



*Type of the Paper (Research Article )*

# Numerical investigations of SiO<sub>2</sub> and TiO<sub>2</sub> nanoparticle's addition impact on performance, combustion features, and emissions characteristics of the diesel engine operating with water diesel emulsified fuel at different lambda values and engine speeds.

**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 TiO<sub>2</sub> (DWTIO<sub>2</sub>), and 95% diesel fuel with 5% water and 50µm SiO<sub>2</sub> (DWSIO<sub>2</sub>). Combustion simulations were done using the Diesel-RK program on a DEUTZ F1L511, single-cylinder, air-cooled, direct-injection diesel engine. The outcomes of the simulation demonstrated that increasing the lambda ratio lowered combustion parameters, including temperature, pressure, heat release rate (HRR), smoke levels, and particulate matter emissions (PM), while NO and CO<sub>2</sub> rose. Moreover, increasing engine speed lowered NO emissions, HRR, pressure, and temperature, while emissions of CO<sub>2</sub> 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, CO<sub>2</sub> emissions increased. Nanomaterials added 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 (DWTIO<sub>2</sub>) surpassed the mixture (DWSIO<sub>2</sub>), highlighting its potential to enhance diesel engine performance and decrease environmental impact.

**Keywords:** water diesel emulsified fuel; TiO<sub>2</sub> and SiO<sub>2</sub> Nano particles; diesel engine; Combustion; Emission; Diesel-RK

## 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 (Vigneswaran et al., 2021; Mahmood et al., 2016; Ghareeb and Anjal, 2024; Niran K. Ibrahim, 2016; Simanjuntak et al., 2024; Tuktin et al., 2024). However, during combustion, diesel engines emit various unwanted pollutants, including particulate matter (PM) and nitrogen oxides (NO<sub>x</sub>). Both the environment and our health are negatively impacted by the emissions and the pollutants. 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 (Mahmood et al.,

For grants, please provide the grant number and the year it was received. Write it as follows: "This work was supported by the 'Name of organization' funded by 'Name of Grant and number' "

<https://doi.org/xx/ijtech.xx>

Received date; Revised date; Accepted date

2021; Watanabe et al., 2017; Abdulhadi, 2011; Hendrarsakti et al., 2025; Mahmood et al., 2024; Aisyah et al., 2023).

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 emission levels of NOX and PM and simultaneously enhance combustion efficiency in diesel combustion engines without needing engine adjustment (Vellaiyan and Amirthagadeswaran, 2016; Vellaiyan and Amirthagadeswaran, 2017). Numerous studies have shown that mixing water with diesel fuel lowers its calorific value and raises the amount of specific fuel consumed. (Mostafa et al., 2023; Khatri and Goyal, 2021; Khatri and Goyal, 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<sub>x</sub>, CO, and PM, as well as enhanced combustion efficiency. Water's ability to generate OH radicals enhances the oxidation of carbon monoxide (CO) to carbon dioxide (CO<sub>2</sub>), resulting in cleaner exhaust emissions. Blending water with 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 while vaporizing. This cooling effect decreases nitrogen oxides (NO<sub>x</sub>), a major pollutant, as well as soot and particulate matter (PM) by removing hotspots and promoting uniform combustion (Mostafa et al., 2023; Khatri and Goyal, 2021; Kumar and Raheman, 2022). Various researchers have investigated several emulsion fuels in diesel engines. Attia and Kulchitskiy (Attia and Kulchitskiy, 2014) looked into the impact of water-diesel emulsion on the three-cylinder engine with varying drop sizes. This study demonstrated that smaller water droplets were less efficient in lowering NO<sub>x</sub> emissions than bigger ones. Still, little droplets are quite effective in reducing HC emissions. Leng et al. (Leng et al., 2015) examined the variations between the features of the water-diesel combination and micro emulsion. The results revealed that the micro-emulsion showed a lower lag and improved combustion efficiency with a declining activation energy. Bidita et al. (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, with a growing need for alternatives to fossil fuels, nanofuels may represent a significant advancement in pursuing more ecologically friendly and efficient fuel technologies. Recently, researchers have looked at using nanomaterials as diesel fuel additions to enhance diesel engine performance and quality (Mahmood et al., 2023; Al-Kayiem et al., 2018; Altaee, 2022; Khan et al., 2022). Nano fuels are a kind of nanofluid that can serve as substitutes for conventional fuels. Nano fuels 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, leading to generating potential power and contributing to reducing the amount of soot creation, as well as decreased ignition delay and duration of combustion. Nouri et al. (Nouri et al., 2021) investigated the effects of Fe<sub>2</sub>O<sub>3</sub>-Al<sub>2</sub>O<sub>3</sub> 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 emissions from the diesel engine. Aalam et al. (Aalam and Alagappan, 2015) conducted a study to examine the impact of CeO<sub>2</sub> nanoparticles as an additive to diesel fuel on engine efficiency. The findings indicated that the incorporation of CeO<sub>2</sub> into diesel fuel enhanced brake thermal efficiency, elevated NO emissions, and reduced HC emissions. Tarek (Altaee, 2022) assessed the effects of integrating nanoparticles (CeO and ZnO) 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, a decrease in unburned hydrocarbons (UHC) and carbon monoxide (CO) emissions, while concurrently enhancing brake thermal efficiency.

Integrating  $\text{TiO}_2$  and  $\text{SiO}_2$  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, studies indicate that nanoparticles such as Titanium Dioxide ( $\text{TiO}_2$ ) and Silicon Dioxide ( $\text{SiO}_2$ ) 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 such as  $\text{SiO}_2$  and  $\text{TiO}_2$  to diesel-water emulsions improves combustion performance by serving as catalysts, minimizing ignition delay, and facilitating more thorough fuel oxidation, vastly boosting the heat release rate (HRR) (Rezaei, 2023; Karisathan 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; Hasannuddin et al., 2018; Khatri and Goyal, 2021; Khatri and Goyal, 2020). Vellaiyan et al. (Vellaiyan et al., 2020) examined the influence of titanium dioxide ( $\text{TiO}_2$ ) 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  $\text{TiO}_2$  nanoparticles enhanced fuel oxidation and reduced  $\text{NO}_x$  emissions, hence improving combustion efficiency. At elevated engine loads, the incorporation of  $\text{TiO}_2$  was observed to reduce smoke opacity and enhance Brake Thermal Efficiency (BTE). Vigneswaran et al. (Vigneswaran et al., 2021) investigated the exhaust properties of a compression ignition engine powered by diesel-water emulsion mixtures with the incorporation of  $\text{TiO}_2$  nanoparticles, maintaining consistent engine speed and lambda values. The results indicated that  $\text{TiO}_2$  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,  $\text{NO}_x$  emissions escalated with elevated  $\text{TiO}_2$  content. Khatria et al. (Khatri and Goyal, 2020) investigated the impact of silicon dioxide ( $\text{SiO}_2$ ) 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  $\text{SiO}_2$  nanoparticles at levels of 50 ppm and 100 ppm markedly diminished  $\text{NO}_x$  and smoke opacity emissions while enhancing the combustion of fuel. The use of  $\text{SiO}_2$  nanoparticles boosts the thermal properties of the fuel, resulting in improved heat distribution inside the engine and thus increasing the efficiency of combustion.

