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ARTICLE

Improving the Combustion Process of Biofuels for Diesel Engines to Reduce Environmental Pollution

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ABSTRACT

Limiting environmental pollution from exhaust emissions from internal combustion engines includes many measures, including encouraging biofuel use because biofuel is environmentally friendly and renewable. A mixture of diesel fuel and vegetable oil is a form of biofuel. However, some properties of the mixed fuel, such as viscosity and density, are higher than those of traditional diesel fuel, affecting the injection and combustion process and reducing power and non-optimal toxic emissions, especially soot emissions. This study uses Kiva-3V software to simulate the combustion process of a diesel-vegetable oil mixture in the combustion chamber of a fishing vessel diesel engine with changes in fuel injection timing. The results show that when increasing the fuel injection timing of a diesel-vegetable oil mixture about 1–2 degrees of crankshaft rotation angle before the top dead center compared to diesel fuel injection timing, the engine power increases, and soot emissions decrease compared to no adjustment. The above simulation research results will help orient the experiments conveniently and reduce costs in the future experimental research process to quantify the fuel system adjustment of fishing vessels' diesel engines when using biofuels, including diesel-vegetable oil mixtures. Thus, the engine's economic indicators will improve, and emissions that pollute the environment will be limited.

Keywords: Diesel Engine; Injection Timing; Biofuel; Soot; Kiva-3V

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1. Introduction

The environment is polluted by various causes, resulting in numerous negative consequences that seriously affect socio-economic development and humanity, especially in developing countries. Therefore, environmental protection is a shared responsibility of every individual and every country worldwide. That is synonymous with protecting human healthcare [1]. This research introduces the causes of environmental pollution from the exhaust gas of internal combustion engines and the solutions implemented to limit pollution, specifically using biofuels for engines. It also introduces the application of diesel blends mixed with original vegetable oils as fuel for diesel engines. It includes adjusting the fuel injection system to optimize combustion and reduce emissions, especially soot emissions, using a simulation method.

The development of vehicles and industrial factories has consumed a lot of petroleum fuel, increasing toxic emissions from combustion; this has caused air pollution, which has seriously affected humans and ecosystems. Without timely and appropriate solutions, it can lead to an increasingly polluted, unsustainable, and difficult-to-remediate environment [1, 2].

Environmental reports from many countries have indicated that air pollution directly affects public health. In large cities, a significant proportion of the population suffers from diseases related to air pollution, with children being the most vulnerable group [2, 3]. A particular concern is PM 2.5 dust (soot), which consists of microscopic particles that are invisible to the naked eye. This pollutant is considered to have the most significant impact on health due to its ability to settle in the lungs, penetrate lung tissue, and even pass through the walls of blood vessels into the human circulatory system [2, 3].

Also, from the current environmental situation, one of the essential things that humanity must do to protect the environment is to reduce the destruction of ecosystems caused by pollution. Humans must protect the environment from pollution and other activities that lead to environmental degradation. Ecological degradation must be detrimental because it threatens the long-term health of animals, humans, and plants. Air and water pollution, global warming, smog, acid rain, etc., are just a few environmental problems humans face. Humans need to take responsibility for taking care of the environment to make the planet friendly for life; simple changes in daily life are all that is necessary to reduce the amount of toxic emissions into the environment, must make ecosystems sustainably connected to create a green environment, a green planet, serving the best interests of humans, to put health first. From the above reasons, it is evident that air pollution is not only one of the harmful factors affecting the environment, but it also affects the quality of food, leading to the ingestion of toxic substances, directly affecting biodiversity, thereby causing negative consequences to important characteristics in maintaining the life cycle of the ecosystem, leading to climate change, severely affecting human life [2, 3].

The negative impacts of environmental pollution show that engine emissions have a huge impact. When internal combustion engines are operating, including diesel engines, the fuel commonly used for internal combustion engines today is petroleum products with components including hydrocarbons (C_nH_m), additives, and impurities [4].

The combustion process in internal combustion engines is a fuel oxidation process that occurs according to very complex mechanisms and is affected by many factors. Among the fuel combustion products in internal combustion engines, many substances directly or indirectly harm human health and the environment at different levels. The essential toxic substances in the exhaust gas of internal combustion engines include carbon monoxide (CO), carbon dioxide (CO_2), hydrocarbons (HC), nitrogen oxides (NO_x), sulfur oxides (SO_x), lead compounds (Pb), soot, etc. The fuel combustion and emission formation process is shown in Equation (1) [4–6].

