



Research Article

Numerical Investigations of SiO₂ and TiO₂ Nanoparticle's Addition Impact on Performance, Combustion Features, and Emission Characteristics of a Diesel Engine Operating with Water Diesel Emulsified Fuel at Different Lambda Values and Engine Speeds

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Abstract: Although several investigations have examined the impacts of nanoparticle addition in diesel and water-diesel emulsified fuel, little research has focused on the implication of nanoparticle inclusion in water-diesel-emulsified fuel, especially under varying engine speeds and lambda values. The current work evaluates the effects of lambda ratios (1.2, 1.4, and 1.6) and engine speeds (2000, 3000, and 4000 rpm) on the combustion efficiency and emissions of diesel engines using three different additives: 95% diesel fuel and water at a 5% ratio (DW), 95% diesel fuel with 5% water and 50µm TiO₂ (DWTiO₂), and 95% diesel fuel with 5% water and 50µm SiO₂ (DWSiO₂). Combustion simulations were performed using the Diesel-RK program on a DEUTZ F1L511, single-cylinder, air-cooled, direct-injection diesel engine. The simulation results demonstrated that increasing the lambda ratio lowered combustion parameters, including temperature, pressure, heat release rate (HRR), smoke levels, and particulate matter emissions (PM), while increasing NO and CO₂ increased. Moreover, increasing the engine speed lowered NO emissions, HRR, pressure, and temperature, whereas the emissions of CO₂ and PM rose. Furthermore, adding water to diesel fuel led to a reduction in NO and PM, along with a slight decrease in HRR. Nonetheless, CO₂ emissions increased. The addition of nanomaterials to the water-emulsified diesel produced the highest peak temperature, pressure, HRR, and NO emissions. Offering improved combustion efficiency and reduced pollution emissions, the mixture (DWTiO₂) surpassed the mixture (DWSiO₂), highlighting its potential to enhance diesel engine performance and decrease environmental impact.

Keywords: Combustion; Diesel engine; Diesel-RK; Emission; TiO₂ and SiO₂ nanoparticles; Water diesel emulsified fuel

1. Introduction

Industrialists, scientists, and researchers have been motivated to focus their research on alternative environmentally friendly fuels due to the growing worldwide need for energy, the harm to the environment, and the objectives of sustainable energy progress. Diesel engines are practical,

sufficient, and more powerful and efficient than spark ignition engines (Ghareeb and Anjal, 2024; Simanjuntak et al., 2024; Tuktin et al., 2024; Vigneswaran et al., 2021; Mahmood et al., 2016; Ibrahim et al., 2016). However, diesel engines emit various unwanted pollutants, including particulate matter (PM) and nitrogen oxides (NO_x), during combustion. Pollutants and emissions adversely impact the environment and human health. The development and production of environmentally sustainable and friendly fuels to enhance human health and the environment is a topic of significant interest because of the air pollution caused by diesel engines (Hendrarsakti et al., 2025; Mahmood et al., 2024; Aisyah et al., 2023; Mahmood et al., 2021; Watanabe et al., 2017; Abdulhadi, 2011).

Emulsified fuel composed of water and diesel is a renewable energy source that has recently garnered attention. Water in diesel emulsion is an intriguing renewable energy source that can minimize NO_x and PM emission levels and simultaneously enhance combustion efficiency in diesel combustion engines without engine adjustment (Vellaiyan and Amirthagadeswaran, 2017; 2016). Numerous studies have shown that mixing water with diesel fuel lowers its calorific value and increases the amount of specific fuel consumed. (Mostafa et al., 2023; Khatri and Goyal, 2021; 2020; Abdollahi et al., 2020). However, this compromise is warranted due to significant environmental and operational benefits, including improved engine performance and reduced harmful emissions such as NO_x, CO, and PM, as well as enhanced combustion efficiency. The ability of water to generate OH radicals enhances the oxidation of carbon monoxide (CO) to carbon dioxide (CO₂), resulting in cleaner exhaust emissions. The combination of water and diesel fuel results in improved energy efficiency and effective emission management, aligning with strict environmental standards and sustainability practices. Incorporating water, often as emulsions or through the injection process, lowers the combustion temperature by absorbing significant heat during vaporization. This cooling effect decreases nitrogen oxides (NO_x), a major pollutant, as well as soot and particulate matter (PM) by removing hotspots and promoting uniform combustion (Mostafa et al., 2023; Kumar and Raheman, 2022; Khatri and Goyal, 2021). Various researchers have investigated several emulsion fuels in diesel engines. Attia and Kulchitskiy (Attia and Kulchitskiy, 2014) investigated the impact of water-diesel emulsion on three-cylinder engines with varying drop sizes. This study demonstrated that smaller water droplets were less efficient than larger ones in lowering NO_x emissions. Nevertheless, small droplets are quite effective in reducing HC emissions. Leng et al. (2015) examined the variations between the features of the water-diesel combination and microemulsion. The micro-emulsion showed a lower lag and improved combustion efficiency with a declining activation energy. Bidita et al. (2016) examined diesel engine combustion emissions employing water-diesel emulsion. The findings showed that compared to diesel fuel, water-diesel emulsion minimized NO and CO emissions.

On the other hand, nanofuels may represent a significant advancement in pursuing more ecologically friendly and efficient fuel technologies with a growing need for alternatives to fossil fuels. Recently, researchers have looked at using nanomaterials as diesel fuel additions to enhance diesel engine performance and quality (Mahmood et al., 2023; Naife, 2022; Khan et al., 2022; Al-Kayiem et al., 2018). Nanofuels are a type of nanofluid that can serve as a substitute for conventional fuels. Nanofuels are produced by mixing solid nanoparticle substances with base fuel, yielding fuels with enhanced calorific value, elevated energy density, and an extensive reactive interfacial region that permits expanded fuel-oxidizer reactions, generating potential power and contributing to reducing the amount of soot creation, as well as decreased ignition delay and combustion duration. Nouri et al. (2021) investigated the effects of Fe₂O₃-Al₂O₃ nanoparticles on the performance and emission characteristics of diesel engines. The findings indicated that the incorporation of nanoparticles into diesel fuel improved combustion efficiency and diminished diesel engine emissions. Aalam and Alagappan (2015) examined the impact of CeO₂ nanoparticles as an additive to diesel fuel on engine efficiency. The findings indicated that the incorporation of CeO₂ into diesel fuel enhanced the thermal efficiency of brakes, elevated NO emissions, and reduced HC emissions. Tarek (Naife, 2022) assessed the effects of integrating CeO₂ and ZnO nanoparticles into diesel fuel on the combustion efficiency and emission characteristics of diesel engines. The findings indicated

that the incorporation of these additive nanoparticles led to a reduction in brake-specific fuel consumption and a decrease in unburned hydrocarbons (UHC) and carbon monoxide (CO) emissions, while simultaneously enhancing brake thermal efficiency.

Integrating TiO_2 and SiO_2 nanoparticles into fuel systems has garnered significant attention for enhancing combustion performance and diminishing hazardous emissions. These nanoparticles are significant for augmenting fuel reactivity, optimizing the air-fuel mixture, and facilitating more thorough combustion. According to literature reviews, nanoparticles such as Titanium Dioxide (TiO_2) and Silicon Dioxide (SiO_2) in water-diesel emulsified fuel boost combustion properties, diminish hazardous emissions, and augment fuel efficiency (Taştan et al., 2024; Ghanati et al., 2024; Doğan et al., 2024). Introducing nanoparticles (NPs) such as SiO_2 and TiO_2 to diesel-water emulsions improves combustion performance by serving as catalysts, minimizing ignition delay, and facilitating more thorough fuel oxidation, vastly boosting the HRR (Rezaei, 2023; Sundararajan and Ammal, 2018). The combustion characteristics are enhanced by the inclusion of nanoparticles in the diesel-water mixture, which causes micro-explosions and finer atomization, which in turn improves the mixing of fuel and air and accelerates vaporization (Al-Sabagh et al., 2012). Additionally, the decreased quenching impacts near the combustion chamber walls and the thermal transmission characteristics of nanoparticles contribute to a more vigorous and efficient combustion procedure than the normal diesel-water blends (Mostafa et al., 2023; Khatri and Goyal, 2021; 2020; Hasannuddin et al., 2018). Vellaiyan et al. (2020) examined the influence of titanium dioxide (TiO_2) nanoparticles combined with water-in-diesel (DWS) emulsion fuel on the engine performance, emissions, and combustion of a single-cylinder diesel engine, maintaining a constant engine speed and lambda value. The results indicated that TiO_2 nanoparticles enhanced fuel oxidation and reduced NO_x emissions, thereby improving combustion efficiency. At elevated engine loads, the incorporation of TiO_2 was observed to reduce smoke opacity and enhanced brake thermal efficiency (BTE). Vigneswaran et al. (2021) investigated the exhaust properties of a compression ignition engine powered by diesel-water emulsion mixtures with the incorporation of TiO_2 nanoparticles, maintaining consistent engine speed and lambda values. The results indicated that TiO_2 nanoparticle mixtures with water-diesel emulsions led to a notable enhancement in brake thermal efficiency (BTE), accompanied by decreases in carbon monoxide (CO) and unburned hydrocarbons (HC). Nonetheless, NO_x emissions escalated with elevated TiO_2 content. Khatria and Goyal (2020) investigated the impact of silicon dioxide (SiO_2) nanoparticles on water-diesel emulsified fuel in a diesel engine at different injection timings, maintaining a constant speed of 1500 rpm. The findings showed that SiO_2 nanoparticles at levels of 50 and 100 ppm markedly diminished NO_x and smoke opacity emissions while enhancing fuel combustion. The use of SiO_2 nanoparticles boosts the thermal properties of the fuel, resulting in improved heat distribution inside the engine and thus increasing the combustion efficiency.