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 assessing and determining combustion performance and emissions. When lambda shifts from stoichiometric conditions ( $\lambda = 1$ ), either towards leaner mixtures ( $\lambda > 1$ ) or richer mixtures ( $\lambda < 1$ ), the combustion specifications can change dramatically, affecting engine performance, the combustion process, and exhaust emissions (Mahmood et al., 2022b). At the same time, different engine speeds create dynamic variations in fuel-air blending, intensity of turbulence, and heat release rates within the combustion chamber. At elevated engine speeds, shorter ignition delays and more significant turbulence may improve dispersion of nanoparticles and reactivity, in turn enhancing combustion stability and increasing the engine's thermal efficiency. However, partial combustion and increased particulate matter emissions can occur at lower engine speeds due to insufficient mixing time, which limits nanoparticle efficiency. Therefore, there is a gap in understanding the influence of engine speed and lambda values on combustion efficiency and emissions when nanoparticles are incorporated into emulsified fuels. Addressing these shortcomings will be essential for improving the usage of nanoparticle-infused emulsified fuels for cleaner and more efficient diesel engine

operation. The aim of this study is to examine the effects of nanoparticles of SiO<sub>2</sub> and TiO<sub>2</sub> 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 numerical analysis of the engine model.

## 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 rpm, 3000 rpm, and 4000 rpm), running on diesel fuel, water-emulsified diesel fuel, water-emulsified diesel fuel with SiO<sub>2</sub>, and water-emulsified diesel fuel with TiO<sub>2</sub>. (Supplementary Table A.1) presents the specifications of nanoparticles (Abdulwahab et al., 2016; Vigneswaran et al., 2021; Khatri and Goyal, 2020), 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 engine's specifications (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 process of combustion, 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; Thokchom, 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 in simulating the evaporation and combustion processes (Gad et al., 2021; Georgiou and Azimov, 2020; Kurse and Nallamotheu, 2022). The Diesel RK model considers fuel particle dimensions, the fuel spray shape, the orientation of the fuel spray, dynamics of growth and development, the process of fuel spray decomposition, the dynamics and forms of swirly patterns, and the relationship of fuel particles to walls of the combustion chamber and swirls. NO<sub>x</sub> emissions are determined by employing the Zeldovich methodology. Furthermore, the modeling process was simulated: compression stroke, fuel injection, combustion procedures, and power stroke (Gumus and Otkur, 2023; Al-Dawody et al., 2023; Islam et al., 2025; Pal and Reddy, 2024; 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 yet increase fuel efficiency; it is a benchmark for measuring the effects of nanoparticles. Also, 50 μm SiO<sub>2</sub> and TiO<sub>2</sub> nanoparticles are adopted, based on previous studies (Vellaiyan et al., 2020; Khatri and Goyal, 2020; Khatri and Goyal, 2021). In modeling diesel-water-nanoparticle blends in Diesel rk software, several simplifying assumptions are required 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 that has 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 inserted manually 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 nanoparticles 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 micro scale heat exchange. Moreover, the evaporation of water is modeled based on standard evaporation models, and nanoparticle evaporation or deposition is ignored (Hamzah et al., 2025). The governing equations utilized in the Diesel RK software are as follows: (Paul et al., 2014; Gad et al., 2021; Adib et al., 2024).

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

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

Where:

m: the entire mass in the system

t: time (s)

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

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

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

Where

$Y_j$  : Mass fraction of species j

$\Omega_i$ : Chemical reaction rate of species i (kmol/m<sup>3</sup> s)

$W_{mw}$ : species Molecular weight (kg/kmol)

$\rho$ : density of Gas (kg/m<sup>3</sup>)

**3-Energy Conservation:** An open thermodynamic system's generalized energy equation 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)

$Q_{ht}$ : Heat transfer rate (W)

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

**4- Lambda ( $\alpha_1$ ):**  $\lambda$  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

$\alpha_1$ : Equivalence ratio (dimensionless).

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

(A/F)<sub>s</sub>: 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 power generated is known as specific fuel consumption, or SFC that is:

:

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

Where

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

Pb: Brake power (W).

## 6- Calculation of heat release

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

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

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

$\tau$ : Ignition delay time (s).

n: Engine speed (rpm).

P: Pressure (Pa).

T: Temperature (K).

Ea: Activation energy (J/mol).

CN: Cetane number of the fuel.

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

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

x: Burned fuel fraction.

$d\sigma_u$ : Unburned fuel mass fraction.

X0: Initial burn fraction.

$m_f$ : Fuel mass (kg).

$V_i$ : Initial spray volume (m<sup>3</sup>).

$\phi_0, \phi_1$ : Combustion efficiency factors

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

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

$\sigma_u$ : Unburned fuel fraction.

$\phi$ : Equivalence ratio.

A2: Mixing-controlled combustion constant.

(d) Phase of late combustion. The HRR is calculated as follows:

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

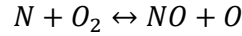
KT: Temperature-dependent rate coefficient.

$\xi_b$ : Burned gas fraction.

$\phi_3$ : Late-phase efficiency factor.

### 7-NOx formation calculation

The nitrogen oxide reaction is:



The reaction is depended on the oxygen concentration. The volumetric of NO concentration is given by:

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

[NO]: Nitric oxide concentration (mol/m<sup>3</sup>).

$\theta$ : Crank angle (degrees).

$T_z$ : Local temperature (K).

$[N_2]_e, [O]_e$ : Equilibrium concentrations of N<sub>2</sub> and O<sub>2</sub>.

$[NO]_e$ : Equilibrium NO concentration.

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

### 8- Soot intensity calculation

Soot consists of minuscule particles of dark carbon dispersed in a gas transporter. Incomplete combustion of hydrocarbons is considered the primary reason for soot formation. Soot particles are formed, grown, and broken down as a result of chemical reactions during combustion. This is linked to common scenarios, including:

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

$[C]_H$ : Hartridge smoke intensity.

[C]: Soot concentration (mg/m<sup>3</sup>).

$\theta_B$ : Start of combustion (crank angle).

$\gamma$ : Pressure exponent (dimensionless).

The Hartidge smoke intensity is determined using the following Equation:

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

Bosch Smoke Number (BSN): Derived from Hartridge smoke intensity.

### 9-Particulate Matter (PM)

The PM level is determined depending on the Bosch smoke number.

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

[PM]: Particulate matter concentration (mg/m<sup>3</sup>).



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

	Diesel	95% Diesel and 5% water	95%Diesel and 5%water with 50 µm SiO <sub>2</sub>	95% Diesel and 5% water with 50 µm TiO <sub>2</sub>
Abbreviation of the symbol	D	DW	DWTiO <sub>2</sub>	DWSiO <sub>2</sub>
Density at 15°C (kg/m <sup>3</sup> )	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	20.263
Air-fuel ratio/ Lambda 1.6	22.88	23.95	23.18	23.158
Molar weight	168	160.5	160.5	160.5
Viscosity at 40°C (mm <sup>2</sup> /sec)	2.41	2.91	2.92	2.93

