progression is affected by factors such as injection timing, mixture composition, and thermodynamic conditions. The initial auto-ignition phase and subsequent flame development are modeled by integrating computational fluid dynamics with chemical kinetics via Fire-Chemkin software.

6.3. Simulation boundary conditions

The simulation setup includes initial parameters such as an inlet pressure of 1.2 bar, an inlet temperature of 360 K, and a fuel-liquid temperature of 353 K. The boundary conditions include wall temperatures ranging from approximately 580 to 590 K, intermittent zeroing of the heat flux, and injection timing at 16° before top dead center. All of these are within a grid consisting of approximately 60,786 cells, each averaging 2.2 mm. The grid is arranged in a Cartesian coordinate system that accounts for piston motion and chamber dynamics through grid movement.

6.4. Reaction rates and kinetics

In this model, reaction velocities follow Arrhenius equations and depend heavily on temperature, pressure, and species concentrations. Meanwhile, the production and penetration terms for various species change dynamically according to the combustion stage. The overall reaction advancement is continuously calculated throughout the simulation by analyzing the specific pathways of methane and n-heptane, including their auto-ignition delays.

This study uses reactive flow equations to model flame front propagation, incorporating the effects of turbulence and species diffusion. The k-ε turbulence model ensures authentic turbulent mixing, which is essential for flame stability and spread. Heat release profiles, derived from reaction rates, directly impact pressure and temperature evolution. All of these processes are integrated within a comprehensive CFD framework that uses detailed chemical kinetics via the GRI 3.The framework uses detailed chemical kinetics, the GRI 3.0 mechanism, turbulence models, and spray behavior models to analyze how injection timing and fuel blend ratios influence ignition, flame development, and emissions in dual-fuel engines. This provides deep insights into combustion dynamics and optimization strategies.

7. Results and discussion

7.1. Validation on experimental data and investigation of the optimal number of field grids

Fig. 2 shows comparative plots evaluating the validation of simulation results against experimental data. The plots focus on pressure and heat release rate (HRR) at engine speeds of 1400 and 2200 RPM. The plots also illustrate the effect of mesh cell numbers on model accuracy. In the combustion study of the OM355 EU2 dual-fuel diesel engine, the optimal mesh configuration was identified as 45,076 cells with an average size of 3 mm. The pressure curves for all mesh densities closely follow the experimental data, especially during the peak combustion phase. This indicates that the model's accuracy is not significantly