Although several investigations have examined the impacts of nanoparticle addition in diesel fuel and water-diesel emulsions fuel, little research has focused on the implication of nanoparticle inclusion in water-diesel-emulsified fuel, especially under varying engine speeds and lambda values. The lambda value, which indicates the air-fuel equivalence ratio, is essential for determining combustion performance and emissions. When lambda shifts from stoichiometric conditions ($\lambda = 1$), either toward leaner mixtures ($\lambda > 1$) or richer mixtures ($\lambda < 1$), the combustion specifications can change dramatically, affecting engine performance, combustion process, and exhaust emissions (Mahmood et al., 2022b). At the same time, different engine speeds create dynamic variations in fuel-air blending, turbulence intensity, and heat release rates within the combustion chamber. At elevated engine speeds, shorter ignition delays and more significant turbulence may improve nanoparticle dispersion and reactivity, thereby enhancing combustion stability and increasing the thermal efficiency of the engine. However, partial combustion and increased particulate matter emissions can occur at lower engine speeds due to insufficient mixing time, which limits the efficiency of nanoparticles. Therefore, understanding the influence of engine speed and lambda values on combustion efficiency and emissions when nanoparticles are incorporated into emulsified

fuels is lacking. Addressing these shortcomings is essential for improving the usage of nanoparticle-infused emulsified fuels for cleaner and more efficient diesel engine operation. This study aims to examine the effects of nanoparticles of SiO_2 and TiO_2 on the efficiency, combustion, and emissions of diesel engines operating with diesel and water-diesel emulsified fuel at different lambda values and engine speeds. The Diesel-Rk Program was employed for the engine model's numerical analysis.

2. Simulation Method and Material

In the present study, the Diesel-RK modeling program is one of the best optimization tools used to test and analyze the performance, combustion, and emissions of diesel engines under different lambda values (1.2, 1.4, and 1.6) and various engine speeds (2000, 3000, and 4000 rpm), running on diesel fuel, water-emulsified diesel fuel, water-emulsified diesel fuel with SiO_2 , and water-emulsified diesel fuel with TiO_2 . (Supplementary Table A.1) presents the specifications of nanoparticles (Vigneswaran et al., 2021; Khatri and Goyal, 2020; Abdulwahab et al., 2016), while Table 1 details the characteristics of diesel with various additives. An air-cooled, single-cylinder, direct-injection diesel engine (Model DEUTZ F1L511) was used for the numerical investigation. Table 2 displays the specifications of the engine (Gad et al., 2021). The Diesel-RK software was used to mimic combustion inside an engine chamber by resolving the governing equations related to the combustion process, mostly by solving the partial differential equations of energy, mass, and temperature and the state equation for open thermodynamic systems (Al-Dawody et al., 2024; Adib et al., 2024; Kumar et al., 2024). Diesel-RK has a sophisticated model for combustion and mixture generation in a diesel engine. The present research employs the physical parameters of fuel blends in simulations of spray generation and evaporation and combustion processes (Kurse and Nallamotheu, 2022; Gad et al., 2021; Georgiou and Azimov, 2020). The Diesel RK model considers fuel particle dimensions, fuel spray shape, fuel spray orientation, growth and development dynamics, fuel spray decomposition process, swirly pattern dynamics and forms, and the relationship of fuel particles to combustion chamber walls and swirls. NOx emissions are determined using the Zeldovich methodology. Furthermore, the following modeling processes were simulated: compression stroke, fuel injection, combustion procedures, and power stroke (Islam et al., 2025; Pal and Reddy, 2024; Gumus and Otkur, 2023; Al-Dawody et al., 2023; Mahmood et al., 2022a). This research uses a fuel mixture of 95% diesel and 5% water because it offers an ideal mixture to minimize emissions while increasing fuel efficiency; it is a benchmark for measuring the effects of nanoparticles. In addition, 50 μm SiO_2 and TiO_2 nanoparticles are adopted, based on previous studies (Khatri and Goyal, 2021; 2020; Vellaiyan et al., 2020). Modeling diesel-water-nanoparticle blends in Diesel-RK software requires several simplifying assumptions due to the software's constraint to simulate multiphase or particulate fuels. Nanoparticles are usually considered to be homogeneously dispersed in the fuel and create a pseudo-single-phase mixture with altered effective thermophysical properties (density, thermal conductivity, and latent heat of vaporization) (Mostafa et al., 2023). These properties can be calculated using empirical or theoretical mixing rules and are manually inserted into the model. Additionally, the fuel mixture is assumed to be homogeneous in the software, which does not account for potential local concentration differences that may alter combustion dynamics (Fadhil et al., 2023). In addition, the catalytic properties of NPs are frequently simplified and replaced by a generalized oxidation acceleration instead of decoding complicated surface interactions. Furthermore, improvements in the thermal conductivity with nanoparticles are added as broad enhancements of the heat transfer efficiency, with no direct modeling of the microscale heat exchange. The evaporation of water is modeled based on standard evaporation models, and nanoparticle evaporation or deposition is ignored (Hamzah et al., 2025). The following are the governing equations used in the Diesel-RK software are as follows: (Adib et al., 2024; Gad et al., 2021; Paul et al., 2014).

1-Mass conservation: The net mass flux across the boundary of any open system is the rate at which the mass changes. In mathematical terms, it may be expressed as follows:

$$\frac{dm}{dt} = \sum_j \dot{m}_j \quad (1)$$

where:

m: The entire mass in the system

t: Time (s)

$\dot{m}_j$: Net mass flow rate of species j (kg/s)

2-Conservation Equation for Species: The mass balance of each species can be expressed as follows:

$$Y_j = \sum_j \left(\frac{\dot{m}_j}{m} \right) (Y_i^j - Y_i^{cyl}) + \frac{\Omega_i W_{mw}}{\rho} \quad (2)$$

where

Y : Mass fraction of j species

Ω_i : Chemical reaction rate of species i (kmol/m³·s)

Wmw: Species molecular weight (kg/kmol)

ρ : Density of gas (kg/m³)

3. Energy Conservation: The generalized energy equation of an open thermodynamic system can be expressed as

$$\frac{d(mu)}{dt} = -p \frac{dv}{dt} + \frac{dQ_{ht}}{dt} + \sum_i \dot{m}_i h_i \quad (3)$$

where

u: Specific internal energy (J/kg)

p: Cylinder pressure (Pa)

Qht: Heat transfer rate (W)

h_i: Specific enthalpy of the stream (J/kg)

4-Lambda (α_1): λ represents the correlation between the actual and stoichiometric air/fuel ratio:

$$\alpha_1 = \frac{\frac{A}{F}}{\left(\frac{A}{F}\right)_s} = \frac{\frac{\dot{m}_a}{\dot{m}_f}}{\left(\frac{\dot{m}_a}{\dot{m}_f}\right)_s} \quad (4)$$

where

α_1 : Equivalence ratio (dimensionless).

A/F: air-to-fuel ratio (kg air/kg fuel).

(A/F)_s: Stoichiometric air-to-fuel ratio.

$\dot{m}_a$: Mass flow rate of air (kg/s).

$\dot{m}_f$: Mass flow rate of fuel (kg/s).

5-Specific Fuel Consumption: The quantity of fuel used per unit of power generated is known as specific fuel consumption (SFC):

:

$$SFC = \frac{\dot{m}_f}{P_b} \quad (5)$$

where

SFC: Specific fuel consumption (kg/J or g/kWh)

Pb: Brake power (W).

6-Calculation of the heat release

The combustion process of the fuel is divided into four phases to determine the heat release during the engine cycle, each exhibiting unique physical and chemical properties that influence the combustion rate. These phases are outlined as follows:

(a) Phase of the ignition delay. The modified Tolstov's equation is used to calculate the auto-ignition delay interval:

$$\tau = 3.8 * 10^{-6} * (1 - 1.6 * 10^{-4} * n) \sqrt{\frac{T}{P}} \cdot \exp\left(\frac{E_a}{8.312T} - \frac{70}{CN + 25}\right) \quad (6)$$

τ : Ignition delay time (s).

n : Engine speed (rpm).

P : Pressure (Pa).

T : Temperature (K).