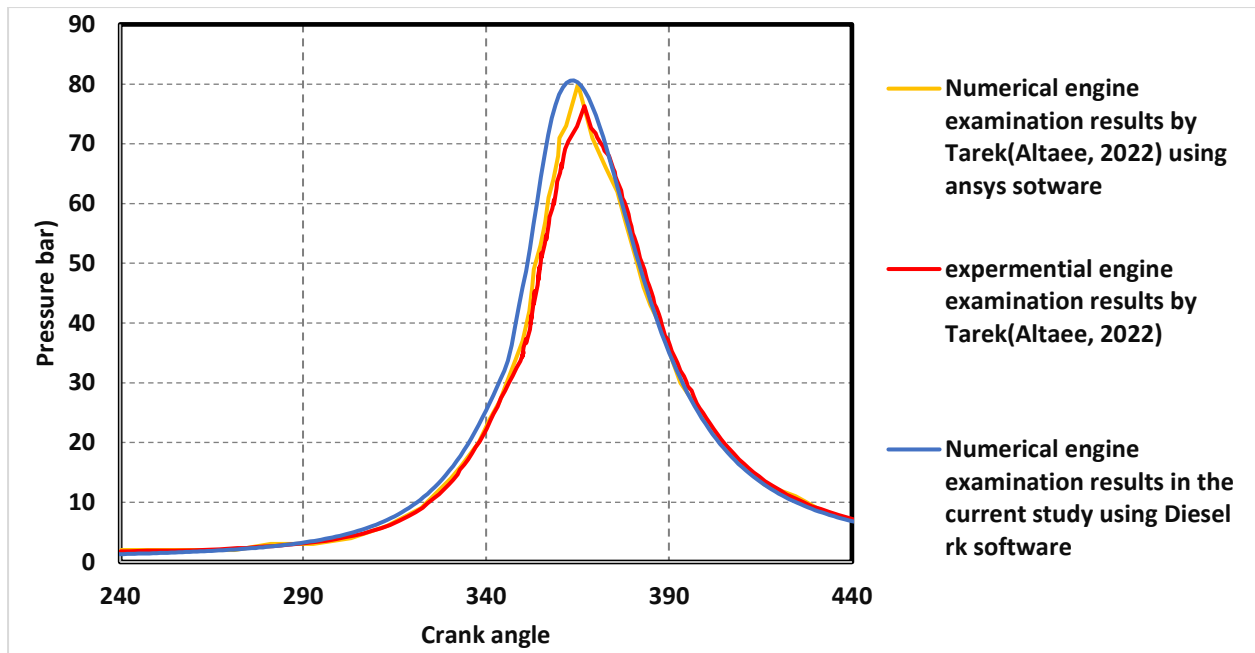
**Table 2** Engine characteristics(Gad et al., 2021).

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. Validations of the models*

A model of a combustion chamber for a single-cylinder, air-cooled, direct-injection diesel engine was developed and evaluated for validation reasons. A mimicked model in this study was compared to the experimental and numerical model developed by Tarek. (Altaee, 2022). The engine specifications and additional data were obtained from the engine specifications identified by Tarek (Altaee, 2022) under particular conditions, including an engine speed of 1500 rpm. The outcomes of the combustion chamber pressure validation are displayed in Figure 1. Tarek's numerical and experimental outcomes and the numerical outcomes in this study seemed to match rather well at most points, generally. Additionally, the mimicked model in this study was compared to Gad et al.'s experiential and numerical results (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, the simulated results in this study demonstrated a strong correlation with the experimental and numerical outcomes by Gad et al (Gad et al., 2021) as shown in Table 3.





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

**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	0.30495
Thermal efficiency, %	27.5	27.8	28.107
Maximum cylinder pressure (bar)	71.2	71.3	68.99

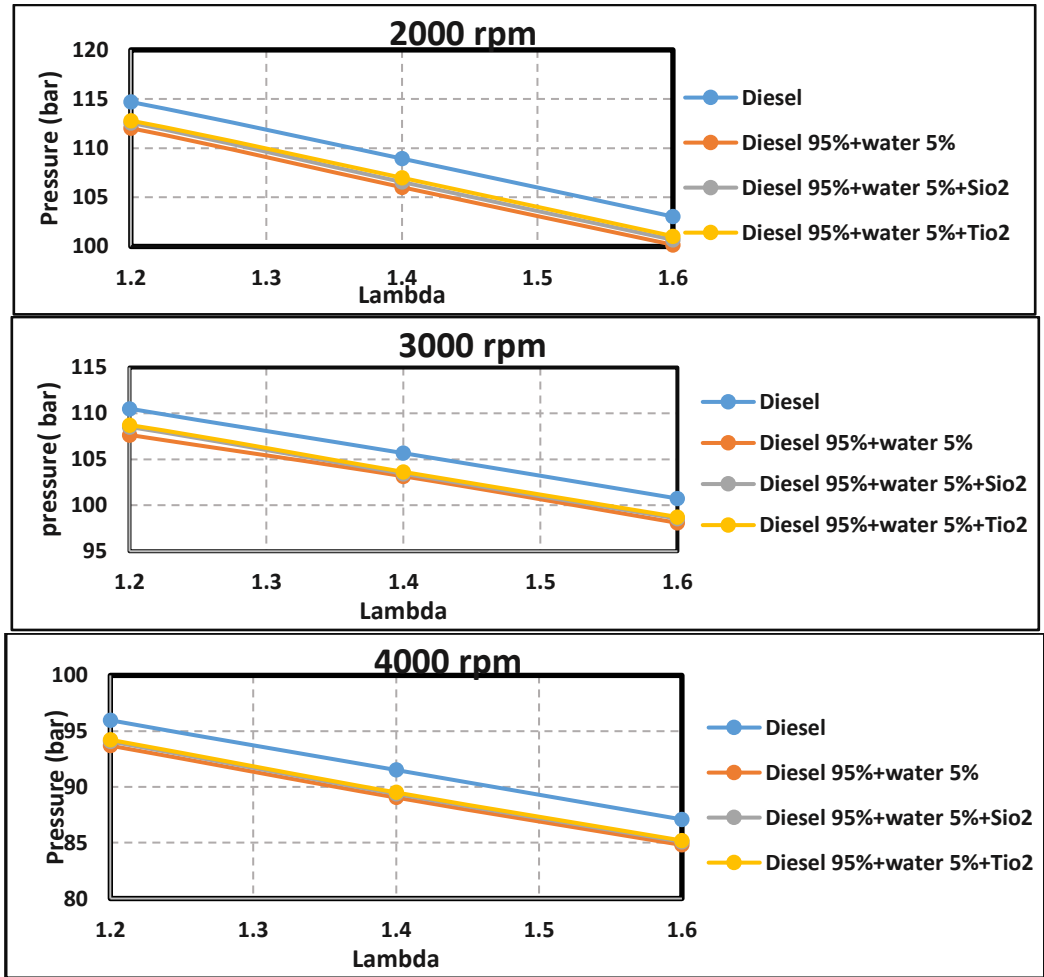
### 3. Results and Discussion

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 rpm, 3000 rpm, and 4000 rpm) on the performance of diesel combustion. 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 various additions (95% diesel fuel and water with a 5% ratio (DW), 95% diesel fuel and 5% water with 50 $\mu$ m TiO<sub>2</sub> (DWTiO<sub>2</sub>) and 95% diesel fuel and 5% water with 50 $\mu$ m SiO<sub>2</sub> (DWSiO<sub>2</sub>)). Below are the simulation findings for the combustion characteristics of diesel fuels with three different additives.