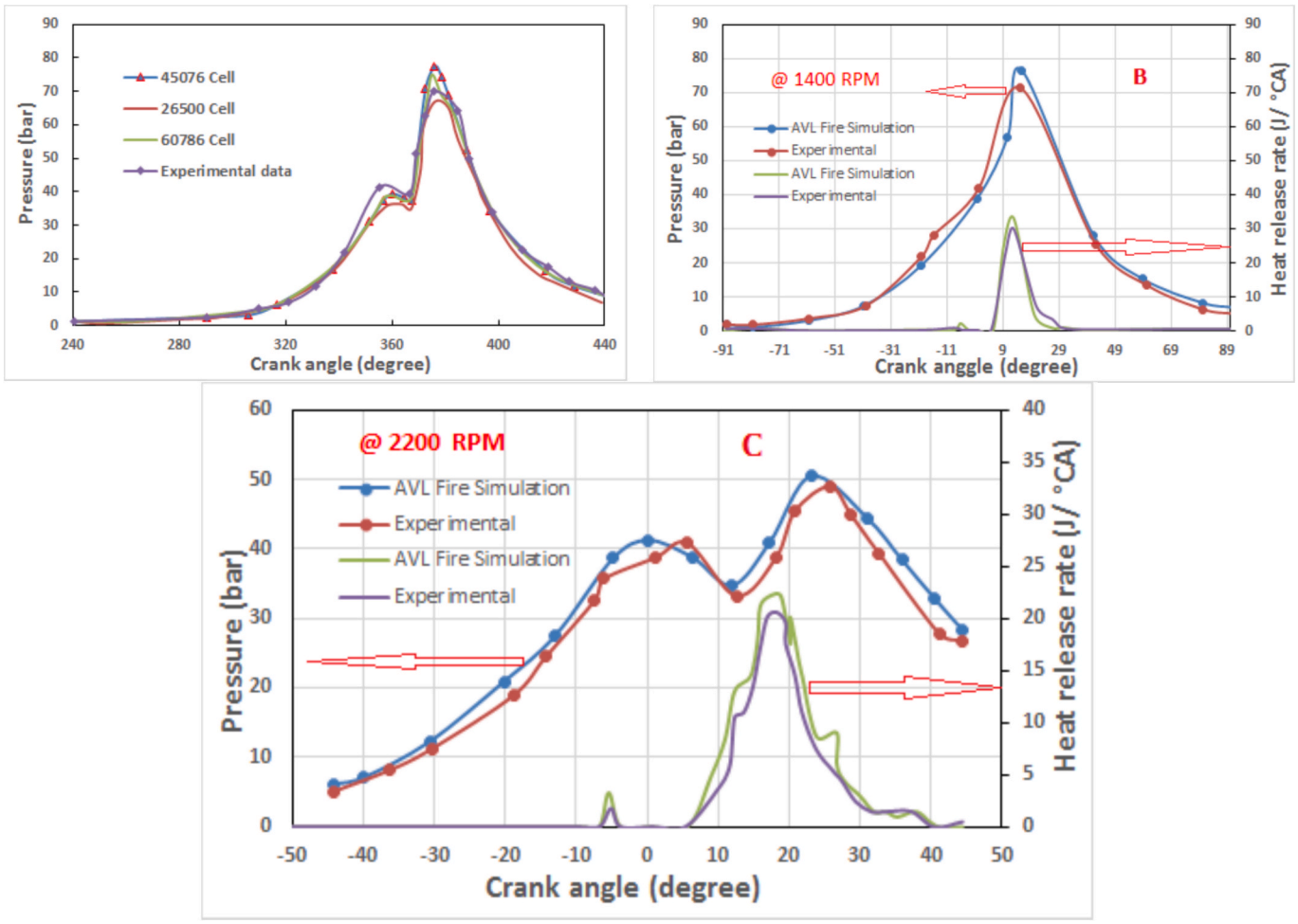

Fig. 2. Comparison between experimental and simulation results for validation of pressure and heat release rates.

affected by mesh size. The mesh with 60,786 cells closely matches the experimental results, suggesting that this mesh density reliably simulates the combustion process.

Comparing simulation and experimental data reveals a high degree of correlation for pressure and HRR at 1400 RPM, showing that the model effectively captures the combustion process at this speed. Similarly, at 2,200 RPM, the simulation results align well with the experimental measurements, confirming the model's validity at higher speeds. Mesh validation indicates minimal deviation among different mesh densities; the denser mesh (60,786 cells) closely matches experimental data.

Overall, the operating conditions for the dual-fuel diesel engine, which used a fuel mixture of 90 % methane and 10 % n-heptane, were validated at 1400 and 2200 RPM, focusing on pressure and heat release rate and show good agreement between simulation and experiment [40]. Key combustion parameters, such as peak pressure and heat release rate (HRR), are accurately represented in the simulations. Increasing the number of cells improved the initial pressure curve results.

7.2. Investigation of the influence of injection timing and fuel mixture on the ignition delay

Previous studies have shown that ignition delay is highly dependent on combustion chamber pressure and temperature parameters, fuel type, and oxygen concentration [45]. Changes in injection time can significantly affect the pressure and temperature within the combustion chamber. Considering that the fuel combustion process in compression-ignition dual-fuel engines is governed by their kinetic characteristics, changes in the fuel mixture percentage can also affect the ignition delay interval [46]. It has been shown that changes in the mixture percentages of the fuels in a dual-fuel diesel engine can affect the chemical and physical ignition delay. As the fuel injection timing is adjusted to occur earlier, a higher temperature is observed, which increases the ignition delay. In dual-fuel diesel engines, the combustion front moves from the center to the walls after fuel injection. If the injection time is shortened, the flame front is pushed toward the walls, leading to insufficient combustion.

Studies show that the centripetal flame front has the best combustion quality. When the injection time is advanced, the heat absorption time of oxygen molecules and gaseous fuel in the combustion chamber is improved, which leads to an even distribution of heat in all particles of the fuel mixture and increases the peak combustion pressure. The results of the numerical analysis showed that the ignition delay decreased by 2 crank angles with the injection advance. Increased heat absorption by the gas particles in the mixture increases the chamber temperature and consequently reduces the ignition delay time. At 2,200 rpm, the injection advance caused the peak ignition pressure to decrease. If the peak ignition pressure occurs before the top dead center, the engine power display will increase.

The findings from the numerical study showed that decreasing the injection duration at 2200 RPM enhanced the performance parameters of the dual-fuel diesel engine. Therefore, it can be concluded that to improve the torque of the dual-fuel diesel engine at a speed of 1400 rpm, the injection advance would increase the peak ignition pressure [47] and improve the output torque. In addition, at a speed of 2200 rpm, the

injection time should be close to the peak ignition pressure. Consequently, shortening the fuel injection duration at 2200 RPM has enhanced the performance metrics of the dual-fuel diesel engine. Fig. 3 illustrates the variations in cylinder pressure at two distinct speeds. Advancing the injection timing has extended the ignition delay and moved the peak of the pressure curve farther from top dead center.