E_a : Activation energy (J/mol).

CN : Cetane fuel number.

(b) Burning time with the premixed fuel. In the premixed combustion phase, the HRR is computed as follows:

$$\frac{dx}{dt} = \phi_0 \left(A_0 \left(\frac{m_f}{V_i} \right) \right) \cdot (\sigma_{ud} - X_0) \cdot (0.1\sigma_{ud} + X_0) + \phi_1 (d\sigma_u/dt) \quad (7)$$

x : Burned fuel fraction.

$d\sigma_u$: Unburned fuel mass fraction.

X_0 : Initial burn fraction.

m_f : Fuel mass (kg).

V_i : Initial spray volume (m³).

ϕ_0, ϕ_1 : Crank angle

(c) Blending-controlled burning stage. The HRR during the blending controlled burning stage can be expressed as follows:

$$\frac{dx}{dt} = \phi_1 \left(\frac{d\sigma_u}{dt} \right) + \phi_2 \left(A_2 \left(\frac{m_f}{V} \right) \right) \cdot (\sigma_u - X)(\phi - X) \quad (8)$$

σ_u : Unburned fuel fraction.

Φ_2 : Crank angle

ϕ : air-fuel ratio

A_2 : Mixing-controlled combustion constant.

(d) Late combustion phase. The HRR is calculated as follows:

$$\frac{dx}{dt} = \phi_3 A_3 K_T (1 - X)(\xi_b \cdot \phi - X) \quad (9)$$

K_T : Temperature-dependent rate coefficient.

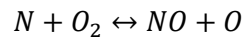
ξ_b : Burned gas fraction.

ϕ_3 : Late-phase efficiency factor.

A3: Empirical constant

7-NO_x formation calculation

The nitrogen oxide reaction is as follows:



The reaction depends on the oxygen concentration. The volumetric NO concentration is given by

$$\frac{d[NO]}{d\theta} = \frac{2.33 * 10^7 p \cdot e^{\frac{38020}{T_z}} [N_2]_e [O]_e ([1 - NO][NO][NO]_e)^2 \left(\frac{1}{rps}\right)}{RT_2 \left(1 + (2365/T_z) \cdot e^{\frac{38020}{T_z}} [NO]/O_e\right)} \quad (10)$$

[NO]: Nitric oxide concentration (mol/m³).

θ : Crank angle (degrees).

T_z : Local temperature (K).

$[N_2]_e, [O]_e$: Equilibrium concentrations of N₂ and O₂.

$[NO]_e$: Equilibrium NO concentration.

rps : Engine revolutions per second (1/s).

8-Soot intensity calculation

Soot consists of minuscule dark carbon particles dispersed in a gas transporter. Incomplete combustion of hydrocarbons is the primary cause of soot formation. Soot particles are formed, grown, and broken down because of combustion-related chemical reactions. This is linked to the following common scenarios:

$$[C]_H = \int_{\theta_B}^{480} \frac{d[C]}{dt} \cdot \frac{d\theta}{6n} \left(\frac{0.1}{p}\right)^\gamma \quad (11)$$

[C]_H: Hartridge smoke intensity.

[C]: Soot concentration (mg/m³).

θ_B : Start of combustion (crank angle).

γ : Pressure exponent (dimensionless).

The Hartridge smoke intensity is determined using the following equation:

$$\text{Hartridge} = 100[1 - 0.9545 \cdot \exp(-2.4226[C])] \quad (12)$$

BSN: Derived from Hartridge smoke intensity.

9-Particulate matter

The PM level is determined based on the number of Bosch smokes.

$$[PM] = 565 \left(\ln \frac{10}{10 - \text{Bosch}} \right)^{1.206} \quad (13)$$

PM: Particulate matter concentration (mg/m³).

Table 1 Fuel properties of diesel with different additives (Vigneswaran et al., 2021; Vellaiyan et al., 2020; Khatri and Goyal, 2021; 2020)

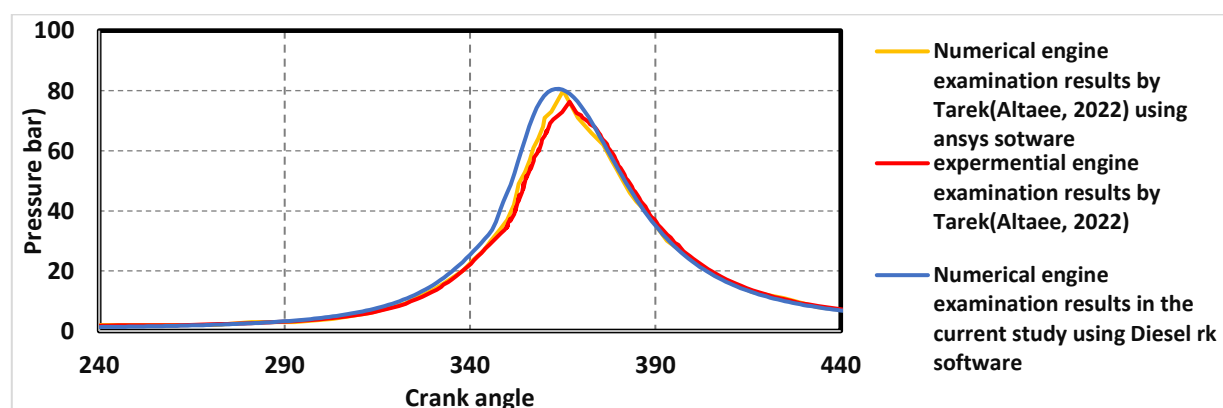
	Diesel	95% Diesel and 5% water	95% Diesel and 5% water with 50 $\mu\text{m SiO}_2$	95% Diesel and 5% water with 50 $\mu\text{m TiO}_2$
Abbreviation of the symbol	D	DW	DWTIO ₂	DWSIO ₂
Density at 15°C (kg/m ³)	830	836.6	846.2	837
Value of Calorific (MJ/kg)	42.9	41.2	41.3	41.4
Point of flash (°C)	62	67	70	69
Cetan number	52.2	50.9	51.4	51.8
Air-fuel ratio /Lambda 1	14.3	14.97	14.49	14.47
Air-fuel ratio /Lambda 1.2	17.16	17.96	17.39	17.36
Air-fuel ratio/ Lambda 1.4	20.02	20.95	20.28	20.26
Air-fuel ratio/ Lambda 1.6	22.88	23.95	23.18	23.15
Molar weight	168	160.5	160.5	160.5
Viscosity at 40°C (mm ² /sec)	2.41	2.91	2.92	2.93

Table 2 Engine characteristics (Gad et al., 2021)

Parameters of the Engine	Characteristics
Type of engine	DEUTZ F1L511
Cycles number	Four-stroke
Number of cylinders	1
Compression ratio	17.5:1
Injector opening pressure (bar)	220
Cooling type	Air-cooled
Bore (mm)	100
Stroke (mm)	105
Rated brake power (kW)	5.775 at 1500 rpm

2.1. Validation of the models

A combustion chamber model for a single-cylinder, air-cooled, direct-injection diesel engine was developed and evaluated for validation purposes. A mimicked model in this study was compared with the experimental and numerical models developed by Tarek (Naife, 2022). The engine specifications and additional data were obtained from the engine specifications identified by Tarek (Naife, 2022) under particular conditions, including an engine speed of 1500 rpm. The combustion chamber pressure validation outcomes are displayed in Figure 1.

**Figure 1** Validation results of combustion chamber pressure

Tarek's numerical and experimental outcomes, along with the numerical outcomes in this study, generally aligned well at most points. Additionally, the mimicked model in this study was

compared to the experiential and numerical results of Gad et al. (Gad et al., 2021). The simulated results in this study demonstrated a strong correlation with the experimental and numerical outcomes by Gad et al. (Gad et al., 2021) under the same operating conditions, similar full engine load conditions, identical fuel properties, the same engine specifications, and an engine speed of 1500 rpm (Table 3).

Table 3 Validation results of combustion chamber model with (Gad et al., 2021)

Parameter	Experiential results by (Gad et al., 2021).	Numerical results by (Gad et al., 2021) using Diesel-RK software	Numerical results in the current study using Diesel Rk software
Specific fuel consumption, kg/ kW.hr	0.31	0.32	0.30
Thermal efficiency, %	27.5	27.8	28.1
Maximum cylinder pressure (bar)	71.2	71.3	68.9

3. Results and Discussion

Three different additives to diesel fuel were used to study the impact of lambda percentages (1.2, 1.4, and 1.6) and different engine speeds (2000, 3000, and 4000 rpm) on diesel combustion performance. The Diesel-RK simulation program was utilized to study the impact of the lambda values and engine speeds on the combustion properties of diesel fuel under three different additions: 95% diesel fuel and water with a 5% ratio (DW), 95% diesel fuel and 5% water with 50 μ m TiO₂ (DWTiO₂), and 95% diesel fuel and 5% water with 50 μ m SiO₂ (DWSiO₂). The simulation findings for the combustion characteristics of diesel fuels with three different additives are presented below.