#### 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 different additives in diesel fuel at various engine speeds. Figure 2 shows the effect of different lambda values on the pressure inside the combustion chamber under different additives in diesel fuel at various engine speeds. According to Figures A.1 and 2, under the same fuel type and same engine speed, it was discovered that the maximum pressure within the combustion chamber drops as the lambda ratio rises. This is because raising the value of lambda 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 drop gradually as the lambda value rises. Furthermore, under the same lambda value and same engine speed, it was determined that

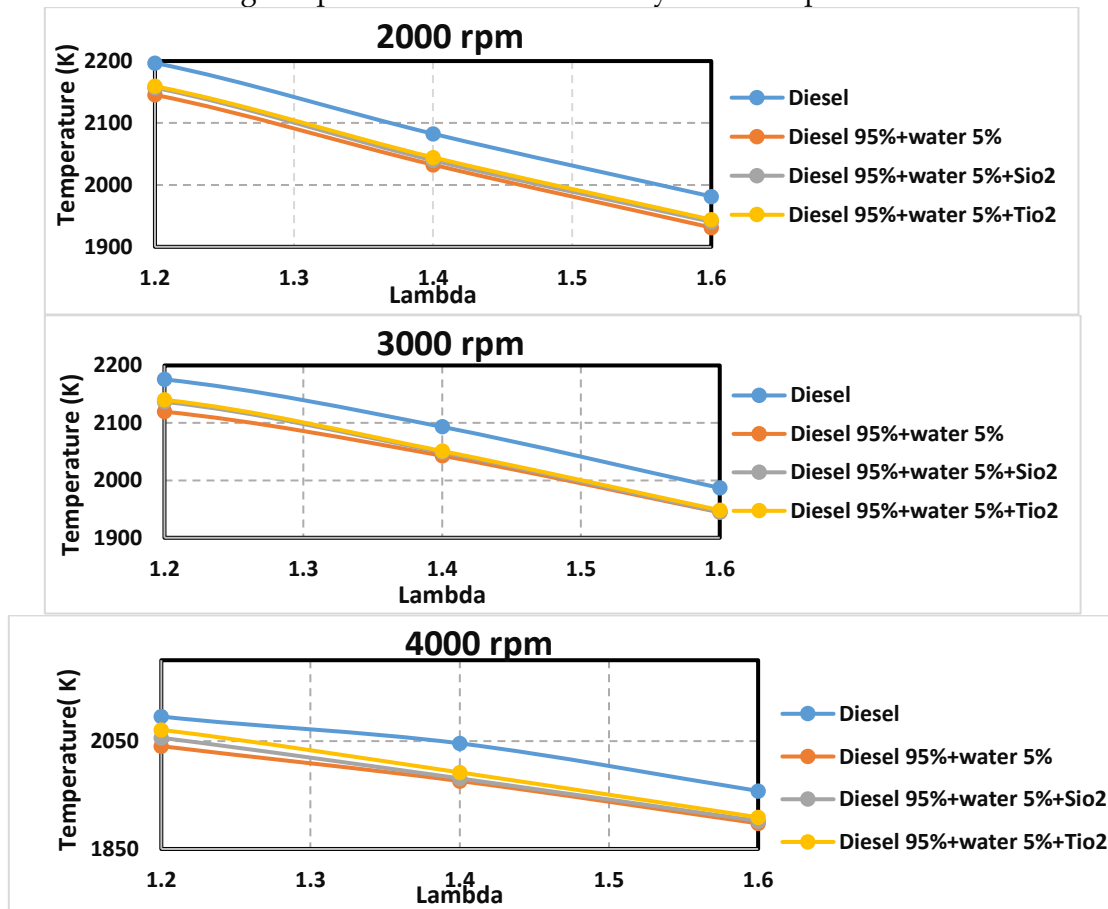
diesel had the greatest peak pressure among many additives to diesel fuel. Also, the peak pressure associated with diesel fuel declines when water is included because of its significant latent heat of vaporization, which cools the combustion process by absorbing thermal energy. Similar outcomes were reported by Watanabe(Watanabe et al., 2017). Moreover, when nanomaterials are introduced, the peak pressure level for water-emulsified diesel fuel rises. According to numerical results, the  $\text{TiO}_2$  nanomaterial exhibits a greater pressure value than the  $\text{SiO}_2$  nanomaterial when combined with water-emulsified diesel fuel. In diesel-water emulsions, integrating nanoparticles such as  $\text{TiO}_2$  and  $\text{SiO}_2$  improves combustion efficiency by serving as catalysts, decreasing ignition delay, and contributing to more thorough fuel oxidation, which raises the heat release rate (HRR) considerably. These nanoparticles enhance thermal conductivity and fuel atomization, improving heat transmission and raising combustion temperatures, 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, peak pressure increases by 0.5% over DW with the  $\text{DWSiO}_2$  mixture and by approximately 0.7% with the  $\text{DWTiO}_2$  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 a 1.6 lambda and 4000 engine speed. In comparison, the maximum cylinder pressure is 114.7 bar when diesel fuel is used at a 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

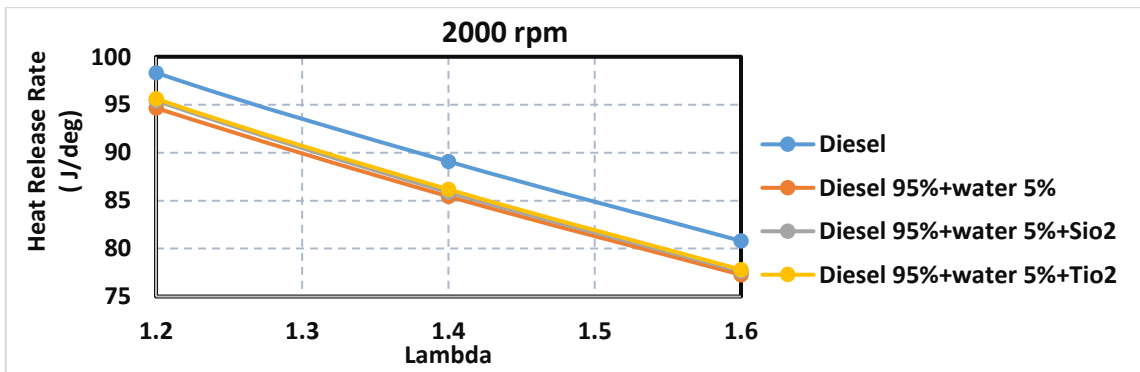
(Supplementary Figure A.2) depicts the linkage between the combustion chamber temperature and the angle of the crank across different lambda values and diesel fuel additives at various engine speeds. Figure 3 depicts the influence of various lambda values on the temperature inside the combustion chamber under different additives in diesel fuel at various engine speeds. Assuming the same fuel type and engine speed, Figures A.2 and 3 indicate that the highest temperature inside the internal combustion chamber goes down as the lambda ratio increases. Furthermore, adding water to diesel fuel lowers the greatest peak temperature because water has a cooling impact that reduces peak combustion temperatures by absorbing heat during combustion. Similar findings were mentioned by Watanabe (Watanabe et al., 2017). However, the greatest peak temperature rises when nanomaterials are introduced to water-emulsified diesel fuel. Furthermore, the  $\text{TiO}_2$  tiny particles exhibit a higher temperature ratio than the  $\text{SiO}_2$  tiny particles when combined with water-emulsified diesel fuel. Including nanoparticles like  $\text{TiO}_2$  and  $\text{SiO}_2$  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 contrasted with diesel, owing to the cooling impact of water, which lowers peak combustion temperatures. However, peak temperatures rise dramatically when  $\text{TiO}_2$  or  $\text{SiO}_2$  nanoparticles are included in the DW combination. More precisely, the DWSiO<sub>2</sub> mixture improves peak pressure by 0.42% above DW, but the DWTiO<sub>2</sub> mixture improves by around 0.59%. Figures A.2 and 3 illustrate that the maximum temperature value drops as 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 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.