At a constant speed, the effects of varying the fuel mixture ratio on the ignition delay were studied. The ignition delay variable was investigated at a speed of 1400 rpm. According to previous studies, engine speed does not have a significant effect on ignition delay [48]. Therefore, the effect of changing the mixture ratio on the drop in peak ignition pressure at higher speeds is critical. Changes in mixture percentages affect chemical ignition delay. By slightly adjusting the fuel blend percentage, the ignition delay was reduced by 1 crank degree. As the percentage of gaseous fuel decreased further, the ignition delay increased by 3 crank degrees and the peak ignition pressure drop occurred.

Raising the proportion of gaseous fuel leads to a higher peak ignition pressure and shifts it further away from TDC. Consequently, the increase in output torque is related to the greater amount of gaseous fuel in the fuel–air mixture. However, as the volume fraction of gaseous fuel decreases—due to its phase transition and the increased molecular weight of the liquid fuel—the peak combustion pressure increases only slightly beyond TDC. In addition, increasing the fraction of liquid fuel in the fuel mixture results in a decrease in the temperature of the combustion chamber; this is an additional factor that can contribute to a reduction in ignition delay in a fuel mixture containing 85 % methane. Fig. 4 shows how the temperature is distributed throughout the region. Increasing the volumetric percentage of gaseous fuel promotes uniform heat distribution throughout the combustor. In addition, a higher peak combustion pressure results in higher temperatures within the cylinder.

7.2.1. Fuel injection and in-cylinder velocity distribution

Fig. 5 shows how different methane and n-heptane fuel mixtures affect in-cylinder flow and spray behavior at 22° BTDC and 1400 RPM. The top row shows the distribution of the fuels during injection; the colors represent the spray velocity and atomization patterns. Higher n-heptane levels produce more energetic and deeper sprays, which promote better mixing. Increased methane, on the other hand, results in gentler and more dispersed sprays. The bottom row depicts velocity fields within the cylinder and reveals that n-heptane-rich mixtures induce stronger turbulence and airflow, which enhances combustion stability. Conversely, higher methane content leads to calmer flow patterns, which could impact efficiency. Overall, altering the fuel composition significantly changes spray dynamics and flow behavior, thereby affecting the ignition, mixing, and combustion processes. These findings are essential for optimizing the performance and emissions of diesel engines using blended or alternative fuels.

7.3. The impact of variations in injection time and mixing percentage on emissions

7.3.1. NOx, and CO emissions

The temperature of the chamber, the time and method of fuel injection, and combustion are among the most significant parameters influencing the emissions produced by dual-fuel diesel engines. The elevated post-combustion temperature has been observed to result in increased emissions of NOx and carbon dioxide. In a dual-fuel system, the emission of NOx is directly correlated with increased the air/fuel ratio. Accordingly, an increase in the air–fuel ratio results in a rise in chamber temperature, which in turn leads to an elevated emission of NOx pollutants [49].

Additionally, the implementation of advanced fuel injection technology has been demonstrated to effectively reduce the levels of carbon monoxide pollution in the environment. Modifications to the injection time resulted in notable alterations to the emission values of the dual-fuel diesel engine. Assuming a constant percentage of fuel mixing, the results demonstrate that advancing the fuel injection time has led to an increase in carbon dioxide and NOx emissions.

The variations in the proportion of fuel mixing have primarily influenced the modifications in the emission parameters [50]. As the injection time approaches the top dead center and the volume percentage of liquid fuel in the fuel mixture increases, incomplete combustion occurs, resulting in an elevated emission of carbon monoxide, a pollutant. The NOx pollutant demonstrates an increasing trend with advancing injection and changing the mixing percentage. However, it exhibits a decreasing trend in the mixing mode of 25–75 %. This is because, in this mixing percentage, the effect of liquid fuel on the combustion process increases, resulting in incomplete combustion. These findings are following the results of previous studies [51]. Fig. 6 illustrates the changes in the emission of NOx, and carbon monoxide pollutants.

7.3.2. HC, and soot emissions

Methane typically produces lower unburned hydrocarbon (HC) emissions than conventional diesel due to its more complete combustion characteristics when properly blended and combusted. In contrast, n-heptane as a hydrocarbon can produce higher HC emissions than methane, with combustion results varying depending on the blending ratio with CH_4; increasing n-heptane concentration can also result in lower HC emissions.

Early injection allows for better mixing with air, promoting more complete combustion and potentially reducing HC emissions. Conversely, late injection can lead to poorer mixing and incomplete combustion, resulting in higher levels of unburned hydrocarbons. In addition, the mixture of CH4 and n-heptane can affect combustion temperature; higher temperatures generally favor more complete combustion, which reduces HC emissions.