3.1. Pressure

(Supplementary Figure A.1) shows the relationship between the pressures inside the combustion chamber and the crank angle under different lambda values and diesel fuel additives at various engine speeds. Figure 2 shows the effect of different lambda values on the pressure inside the combustion chamber under diesel fuel additives at various engine speeds. Figures A.1 and 2 show that under the same fuel type and engine speed, the maximum pressure within the combustion chamber drops as the lambda ratio rises. This is because raising the lambda value permits the quantity of air to grow and the amount of fuel to decrease, thus lowering the energy generated by the fuel and air combination within the combustion chamber. Thus, the pressure and temperature in the combustion chamber gradually decrease as the lambda value rises. Furthermore, under the same lambda value and engine speed, it was determined that diesel had the greatest peak pressure among many additives to diesel fuel. Also, the peak pressure associated with diesel fuel declines when water is included because of its significant latent heat of vaporization, which cools the combustion process by absorbing thermal energy. Watanabe et al. (2017) obtained analogous outcomes. Moreover, when nanomaterials are introduced, the peak pressure level for water-emulsified diesel fuel rises. According to numerical results, the TiO₂ nanomaterial exhibits a greater pressure value than the SiO₂ nanomaterial when combined with water-emulsified diesel fuel. In diesel-water emulsions, integrating nanoparticles such as TiO₂ and SiO₂ improves combustion efficiency by serving as catalysts, decreasing ignition delay, and contributing to more thorough fuel oxidation, which considerably raises the HRR. These nanoparticles enhance thermal conductivity and fuel atomization, thereby improving heat transmission and raising combustion temperatures, thereby increasing the pressure inside the engine. The DW combination shows a lower peak pressure of around 2.58% than diesel because water has a cooling effect that lowers peak combustion temperatures. Additionally, the peak pressure increases by 0.5% over DW with the DWSiO₂ mixture and by approximately 0.7% with the DWTiO₂ mixture. Figures A.1 and 2 illustrate

that when engine speed expands, the peak pressure value drops for a similar fuel type and lambda value. In addition, the minimum cylinder pressure is 85.05 bar, which is achieved by water-emulsified diesel fuel at 1.6 lambda and 4000 engine speed. In comparison, the maximum cylinder pressure is 114.7 bar when diesel fuel is used at 1.2 lambda and 2000 engine speed.

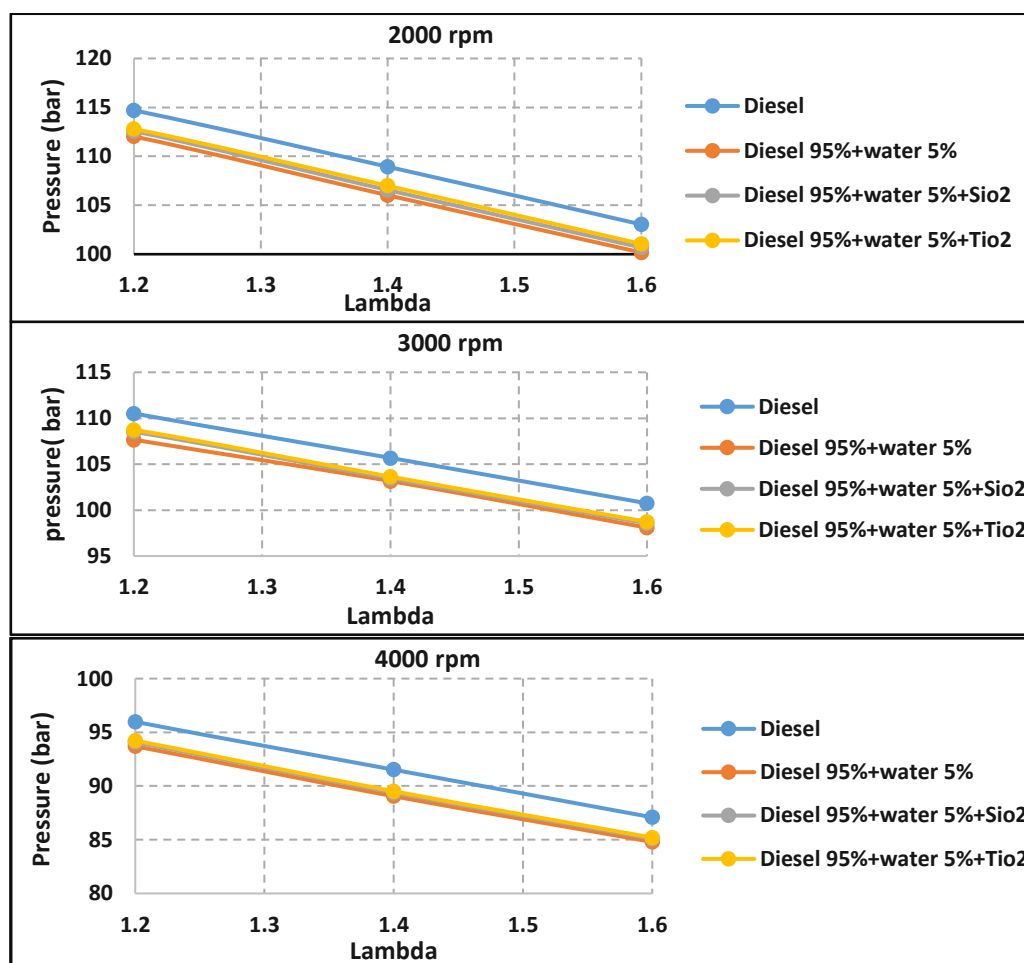


Figure 2 The relationship between the pressures and the lambda values at different additions in diesel fuel and various engine speeds

3.2. Temperature

(Supplementary Figure A.2) depicts the linkage between the combustion chamber temperature and crank angle across different lambda values and diesel fuel additives at various engine speeds. Figure 3 depicts the influence of various lambda values on the temperature inside the combustion chamber under diesel fuel additives at various engine speeds. Assuming the same fuel type and engine speed, Figures A.2 and 3 show that the highest temperature inside the internal combustion chamber decreases as the lambda ratio increases. Furthermore, adding water to diesel fuel lowers the highest peak temperature because water has a cooling effect that reduces peak combustion temperatures by absorbing heat during combustion. [Watanabe et al. \(2017\)](#) reported similar findings. However, the highest peak temperature rises when nanomaterials are introduced to EEDF. Furthermore, the TiO₂ tiny particles exhibit a higher temperature ratio than the SiO₂ tiny particles when combined with water-emulsified diesel fuel. Including nanoparticles like TiO₂ and SiO₂ in diesel-water emulsions improves engine performance by decreasing ignition delay and improving fuel atomization, which contributes to higher HRR and increased combustion temperatures due to their superior thermal conductivity and catalytic activity. The DW blend has lower peak temperatures by approximately 2.42% when compared with diesel because of the

cooling impact of water, which lowers peak combustion temperatures. However, the peak temperatures increase dramatically when TiO_2 or SiO_2 NPs are included in the DW combination. More precisely, the DWSiO_2 mixture improves peak pressure by 0.42% above DW, but the DWTiO_2 mixture improves by around 0.59%. Figures A.2 and 3 show that the maximum temperature value drops as the engine speed increases when the same lambda value and fuel type are applied. Diesel fuel with a 1.2 lambda value and 2000 engine speed of 2000 achieves a maximum cylinder temperature of 2196.9 K. In contrast, water-emulsified diesel fuel with a 1.6 lambda value and 4000 engine speed attains a minimum cylinder temperature of 1897.5 K.