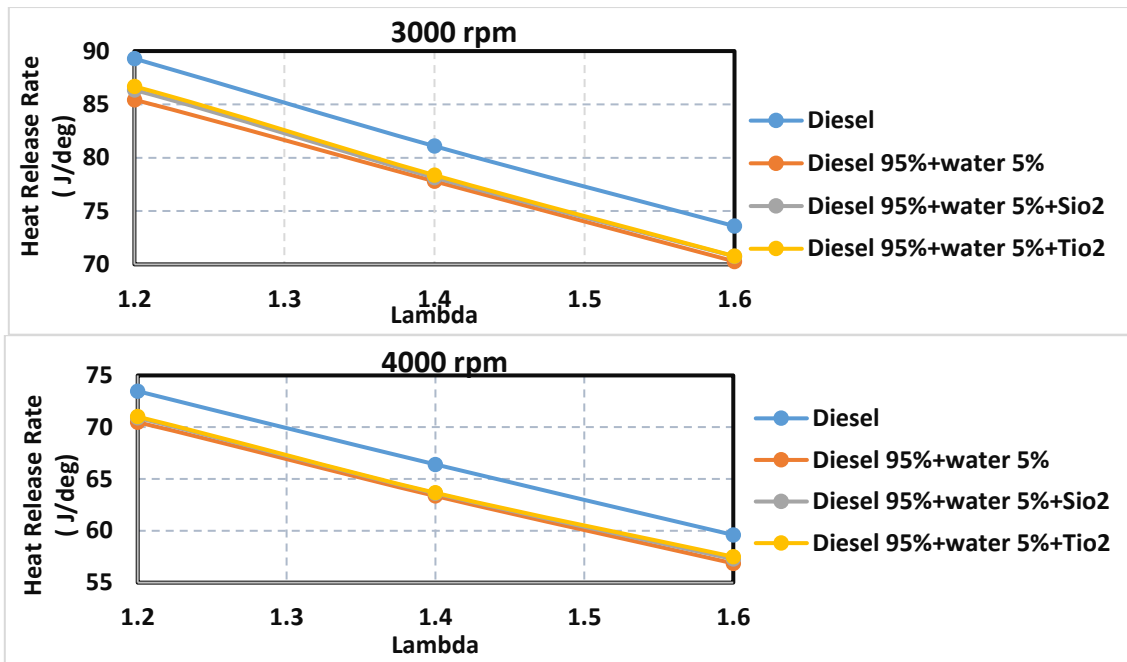


**Figure 3** The relationship between the temperature and the lambda values at different additions in diesel fuel and various engine speeds (2000 rpm, 3000 rpm, and 4000 rpm)

3.3. The heat release rate (HRR)

(Supplementary Figure A.3) illustrates the relationship between the crank angles and the heat release rate with various lambda values, engine speeds, and different additives in diesel fuel. Figure 4 shows the heat release rate analysis per lambda with multiple engine speeds and different additives for diesel fuel. As demonstrated in Figures 4 and A.3, utilizing the identical fuel type and maintaining a consistent engine speed, the value of 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. 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), there is more air than fuel in the combustion mixture, which reduces the amount of fuel available for combustion. As a result, less energy is released during the combustion process, which causes the HRR to decrease. As demonstrated in Figures 4 and A.3, under the same lambda and same engine speed, the findings reveal that diesel has the highest heat release rate compared with different additives in diesel fuel. Moreover, adding 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. Water addition to diesel fuel (DW) reduces HRR by 4.10% at 2000 rpm, 4.45-4.63% at 3000 rpm, and 4000 rpm. However, the peak heat release rate value is increased when nanomaterials are incorporated to water-emulsified diesel fuel. The presence of nanoparticles involving SiO<sub>2</sub> and TiO<sub>2</sub> 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 heat release rate (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 nanoparticles' enhancement of thermal conductivity and fuel atomization(Karisathan Sundararajan and Ammal, 2018). TiO<sub>2</sub> addition to water-emulsified diesel fuel (DWTiO<sub>2</sub>) improves HRR by 1.27% at 2000 rpm, 1.14% at 3000 rpm, and 0.84% at 4000 rpm. In addition, SiO<sub>2</sub> addition in water-emulsified diesel (DWSiO<sub>2</sub>) provides a 0.6- 0.91% improvement over water-emulsified diesel fuel DW but with a smaller effect than TiO<sub>2</sub>. As demonstrated 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 with an increase in the engine speed. The results reveal that the highest value of heat release was 98.34 J/deg obtained by diesel fuel at 1.2 lambda value and 2000 rpm engine speed. In comparison, the minimum value of heat release was 57.5 J/deg obtained by water-emulsified diesel fuel at a 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.





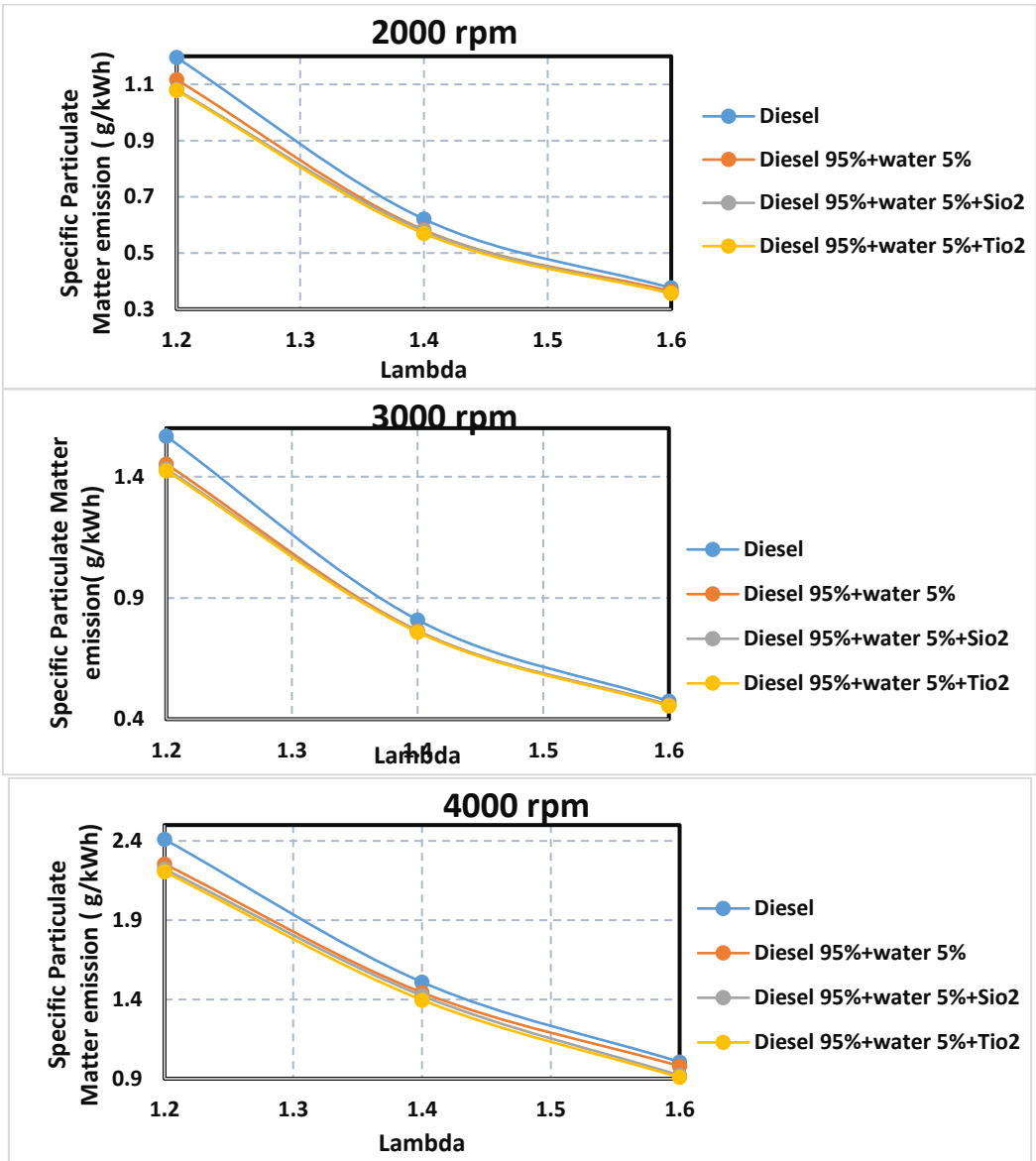
**Figure 4** The relationship between heat release rate and the lambda values at different additions in diesel fuel and various engine speeds.