However, the effects of fuel substitution and injection timing on HC

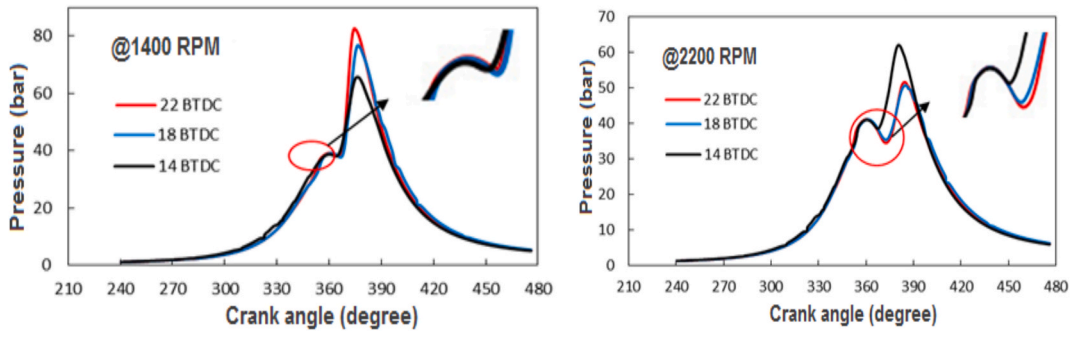

Fig. 3. Cylinder pressure variations relative to crank angle at 1400 and 2200 RPM.

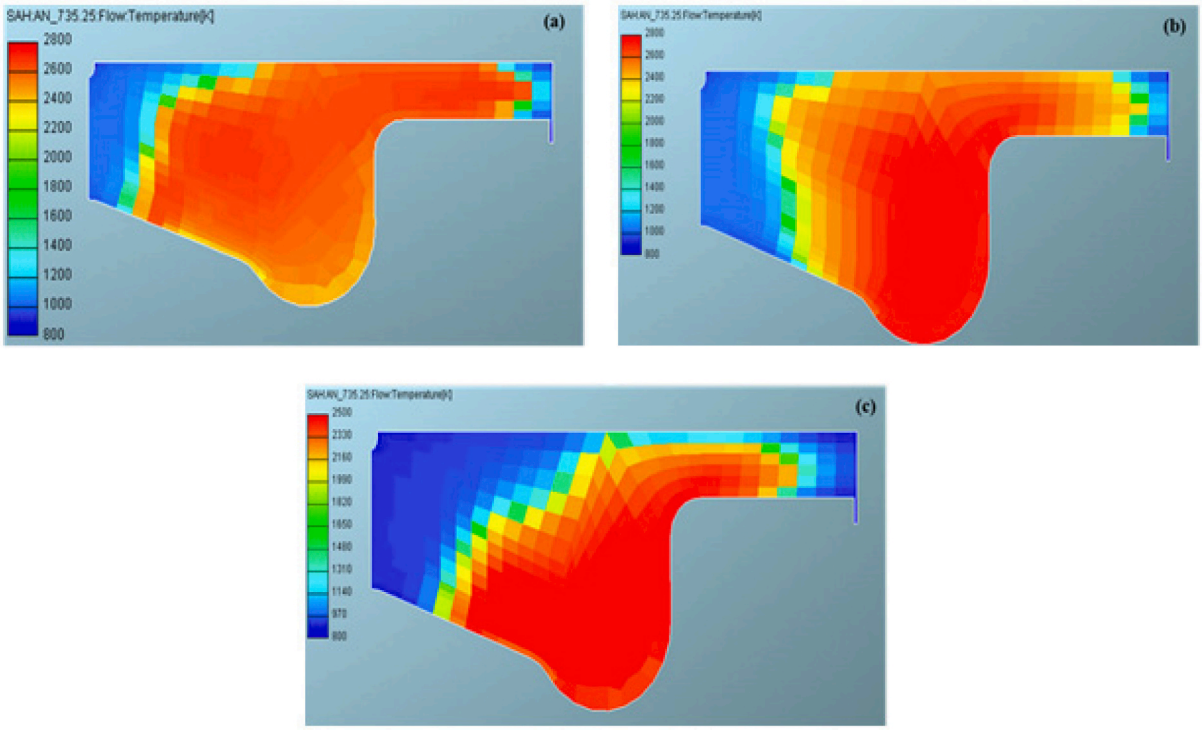

Fig. 4. Distribution of temperature in the solution field. (a) 90 % methane–10 % n-heptane, (b) 85 % methane–15 % n-heptane, (c) 75 % methane–25 % n-heptane.