Carbon monoxide (CO) is a colorless gas formed by the incomplete oxidation of hydrocarbons without oxygen [6].

When entering the body, CO combines with iron in the blood to form a compound that prevents the absorption of oxygen by hemoglobin in the blood.

Carbon dioxide (CO_2) is a colorless, tasteless gas. CO_2 is one of the organic components of the Earth's atmosphere. In clean air, CO_2 accounts for about 0.03% of the volume, equivalent to 598 mg/m^3.

Hydrocarbons (HC) are present in exhaust gases due to incomplete combustion or other abnormal combustion phenomena. Aromatic hydrocarbons (C_nH_{2n-6}) are the hydrocarbon group that has the most substantial impact on human health.

Sulfur (S) is one of the most significant impurities in petroleum-based fuels, especially in heavy fuels used for low-speed diesel engines. During combustion, sulfur is oxidized to SO_2, a colorless gas that can enter the respiratory tract and reduce the body's resistance. Part of SO_2 is further oxidized to SO_3 under the catalytic action of iron oxide (Fe_2O_3) and some other substances in the fuel according to the (2, 3) reactions [6].

Nitrogen oxide (NO_x) is a product of nitrogen oxidation (N_2) at high temperatures above 1100°C. Nitrogen oxide exists mainly in NO and NO_2 (NO_x), of which NO accounts for the most significant proportion. NO is a colorless, odorless gas that quickly transforms into NO_2 under natural conditions and harms humans. The allowable content is [NO] = 9 mg/m^3, [NO_2] = 9 mg/m^3 [6, 7].

Particulate Matter (PM), commonly known as soot or carbon black, is a pollutant of particular concern in the exhaust of diesel engines. Soot exists mainly in particles with an average diameter of about 0.3 μm, so it quickly penetrates the lungs, causing damage to the respiratory system. Soot is also an agent that causes smog and dust in the air. The composition of soot can include carbon, lubricating oil, unburned or incompletely burned fuel, and solid particles such as sulfate, sulfur, calcium, phosphorus, etc [6, 7].

Soot formation begins with the agglomeration of particles with a size of 20 – 30 nm and containing about 105 – 106 C atoms (Precursor Radical particles). These precursor radical particles connect to form spherical crystalline nuclei with a super static structure to form soot particles and are usually composed of three main groups [6, 7]:

- Solid fraction (SOL): Carbon and ash particles (46%).
- Soluble organic fraction (SOF): Organic materials derived from lubricating oils and diesel (32%).
- Sulfate particulates (SO_4): Sulfuric acid and water (14%).

The composition of soot particles also depends on the fuel's properties, the fuel's sulfur content, the combustion process's characteristics, the engine's technical condition, the engine's type, and the engine's age. The soot component in the combustion products of fuels with high sulfur content is more significant than that of low sulfur content [7].

The soot content after the exhaust valve of the engine is the difference between the amount of soot formed and then oxidized. The amount of soot formed depends on the properties of the fuel and the formation of the combustible mixture, in which the fuel injection process of the engine to create the combustible mix has the most significant influence. If the fuel injection is too late, the soot formed is significant; due to the short combustion delay, the incomplete primary combustion process has entered the exhaust stroke [7, 8].

Thus, to organize the combustion process well to reduce pollution caused by substances such as NO_x, CO, HC, and soot right at the source (in the cylinder), it is necessary to have measures related to optimizing the structure of the details, detail clusters and systems that affect the combustion process, such as designing the piston crown and cylinder head to create a vortex effect, increasing the ability to mix fuel and air better, the combustion process takes place faster, this applies well to direct fuel injection diesel engines; using a turbocharger system, increasing the valve diameter, reducing losses on the intake line to increase intake efficiency; calculating and designing the optimal early opening time of the exhaust valve; using electronically controlled fuel injection systems, pilot injection, main injection and additional injection. Although these are very effective measures, they alone cannot help the engine meet increasingly stringent pollution reduction standards [7, 8].