### 3.4. Particulate matter emissions (PM)

Figure 5 likely illustrates the relationship between particulate matter (PM) emissions and lambda values at varying engine speeds and fuel additives. As demonstrated in Figure 5, under the same lambda and same fuel type, the predicted results showed that the PM emissions of all the fuels tested increase with an increase in engine speed. Moreover, as shown in Figure 5, under the same fuel type and same 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 same 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 the PM emissions. Similar results were mentioned by Watanabe et al (Watanabe et al., 2017). Water addition to diesel fuel (DW) decreases PM by 5.36% at 2000 rpm, 5.31- 4.48% at 3000 rpm, and 4000 rpm. On the other hand, adding nanomaterials ( $\text{TiO}_2$  and  $\text{SiO}_2$ ) to water-emulsified diesel fuel (DW) decreases PM emissions. In addition, the  $\text{TiO}_2$  nanomaterial has a low PM emissions value compared with the  $\text{SiO}_2$  nanomaterial when mixed with water-emulsified diesel fuel, highlighting its potential to reduce PM's environmental impact.  $\text{TiO}_2$  addition to water-emulsified diesel fuel (DWTIO<sub>2</sub>) reduces pm by 2.61 % at 2000 rpm and 1.28 - 4.47 % at 3000 rpm and 4000 rpm. In addition,  $\text{SiO}_2$  addition (DWSIO<sub>2</sub>) reduces pm by 1.9% at 2000 rpm, 0.61-3.07 % at 3000 rpm, and 4000 rpm. Several factors impact particulate matter emissions from diesel engines, such as fuel formulation, air-fuel proportion, mixing efficiency, pressure, and temperature. Although 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 surpasses available oxygen. Furthermore, inadequate fuel-air mixing, a typical problem in compression-ignition engines, contributes to soot generation, diminishing the advantages of high temperatures. On the other hand, mixtures of diesel with water or additives such as  $\text{SiO}_2$  and  $\text{TiO}_2$  exhibit markedly reduced PM emissions. Additionally, water enhances fuel-air mixing by dispersing the fuel spray into smaller droplets, resulting in a more uniform distribution of combustion. Adding nanoparticles such as  $\text{SiO}_2$  and  $\text{TiO}_2$  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 is 0.355 g/kWh obtained by DWTiO<sub>2</sub> fuel at a 1.6 lambda value and 2000 engine speed.

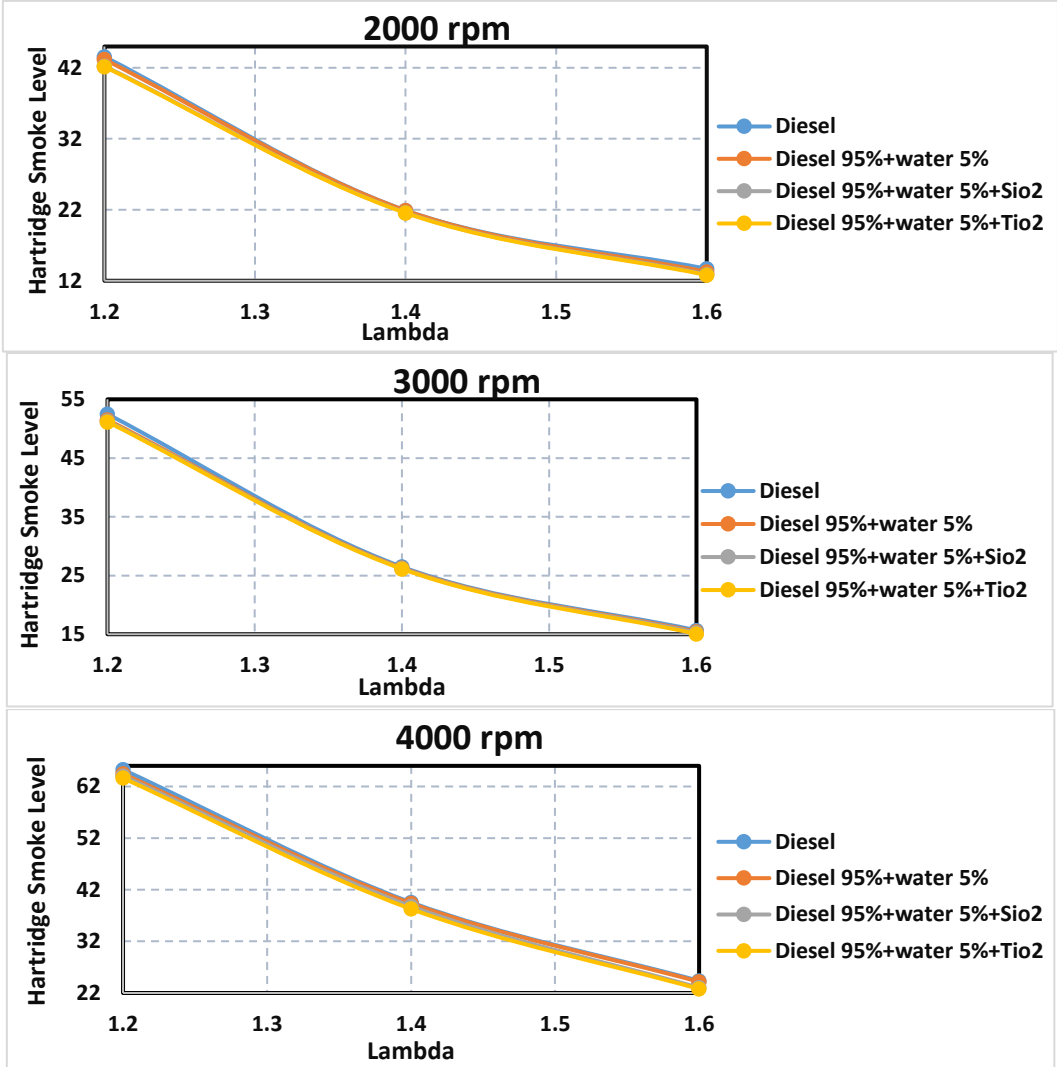


**Figure 5** The relationship between PM emissions and the lambda values at different additions in diesel fuel and various engine speeds

3.5. Hartridge smoke level:

Figure 6 presents the relation between the Hartridge smoke level and the lambda values for various engine speeds and different additives at diesel fuel. As exhibited in Figure 6, under the same fuel type and same engine speed, the smoke level emission decreases with an increase in lambda values. In addition, the smoke level emission concentration rises with an increase in engine speed at the same lambda and fuel type. As shown in Figure 6 under the same lambda and same engine speed, it was found that diesel has a high smoke level compared with different additives in diesel fuel. Moreover, adding water to diesel fuel decreases the smoke emission concentration rate. On the other hand, adding nanomaterials to water-emulsified diesel fuel decreases the smoke emission level. In addition, the TiO<sub>2</sub> nanomaterial gives low smoke level compared with sio<sub>2</sub> nanomaterial during mixing with water-emulsified diesel fuel. Similar results were mentioned by Khatri et al and Vigneswaran et al (Khatri and Goyal, 2021; Vigneswaran et al., 2021). Water addition to diesel fuel (DW) reduces smoke level by 1.36% at 2000 rpm, 1.38% at 3000 rpm, and 0.82% at 4000 rpm. TiO<sub>2</sub>

addition to water-emulsified diesel fuel (DWTIO<sub>2</sub>) reduces smoke level by 2.51% at 2000 rpm, 1.5-3.4% at 3000 rpm, and 4000 rpm. Moreover, SiO<sub>2</sub> addition (DWSIO<sub>2</sub>) reduces smoke level by a 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 obtained by diesel fuel at a 1.2 lambda and engine speed of 4000 rpm, while the minimum Hartridge smoke level is 12.8 obtained by DWTIO<sub>2</sub> fuel at a 1.6 lambda and engine speed of 2000rpm.