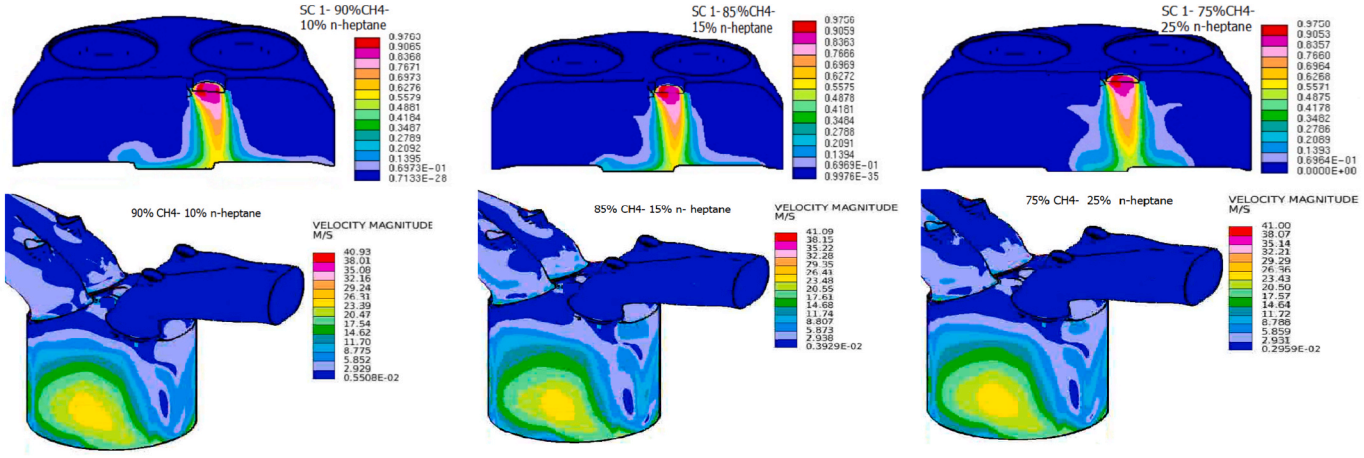

Fig. 5. Fuel injection and in-cylinder velocity distribution at varying fuel percentages of CH_4 and n-heptane.

emissions also depend on engine operating conditions such as load and speed, as these factors can alter combustion dynamics and consequently the emissions profile. Understanding these interactions is critical to optimizing engine performance and minimizing emissions.

N-Heptane improves combustion efficiency and reduces soot emissions due to its clean burning properties and high cetane number. Methane also reduces soot emissions due to its higher hydrogen content, although it has a lower energy density than n-heptane. Fig. 7 illustrates the changes in the emission of HC, and soot pollutants.

In summary, increasing the amount of n-heptane in the fuel mixture and fine-tuning early injection timing are effective methods for reducing soot emissions in diesel engines. Although methane's chemical structure helps reduce soot, its energy content and engine performance must be carefully evaluated. Achieving a balance between these elements is essential to maximize combustion efficiency and minimize soot formation.

7.4. The effect of changes in the mixture ratio of the fuels and the timing of the fuel injection on the performance characteristics of a dual fuel diesel engine

Performance parameters in diesel engines include output torque, indicated power, and specific fuel consumption. The two parameters of torque and indicated power are generally dependent on the changes in the pressure and temperature diagram of the combustion chamber. The output torque is related to the area under the crank angle-pressure curve. As the injection time approaches the top dead point, the ignition delay increases, which causes a drop in pressure peak and, consequently, a decrease in torque.

A notable decline in the pressure curve and torque values occurs when the percentage of fuel mixing is varied. An increase in the volume percentage of liquid fuel in the mixture is associated with a corresponding rise in pressure drop. Findings indicate that, despite an