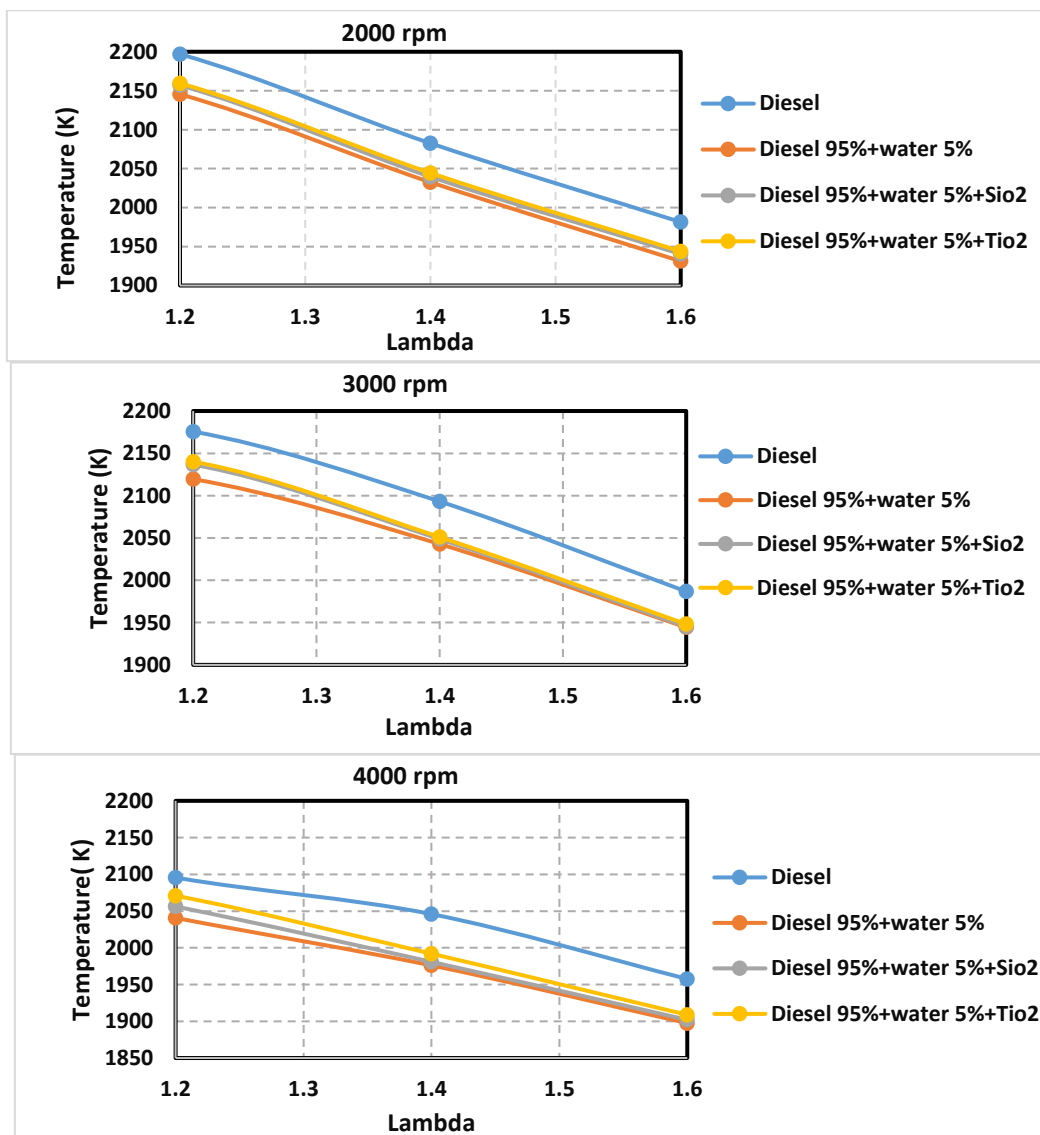


Figure 3 The relationship between the temperature and the lambda values at different additions in diesel fuel and various engine speeds (2000 rpm, 3000 rpm, and 4000 rpm)

3.3. Heat release rate (HRR)

(Supplementary Figure A.3) illustrates the relationship between the crank angles and the HLR with various lambda values, engine speeds, and different additives in diesel fuel. Figure 4 shows the analysis of the heat release rate per lambda with multiple engine speeds and different additives for diesel fuel. As shown in Figures 4 and A.3, the heat release rate decreases with an increase in the lambda ratio due to the reduction in the fuel content and the overall energy released during combustion when using the identical fuel type and maintaining a consistent engine speed. The lambda ratio indicates the air-fuel ratio in relation to the stoichiometric air-fuel ratio. When the

lambda ratio is greater than 1 (leaner mixture), the combustion mixture contains more air than fuel, which reduces the amount of fuel available for combustion. As a result, less energy is released during the combustion process, which decreases the HRR. As shown in Figures 4 and A.3, under the same lambda and engine speed, diesel has the highest heat release rate compared with the different additives in diesel fuel. Moreover, the addition of water to diesel fuel (DW) generally leads to a reduction in the heat release rate (HRR), as water has a cooling effect that absorbs heat during combustion, lowering peak combustion temperatures. The addition of water to diesel fuel (DW) reduces the HRR by 4.10% at 2000 rpm, 4.45-4.63% at 3000 rpm, and 4000 rpm.

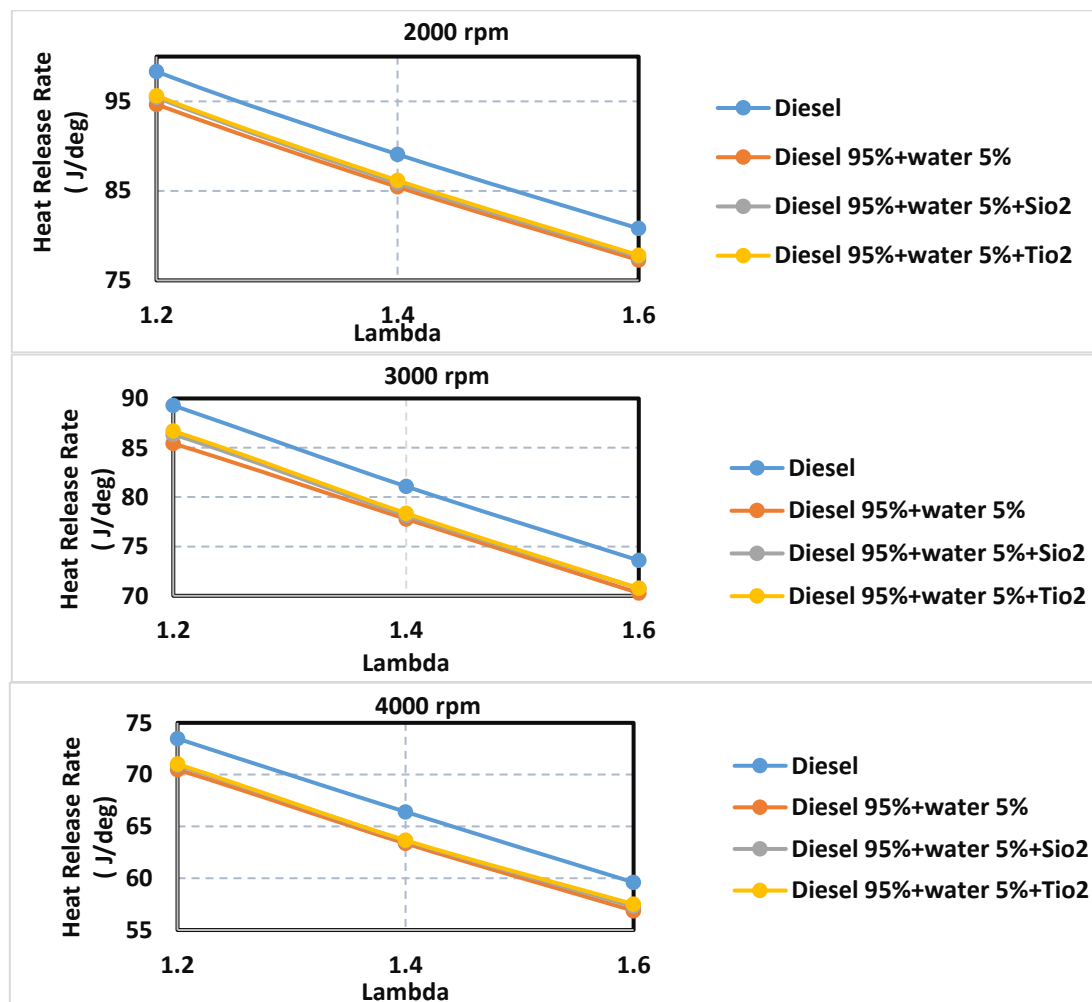


Figure 4 Relationship between the heat release rate and the lambda values at different diesel fuel additions and engine speeds

However, when nanomaterials are incorporated into water-emulsified diesel fuel, the peak heat release rate value increases. The presence of nanoparticles involving SiO_2 and TiO_2 in diesel-water emulsions expands combustion efficiency by lowering the delay of ignition while stimulating more thorough fuel oxidation, which leads to a rise in the HRR. The combustion characteristics are enhanced by the inclusion of nanoparticles in the diesel-water mixture, which causes micro-explosions and finer atomization, which in turn improves the mixing of fuel and air and accelerates vaporization. Improved heat transfer, greater combustion temperatures, and increased pressure within the combustion chamber result from the enhancement of thermal conductivity and fuel atomization by the nanoparticles (Sundararajan and Ammal, 2018). TiO_2 addition to water-emulsified diesel (DWTiO_2) improves the HRR by 1.27%, 1.14%, and 0.84% at 2000, 3000, and 4000 rpm, respectively. In addition, SiO_2 addition in water-emulsified diesel (DWSiO_2) provides a

0.6- 0.91% improvement over water-emulsified diesel fuel DW but with a smaller effect than TiO_2 . As shown in Figures 4 and A.3, with identical fuel type and the same lambda value, the results explain that the value of the heat release rate decreases as the engine speed increases. The results reveal that the highest value of heat release was 98.34 J/deg obtained from diesel fuel at 1.2 lambda and 2000 rpm engine speed. In comparison, the minimum value of heat release was 57.5 J/deg obtained from water-emulsified diesel fuel at 1.6 lambda and 4000 engine speed. Figures A.4 - A.6 illustrate the simulation findings for spray evolution in the combustion chamber with a 1.2 lambda value, variable diesel fuel additions, and different engine speeds.