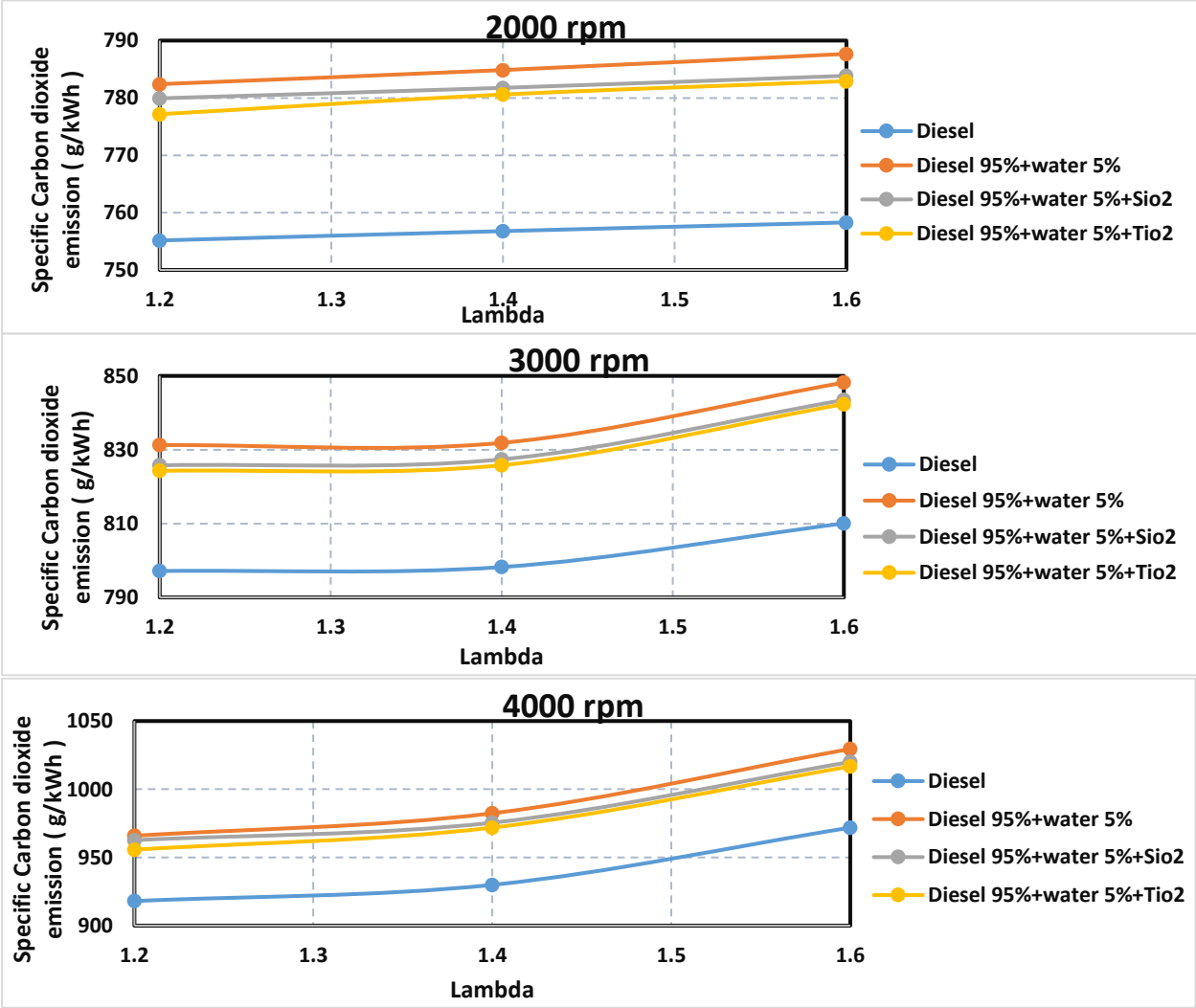
**Figure 6** The relationship between smoke level and the lambda values at different additions in diesel fuel and various engine speeds

3.6. Carbon dioxide (CO<sub>2</sub>)

Figure 7 illustrates the correlation between CO<sub>2</sub> and lambda levels across various engine speeds and distinct additives in diesel fuel. The combustion strategy within the combustion chamber, as well as the fuel's oxygen content, impacts CO<sub>2</sub> emissions. An increased CO<sub>2</sub> content indicates that the fuel has been virtually completely burned within the engine. Additionally, the temperature within the combustion chamber influences CO<sub>2</sub> emissions. A more efficient combustion process also leads to higher CO<sub>2</sub> emissions. As exhibited in Figure 7, under the same fuel type and same engine speed, the CO<sub>2</sub> emission increases with an increase in lambda values. In addition, the CO<sub>2</sub> emission concentration rises with an increase in engine speed at the same lambda and fuel type. As shown in Figure 7, under the same lambda and same engine speed, it was found that diesel has the minimum CO<sub>2</sub> emission concentration compared with different additives in diesel fuel. Moreover, adding water to diesel fuel rises the CO<sub>2</sub> emission concentration rate. On the other hand, adding