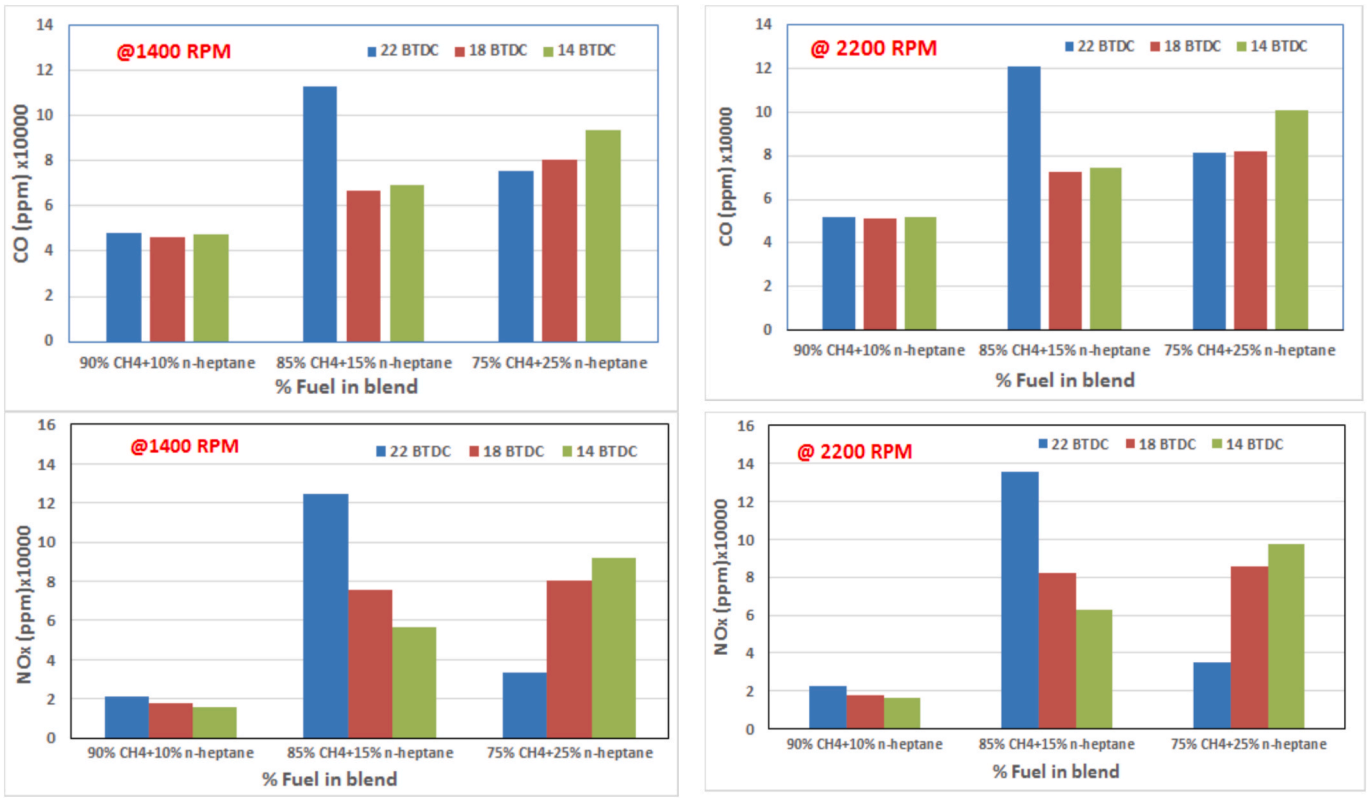

Fig. 6. Variations in the emission of NOx, and carbon monoxide versus % fuel in blend and injection timing.