3.4. Particulate matter emissions

Figure 5 illustrates the relationship between PM emissions and lambda values at varying engine speeds and fuel additives. As demonstrated in Figure 5, under the same lambda and fuel type, the predicted results showed that the PM emissions of all the tested fuels increase with an increase in engine speed. Moreover, as shown in Figure 5, under the same fuel type and engine speed, as the lambda value increases from 1.2 to 1.6, a leaner air-fuel mixture is achieved, which leads to lower PM emissions. As depicted in Figure 5, under the same lambda and engine speed, the results show that diesel has the highest PM emissions compared with different additives in diesel fuel. Moreover, adding water to diesel fuel reduces PM emissions. [Watanabe et al. \(2017\)](#) reported similar results. The addition of water to diesel fuel (DW) decreases PM by 5.36% at 2000 rpm, 5.31- 4.48% at 3000 rpm, and 4000 rpm.

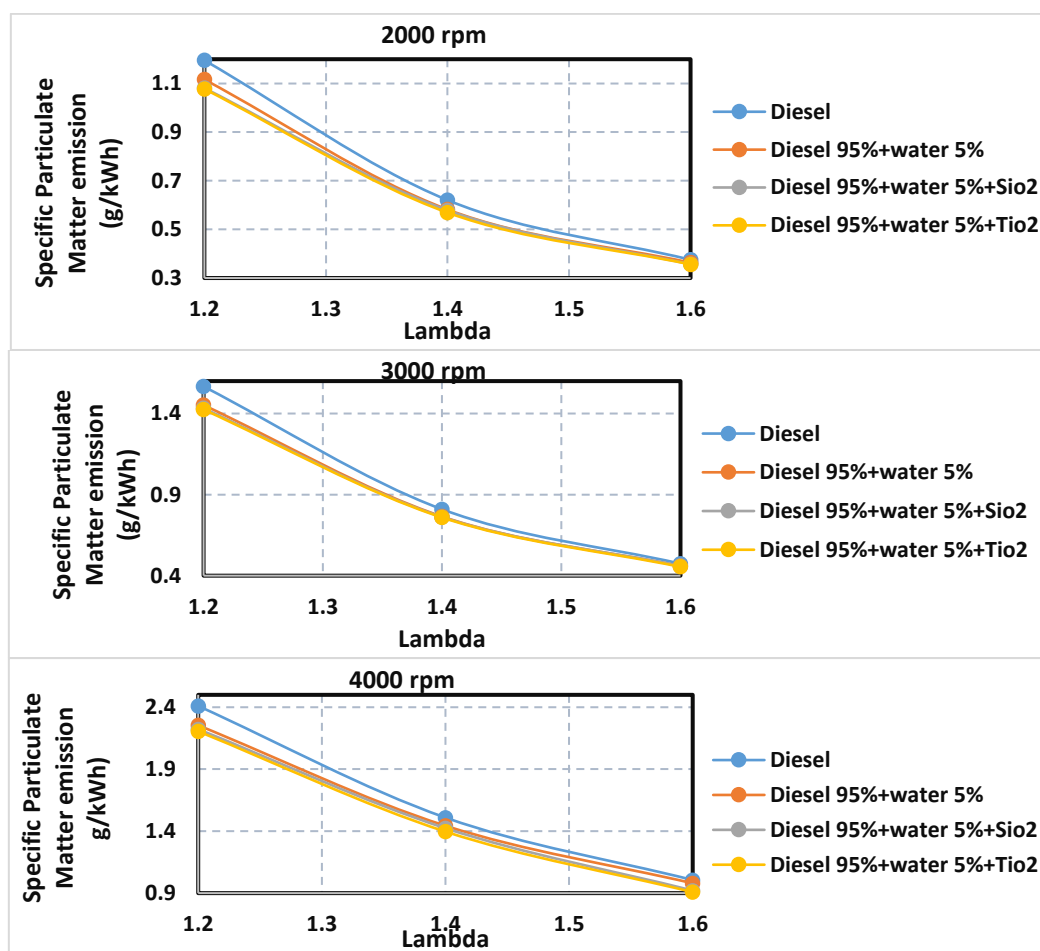


Figure 5 The relationship between PM emissions and the lambda values at different additions in diesel fuel and various engine speeds

Adding nanomaterials (TiO_2 and SiO_2) to water-emulsified diesel fuel (DW) decreases PM emissions. In addition, the TiO_2 nanomaterial has a lower PM emissions value than the SiO_2 nanomaterial when mixed with water-emulsified diesel fuel, highlighting its potential to reduce PM's environmental impact. TiO_2 addition to water-emulsified diesel fuel (DWTIO₂) reduces PM emissions by 2.61 % at 2000 rpm and 1.28 - 4.47 % at 3000 and 4000 rpm. In addition, SiO_2 addition (DWSIO₂) reduces pm by 1.9% at 2000 rpm, 0.61-3.07 % at 3000 rpm, and 4000 rpm. Several factors, such as fuel formulation, air-fuel proportion, mixing efficiency, pressure, and temperature, affect particulate matter emissions from diesel engines. Despite the elevated combustion temperatures, diesel fuel generates more PM due to its intricate composition and the dynamics of the combustion process. Diesel's high carbon-to-hydrogen percentage and lengthy hydrocarbon chains make it susceptible to incomplete and insufficient combustion, particularly in rich spots where fuel intensity exceeds available oxygen.

Furthermore, inadequate fuel-air mixing, a typical problem in compression ignition engines, contributes to soot generation, diminishing the advantages of high temperatures. However, diesel mixtures with water or additives such as SiO_2 and TiO_2 exhibit markedly reduced PM emissions. Additionally, water enhances fuel-air mixing by dispersing the fuel spray into smaller droplets, resulting in a more uniform combustion distribution.

Adding nanoparticles such as SiO_2 and TiO_2 to diesel-water emulsions improves combustion performance by serving as catalysts and facilitating more thorough fuel oxidation, vastly boosting the heat release rate. The highest cylinder PM emissions are 2.410 g/kWh obtained by diesel fuel at a 1.2 lambda value and 4000 rpm engine speed, while the minimum PM emissions are 0.355 g/kWh obtained by DWTIO₂ fuel at a 1.6 lambda value and 2000 engine speed.

3.5. Hartridge smoke level

Figure 6 presents the relation between the Hartridge smoke level and the lambda values for various engine speeds and diesel fuel additives. As exhibited in Figure 6, under the same fuel type and engine speed, the smoke level emission decreases with an increase in the lambda values. In addition, the smoke level emission concentration increases with an increase in engine speed at the same lambda and fuel type. As shown in Figure 6, under the same lambda and engine speed, diesel has a higher smoke level than different additives in diesel fuel. Moreover, adding water to diesel fuel decreases the smoke emission concentration rate.

However, adding nanomaterials to water-emulsified diesel fuel decreases the smoke emission level. In addition, the TiO_2 nanomaterial gives a lower smoke level than the SiO_2 nanomaterial when mixed with water-emulsified diesel fuel. Khatri and Goyal, with Vigneswaran et al. (2021) reported similar results (Khatri and Goyal, 2021; Vigneswaran et al., 2021). The addition of water to DW reduces the smoke level by 1.36% at 2000 rpm, 1.38% at 3000 rpm, and 0.82% at 4000 rpm. TiO_2 addition to water-emulsified diesel fuel (DWTIO₂) reduces smoke level by 2.51% at 2000 rpm, 1.5-3.4% at 3000 rpm, and 4000 rpm. Moreover, SiO_2 addition (DWSIO₂) reduces smoke level by 2.1% at 2000 rpm and 0.6-2.38% at 3000 rpm and 4000 rpm. The maximum Hartridge smoke level inside the engine is 64.45, which is obtained by diesel fuel at a 1.2 lambda and engine speed of 4000 rpm, while the minimum Hartridge smoke level is 12.8, which is obtained by DWTIO₂ fuel at a 1.6 lambda and engine speed of 2000 rpm.

3.6. Carbon dioxide (CO_2)

Figure 7 illustrates the correlation between CO_2 and lambda levels across various engine speeds and distinct additives in diesel fuel. The combustion strategy within the combustion chamber and the oxygen content of the fuel affect CO_2 emissions. The increased CO_2 content indicates that the fuel has been virtually completely burned within the engine. Additionally, the temperature within the combustion chamber influences CO_2 emissions. A more efficient combustion process also results in higher CO_2 emissions. As exhibited in Figure 7, under the same fuel type and engine speed, the CO_2 emission increases with an increase in the lambda values.