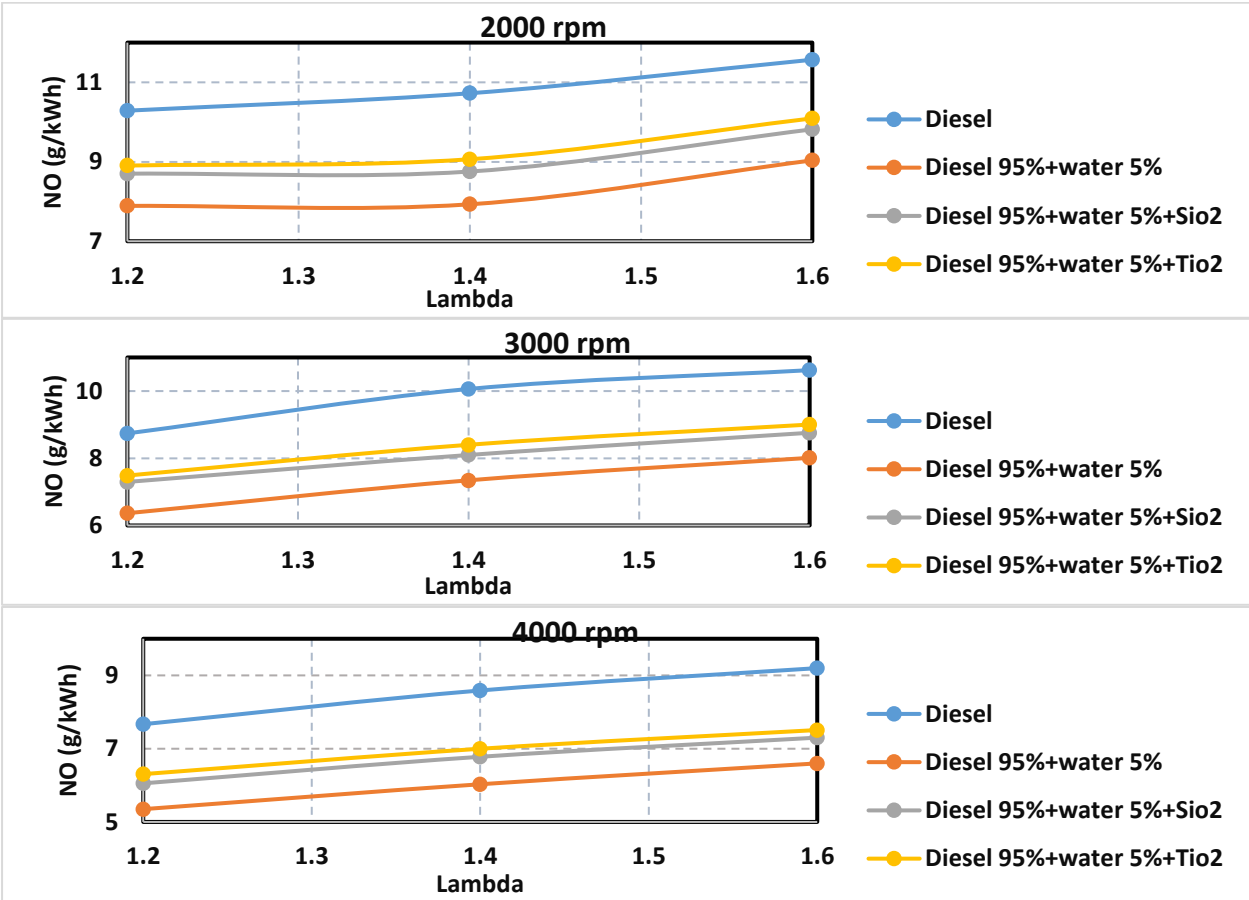
nanomaterials to water-emulsified diesel fuel decreases the CO<sub>2</sub> emission concentration rate. Hoseini et al and Abdollahi et al observed similar findings(Hoseini and Sobati, 2019; Abdollahi et al., 2020). This is because the water vapor in diesel fuel produces an OH radical during combustion, which facilitates the combination of oxygen and CO, thereby increasing the amount of CO<sub>2</sub> emissions. On the other hand, incorporating nanomaterials into water-emulsified diesel fuel lowers CO<sub>2</sub> 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 numerical results, the TiO<sub>2</sub> nanomaterial gives low the CO<sub>2</sub> emission concentration rate compared with SiO<sub>2</sub> nanomaterial during mixing with water-emulsified diesel fuel. Water addition to diesel fuel (DW) increases CO<sub>2</sub> by 3.73% at 2000 rpm, 4.39- 5.60% at 3000 rpm, and 4000 rpm. TiO<sub>2</sub> addition to water-emulsified diesel fuel (DWTIO<sub>2</sub>) reduces CO<sub>2</sub> by 0.61 % at 2000 rpm, 0.74-1.13 % at 3000 rpm, and 4000 rpm. In addition, SiO<sub>2</sub> addition (DWSIO<sub>2</sub>) reduces CO<sub>2</sub> by 0.4% at 2000 rpm and 0.57-0.66 % at 3000 rpm and 4000 rpm. The maximum CO<sub>2</sub> 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 CO<sub>2</sub> 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 CO<sub>2</sub> 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 lambda value. This is because the amount of nitric oxide generated depends on the maximum temperature inside the engine, residence duration, and content of oxygen. Consequently, nitric oxide contaminants in the engine gradually rise as the lambda level rises. As illustrated in Figure 8, diesel has the highest NO mass fraction value compared to other diesel fuel additives at similar lambda and engine speeds. Additionally, the NO mass fraction value is decreased when water is introduced to diesel fuel. However, the NO mass fraction percentage rises when nanomaterials are included in water-emulsified diesel fuel. Furthermore, when combined with water-emulsified diesel fuel, the  $\text{TiO}_2$  nanomaterial yields a higher NO mass fraction value than the  $\text{SiO}_2$  nanomaterial. Similar results were mentioned by Vigneswaran et al and Khatri et al (Vigneswaran et al., 2021; Khatri and Goyal, 2021) . Water addition to diesel fuel (DW) reduces NO emission by 23.75% at 2000 rpm, 26.25 - 29.44% at 3000 rpm, and 4000 rpm.  $\text{TiO}_2$  addition to water-emulsified diesel fuel (DWTiO<sub>2</sub>) increases NO emission by 11.46 % at 2000 rpm, 12.86 % at 3000 rpm and 13.71% at 4000 rpm. Moreover,  $\text{SiO}_2$  addition in water-emulsified diesel (DWSiO<sub>2</sub>) increases NO emission by 8.90% at 2000 rpm, 10.20% at 3000 rpm, and 10.77% at 4000 rpm, but with a smaller effect than  $\text{TiO}_2$ . As seen in Figure 8, the concentration of nitric oxide emissions decreases as 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 rpm, 3000rpm and 4000 rpm) on the combustion efficiency and emissions of diesel engines operating under diesel fuel with three different additive (water with 5% ratio, 5% water with 50 $\mu$ m TiO<sub>2</sub> and 5% water with 50 $\mu$ m SiO<sub>2</sub>). Diesel-RK software was used to model and simulate the combustion of fuel inside the engine. Numerical computations were performed on a DEUTZ F1L511 cooled by air, single-cylinder, and direct-injection diesel engine. Based on the numerical findings, with the same fuel types and engine speeds, when the lambda ratio is increased from 1.2 to 1.6, the maximum pressure, maximum temperature, heat release rate, particulate matter emissions, and smoke level inside the combustion chamber also decreased. In contrast, carbon dioxide as well as, nitric oxide also rose. Moreover, under the same lambda and same fuel type, nitric oxide emission concentration, the heat release rate, the maximum pressure, and the maximum temperature reduced with increased engine speed from 2000 rpm to 4000 rpm, while carbon dioxide emission, Hartridge smoke level, and particulate matter emissions increased. In addition, 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% at 2000 rpm, 1.38% at 3000 rpm and 0.82% at 4000 rpm. Particulate matter emissions decline by 5.36% at 2000 rpm, 5.31% and 4.48% at 3000 rpm and 4000 rpm. The heat release rate drops by 4.10% at 2000 rpm and by 4.45% to 4.63% at 3000 rpm and 4000 rpm. However, adding water to diesel (DW) increases carbon dioxide emissions, with a rise of 3.73% at 2000 rpm and 4.39% to 5.60% at higher speeds (3000 rpm 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, while particulate matter emissions, carbon dioxide, and smoke level emissions decrease. The mixture of 95% diesel fuel and 5% water with 50 $\mu$ m TiO<sub>2</sub> (DWTIO<sub>2</sub>) has a higher value of temperature, pressure, heat release rate, and nitric oxide emission than the DWSIO<sub>2</sub> mixture of 95% diesel fuel and 5% water with 50 $\mu$ m SiO<sub>2</sub>. Moreover, the DWTIO<sub>2</sub> mixture gives a low value of carbon dioxide emissions, particulate matter emissions, and concentration rate compared to the DWSIO<sub>2</sub> mixture.

#### 5. Future works

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

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