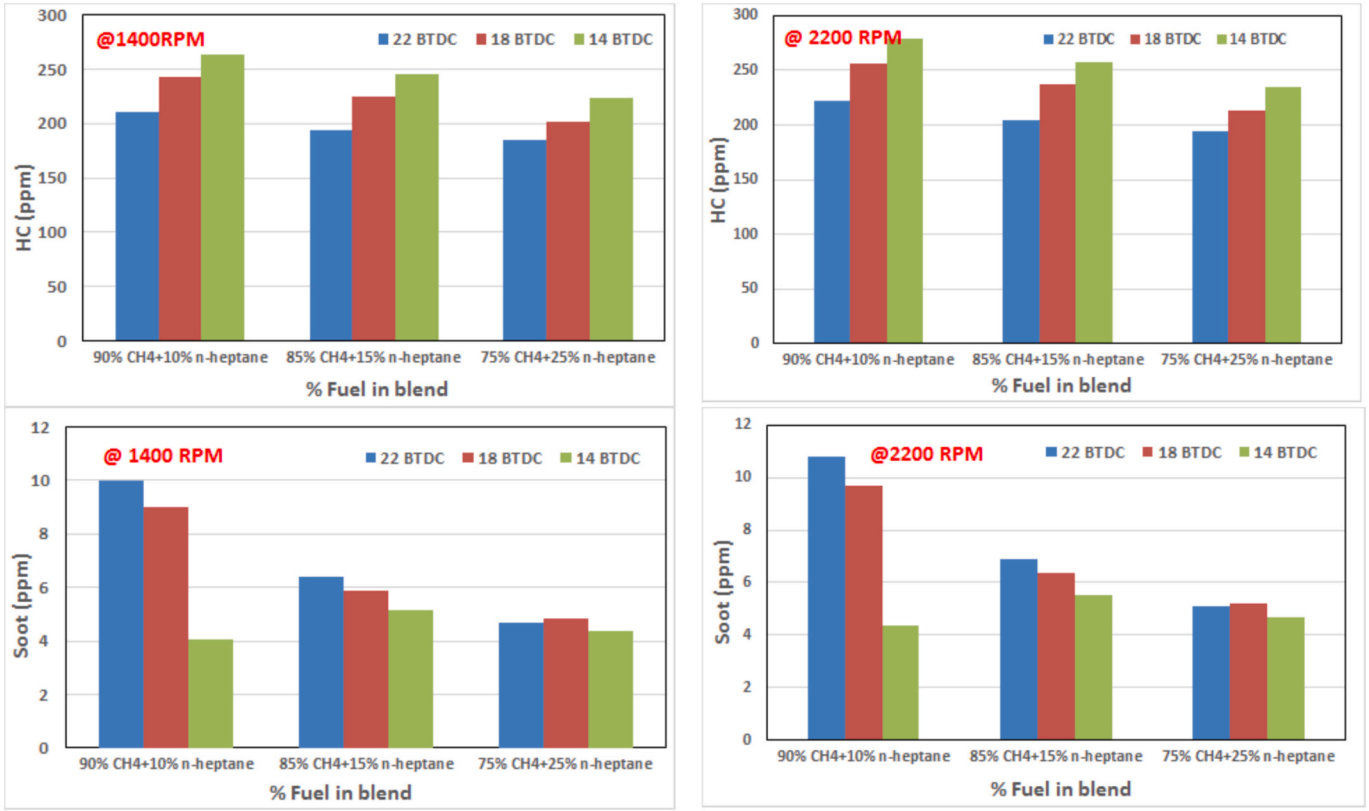

Fig. 7. Variations in the emission of HC, and soot monoxide versus % fuel in blend and injection timing.

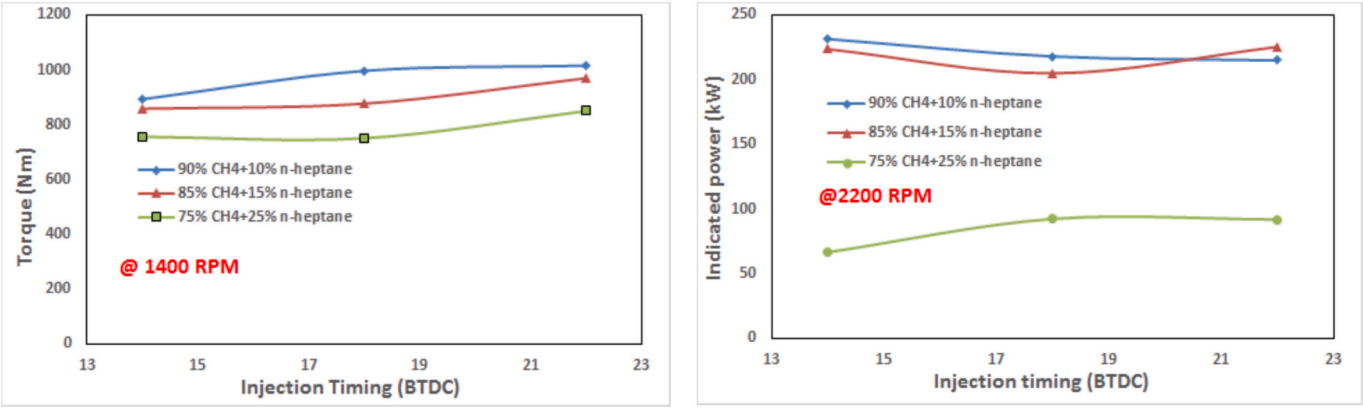

Fig. 8. The impact of varying injection timing and fuel mixing percentages on the output torque and indicated power.

increase in the proportion of injected fuel, there was a 25 % reduction in maximum torque and a 5.3 % reduction in maximum power at a fuel mixing ratio of 75 % methane- 25 %n-heptane. Fig. 8 shows how the output torque and indicated power of the OM355 EU2 dual-fuel engine change with different injection timing and fuel mixing percentages.

The indicated power is subject to influence by the variations in heat release rate demonstrated by the cylinder temperature curve.

Fig. 9 illustrates the evolution of the heat release rate parameter and the specific fuel consumption of the OM355 EU2 dual-fuel engine at varying injection times and fuel mixture percentages. As the indicated power rises, the heat release rate also increases, as shown in Figs. 8 and 9. The heat release rate values in the OM355-EU2 dual-fuel diesel engine demonstrate an increase as the fuel injection time approaches top dead center. Consequently, reducing the fuel injection time at 2,200 RPM increased the indicated power by 1.24 %. Numerical studies indicated that advancing the fuel injection time reduced the indicated power parameter of the dual-fuel diesel engine by 25 %. Therefore, advancing the injection time at 2,200 RPM significantly impacts the power output of the dual-fuel diesel engine. Increasing the volume percentage of liquid fuel creates a greater distance between the heat release peak and top dead center. This leads to a reduction in indicated power. Injection advance results in elevated specific fuel consumption as the combustion process progresses and a greater quantity of the mixture burns within the combustion chamber. When the volume percentage of liquid fuel in the fuel mixture increases, specific fuel consumption declines due to deteriorating combustion in the combustion chamber.

The findings of this study indicate that the impact of engine speed and fuel mixing percentage on fuel consumption in dual-fuel diesel engines is not linear. Rather, several physical factors influence combustion flow.