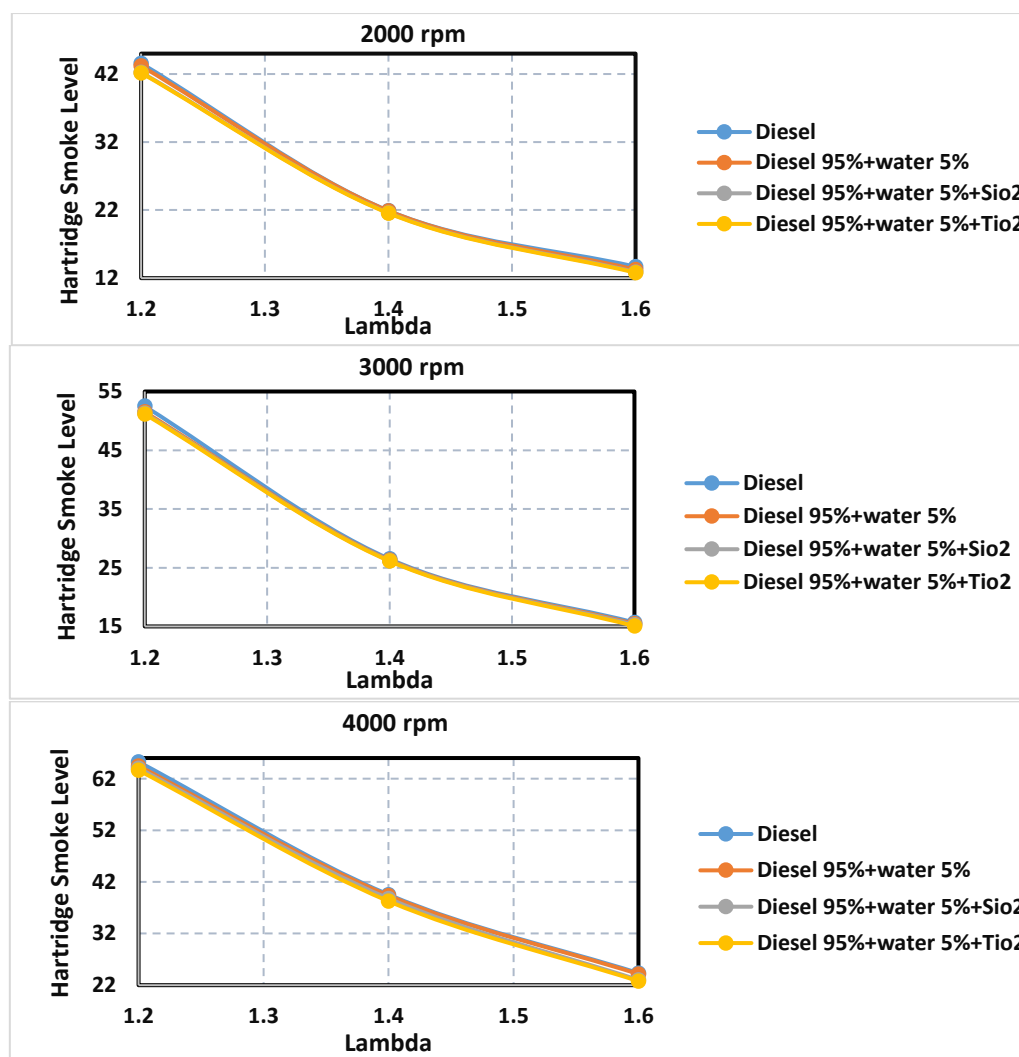


Figure 6 The relationship between smoke level and the lambda values at different additions in diesel fuel and various engine speeds

In addition, the CO₂ emission concentration increases with an increase in engine speed at the same lambda and fuel type. As shown in Figure 7, under the same lambda and engine speed, diesel has the minimum CO₂ emission concentration compared with different additives in diesel fuel. Moreover, adding water to diesel fuel increases the CO₂ emission concentration rate. However, adding nanomaterials to water-emulsified diesel fuel decreases the CO₂ emission concentration rate. [Hoseini and Sobati \(2019\)](#) and [Abdollahi et al. \(2020\)](#) observed similar findings. This is because the water vapor in diesel fuel produces an OH radical during combustion, which facilitates the combination of oxygen and CO, thereby increasing the amount of CO₂ emissions. Incorporating nanomaterials into water-emulsified diesel fuel lowers CO₂ emission levels. Incorporating nanoparticles into the diesel-water emulsion enhances combustion dynamics by increasing micro-explosions and finer atomization, which increase fuel-air mixing and expedite vaporization. According to the numerical results, the TiO₂ nanomaterial has a lower CO₂ emission concentration rate than the SiO₂ nanomaterial when mixed with water-emulsified diesel fuel. The addition of water to DW increases CO₂ by 3.73% at 2000 rpm, 4.39- 5.60% at 3000 rpm, and 4000 rpm. TiO₂ addition to water-emulsified diesel fuel (DWTIO₂) reduces CO₂ by 0.61 % at 2000 rpm, 0.74-1.13 % at 3000 rpm, and 4000 rpm. In addition, SiO₂ addition (DWSIO₂) reduces CO₂ by 0.4% at 2000 rpm and 0.57-0.66 % at 3000 and 4000 rpm. The maximum CO₂ emission concentration inside the engine is 1029.5 g/kWh obtained by water-emulsified diesel fuel at a 1.6 lambda and engine speed of 4000

rpm, while the minimum CO₂ emission concentration is 755.1 g/kWh obtained by diesel fuel at a 1.2 lambda and engine speed of 2000 rpm.

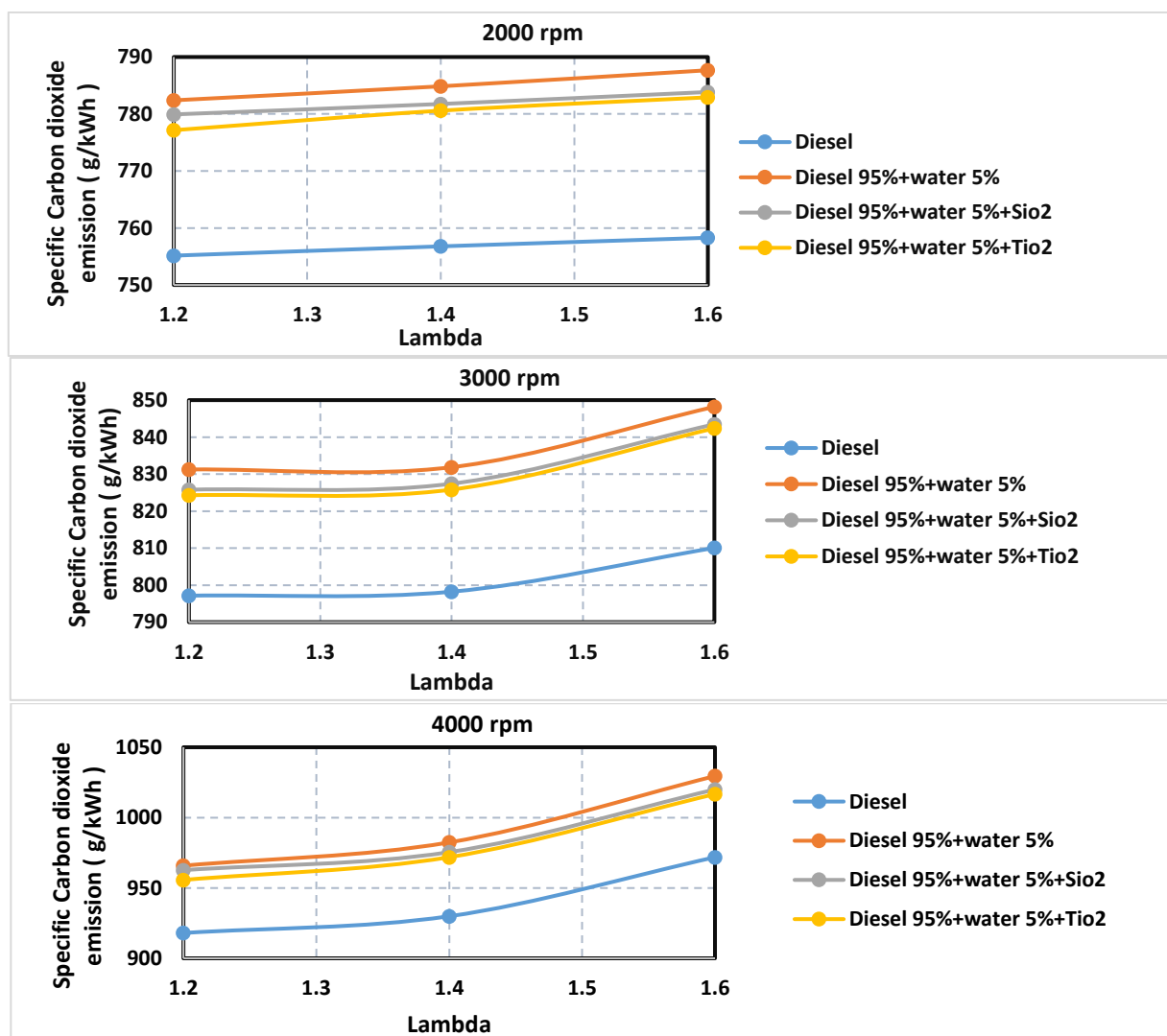


Figure 7 The relationship between CO₂ and the lambda values at different additions in diesel fuel and various engine speeds

3.7. Nitric oxide emission (NO)

Figure 8 depicts the influence of lambda ratios on nitric oxide emissions while using diverse additives in diesel fuel at different engine speeds. Figure 8 demonstrates that for the same fuel type and engine speed, nitric oxide emissions increment with each increase in the lambda value. This is because the amount of nitric oxide generated depends on the engine's maximum temperature, residence duration, and oxygen content. Consequently, nitric oxide contaminants in the engine gradually increase as the lambda level increases. As illustrated in Figure 8, diesel has the highest NO mass fraction value compared with other diesel fuel additives at similar lambda and engine speeds. Additionally, the NO mass fraction value decreases when water is introduced into diesel fuel. However, when nanomaterials are included in water-emulsified diesel fuel, the NO mass fraction percentage rises. Furthermore, when combined with water-emulsified diesel fuel, the TiO₂ nanomaterial yields a higher NO mass fraction value than the SiO₂ nanomaterial. Vigneswaran et al. and Khatri and Goyal reported similar results (Vigneswaran et al., 2021; Khatri and Goyal, 2021). The addition of water to DW reduces NO emission by 23.75% at 2000 rpm, 26.25 - 29.44% at 3000 rpm, and 4000 rpm. TiO₂ addition to water-emulsified diesel fuel (DWTIO₂) increases NO

emission by 11.46 % at 2000 rpm, 12.86 % at 3000 rpm, and 13.71% at 4000 rpm. Moreover, SiO_2 addition in water-emulsified diesel (DWSIO₂) increases NO emission by 8.90%, 10.20%, and 10.77% at 2000, 3000, and 4000 rpm, respectively, but with a smaller effect than TiO_2 . Figure 8 shows that the concentration of nitric oxide emissions decreases as the engine speed increases for the same fuel type and lambda. Diesel fuel with a 1.6 lambda and engine speed of 2000 rpm produced the highest NO mass fraction value within the engine, 11.569 g/kwh, whereas water-emulsified diesel fuel with a 1.2 lambda and engine speed of 4000 rpm produced the lowest NO mass fraction value, 5.34 g/kwh.

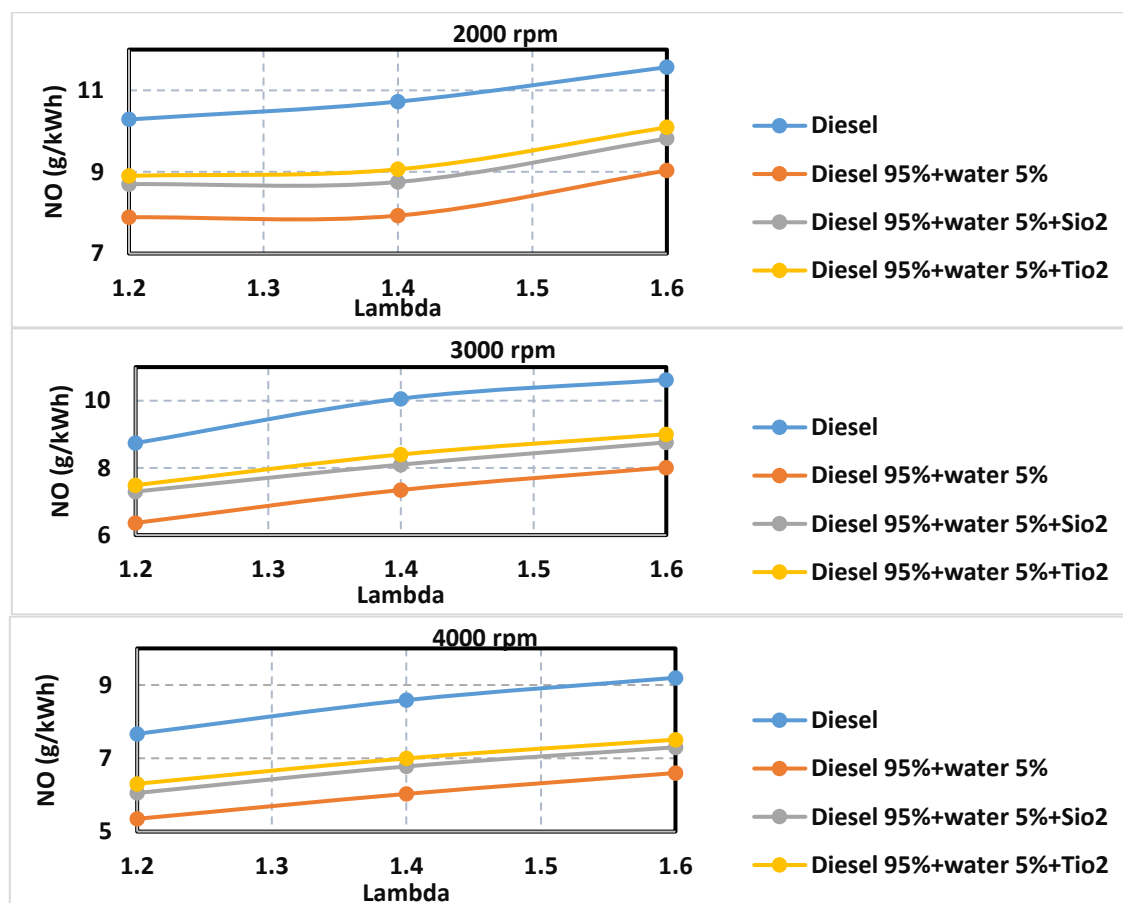


Figure 8 The relationship between NO and the lambda values at different additions in diesel fuel and various engine speeds

4. Conclusions

The current work presents the impact of lambda percentages (1.2, 1.4, and 1.6) and different engine speeds (2000, 3000, and 4000 rpm) on the combustion efficiency and emissions of diesel engines operating under diesel fuel with three different additives (water with 5% ratio, 5% water with 50 μm TiO_2 and 5% water with 50 μm SiO_2). Diesel-RK software was used to model and simulate fuel combustion inside the engine. Numerical computations were performed on a single-cylinder, DEUTZ F1L511 cooled by air, and direct-injection diesel engine. Based on the numerical findings, with the same fuel types and engine speeds, the maximum pressure, maximum temperature, heat release rate, particulate matter emissions, and smoke level inside the combustion chamber decreased when the lambda ratio was increased from 1.2 to 1.6. In contrast, carbon dioxide and nitric oxide also rose. Moreover, under the same lambda and fuel type, the nitric oxide emission concentration, heat release rate, maximum pressure, and maximum temperature reduced with increased engine speed from 2000 to 4000 rpm, whereas carbon dioxide emission, Hartridge smoke level, and particulate matter emissions increased. When water is added to diesel fuel, engine

performance and emissions show appreciable changes over pure diesel: The rate of nitric oxide emission drops by 23.75% at 2000 rpm and 26.25%–29.44% at 3000 rpm and 4000 rpm. The smoke level falls by 1.36%, 1.38%, and 0.82% at 2000, 3000, and 4000 rpm, respectively. Particulate matter emissions decline by 5.36% at 2000 rpm, 5.31%, and 4.48% at 2000, 3000, and 4000 rpm, respectively. The heat release rate drops by 4.10% at 2000 rpm and by 4.45% to 4.63% at 3000 and 4000 rpm. However, adding water to diesel (DW) increases carbon dioxide emissions by 3.73% at 2000 rpm and by 4.39% to 5.60% at higher speeds (3000 and 4000 rpm). On the other hand, adding nanomaterials to water-emulsified diesel fuel increases the highest peak temperature, the highest peak pressure, the heat release rate, and nitric oxide emission, whereas particulate matter, carbon dioxide, and smoke level emissions decrease. The mixture of 95% diesel fuel and 5% water with 50µm TiO₂ (DWTiO₂) has a higher temperature, pressure, heat release rate, and nitric oxide emission value than the DWSiO₂ mixture of 95% diesel fuel and 5% water with 50µm SiO₂. Moreover, the DWTiO₂ mixture yields a lower carbon dioxide emissions, particulate matter emissions, and concentration rate than the DWSiO₂ mixture.

5. Future works

Future studies will involve more detailed numerical and experimental studies with different lambda values, engine speed, and varying air-diesel mixture ratios with water and nanoparticles. The results will enable a more exact characterization of combustion characteristics and emission parameters. This approach would facilitate more accurate curve fitting and diminish dependence on visual interpolation.

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Author Contributions

Hussein A. Mahmood: The authorship and writing of the initial manuscript. Osama H. Attia: Evaluating and validating the results. Ali O. Al-Sultani: Review and evaluate the writing approach used in the original draft.

Conflict of Interest

The contributors to the article confirm that there are no conflicts or disagreements of interest regarding its publication.

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