8. Conclusions

This study conducts a numerical analysis of the combustion characteristics of the OM355 EU2 diesel engine operating in dual-fuel mode (n-heptane/methane). The objective is to investigate how changes in fuel injection timing and fuel mixture ratios affect ignition delay, performance metrics, and emissions for the OM355 EU2 diesel engine. The combustion parameters of dual-fuel diesel engines have been studied by computational fluid dynamics using a coupling with Fire-Chemkin software, leading to the following findings:

- In dual-fuel diesel engines, the duration of the ignition delay affects cylinder pressure and thermal peaks, and advanced injection timing increases the ignition delay by up to 2° crank angle.
- At 1400 rpm, advancing the injection timing resulted in a 16 % increase in maximum cylinder pressure, which increased torque output. This change in injection timing also increased ignition delay.
- Earlier injection timing at higher engine speeds increases ignition delay and reduces peak cylinder pressure, so the reduction in power loss is noticeable at 2200 rpm.
- As the liquid fuel proportion in the mixture increases, engine torque output decreases. With constant injection timing, raising the liquid fuel percentage from 10 % to 25 % leads to a 17 % torque reduction.
- Advancing injection timing raised combustion chamber temperature, causing a 70 % drop in indicated power and a 13 % increase in specific fuel consumption when the liquid fuel percentage was changed from 10 % to 25 %.
- Advancing the timing of fuel injection (moving it closer to top dead center) increases NOx emissions due to higher combustion

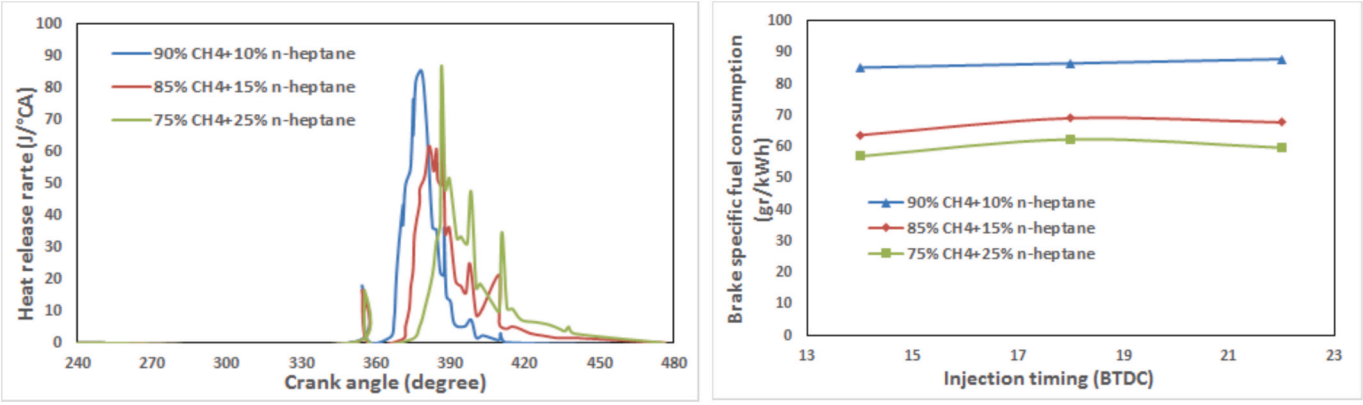

Fig. 9. The impact of the heat release rate parameter and the specific fuel consumption versus variation of injection timing and fuel mixture percentages.

temperatures. However, it also decreases soot emissions by promoting more complete combustion.
- Increasing the proportion of methane in the fuel blend significantly reduces NOx emissions by up to 31 % and decreases HC and CO emissions, thereby improving combustion efficiency and emissions performance.
- Higher n-heptane content tends to increase soot emissions, but it can reduce NOx and HC emissions when properly optimized. Thus, carefully adjusting fuel mixture ratios is essential for balancing emissions.

Optimal injection timing at 22° BTDC, combined with a fuel blend of 85 % methane – 15 % n-heptane, substantially reduces NOx and soot emissions by around 31 % and 16 %, respectively. This illustrates the significance of tuning injection parameters and fuel composition for emission control.

Setting the fuel injection timing earlier, specifically at 22° BTDC, significantly increases torque and power in a dual-fuel diesel engine. Numerical simulations showed a 16 % increase in output torque due to higher peak cylinder pressure. Additionally, early fuel injection resulted in improved emissions, reducing nitrogen oxides (NOx) by 31 % and carbon monoxide (CO) by 16 %. However, increasing the amount of liquid fuel (75 % methane and 25 % n-heptane) in the mixture negatively affected ignition delay. This resulted in a 17 % reduction in output torque and a 70 % reduction in indicator power. In summary, optimizing injection timing and mixture ratios can enhance the performance of dual-fuel diesel engines while reducing emissions.

CRediT authorship contribution statement

Javad Zareei: Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **John William Grimaldo Guerrero:** Writing – review & editing, Writing – original draft, Formal analysis, Data curation, Conceptualization. **José R. Nuñez-Alvarez:** Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Grether Lucía Real-Pérez:** Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Ramon A. Zambrano-Mero:** Writing – review & editing, Writing – original draft, Visualization, Validation, Investigation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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