Therefore, exhaust gas treatment is needed. These measures ensure that the content of toxic substances in exhaust gas before being discharged into the environment is less than the permissible limits prescribed in the regulations. There are many different technologies for exhaust gas treatment, such as 3-way catalytic exhaust gas treatment (neutralizing three essential components in exhaust gas: CO, HC, and NO_x), soot filter, oxidation exhaust gas treatment for diesel engines, accumulation NO_x treatment, etc. [7, 8].

In addition, a combination of auxiliary systems, such as closed-loop control systems (exhaust gas recirculation), intake air temperature assurance systems, and air injection systems (oxygen), can support reactions on the exhaust line, etc. Ensuring compatibility between the engine and fuel is also one of the essential solutions, such as improving fuel quality (fewer impurities and toxic additives), using biofuels and alternative fuels, using additives in fuel, etc. [7, 8].

Numerous policies have been suggested to support the development of new fuels to alternative traditional fuels for engines in many countries, including encouraging less polluting fuels and stringent emission standards. These factors require fuel production companies, engine manufacturers, and users to find solutions to help protect the environment and contribute to maintaining a green planet. In addition, using new energy will encourage the development of agriculture and forestry, create many sustainable ecosystems, and keep abundant raw materials to produce new energy, including biofuel for diesel engines [7, 8].

Based on the theoretical basis of the working cycle of diesel engines, in recent years, many new techniques have been developed to make the engine burn cleanly, but without increasing the cost too much, to ensure economic indicators are suitable for users. In response to the above requirements from reality, many engine manufacturers have applied advanced technology to engines, meeting strict market standards. Typically, the two main directions to provide solutions to improve the combustion process for engines include internal engine treatment (adjusting the intake process, adjusting the fuel injection process, adjusting the shape of the engine's combustion chamber) and external engine treatment (using catalyst filters and soot filters) [7, 8].

Optimization and the development of optimization theory in engineering, particularly in the diesel engine field, have brought practical results, ensuring that the engine meets environmental standards. However, optimization can also degrade other factors. Tuning a diesel engine to the optimum level must accept this conflict.

Improving the combustion process means improving the quality of fuel injection. Each diesel engine has an optimal injection timing for a fuel type (standard injection timing specified by the manufacturer). When changing the fuel properties, the injection system must be adjusted accordingly so that the fuel spray structure develops and vaporizes to form the best combustion mixture, reducing soot emissions and increasing power [8, 9].

Adjusting the injection system will affect the structure and penetration depth of the spray (s). In this case, if there is no specific adjustment range, there may be a phenomenon of the spray colliding with the wall cylinder, forming a liquid film. This fluid film harms the exhaust gas because it evaporates more slowly and cannot be wholly burned. The incomplete combustion causes the content of impurities to exist, in which the concentration of soot is significant, which is one factor that increases emissions [8, 9].

To reduce environmental pollution caused by exhaust fumes from internal combustion engines. Biofuels are particularly interesting among the new energy sources replacing petroleum fuels for engines because they are environmentally friendly, burn cleanly, and limit pollution. Emissions, including soot, will be reduced when diesel engines use biofuels (biodiesel, vegetable oil, etc.) because biofuels contain many oxygen components and low carbon and sulfur content.

However, biofuels used for diesel engines are diverse, as are measures to enhance the combustion process to reduce exhaust pollution. For example, using oxyhydrogen (HHO) with diesel and biodiesel can increase combustion efficiency and reduce HC and soot emissions. Still, it also increases CO_2 and NO_x emissions because the additional hydrogen and oxygen in HHO gas promote more complete combustion with higher combustion temperatures [10].

In addition to reducing emissions and meeting legal regulations, many studies have used Hybrid powertrains for internal combustion engines combined with compression ratios and variable fuel injection timing, reducing fuel consumption and emissions [11]. Some studies add a mixture of methane-hydrogen (hythane) and water in diesel emulsions when the engine uses dual fuel mode, significantly reducing NO_x emissions due to the evaporation of water particles in the combustion chamber, causing a lower combustion temperature. Therefore, using hythane as a secondary fuel has reduced emissions, but without decreasing the engine's thermal efficiency. The experimental results show that the water concentration in diesel emulsions can reach 5–15%, and the remainder is diesel fuel [12].

Similar to the above studies, according to Ajith Damodaran et al. [13], diesel engines using biofuels with different properties and at each operating mode will have different levels of emission reduction. For example, when using Margosa biodiesel (M100) as fuel for the engine at low load mode, it can only reduce soot emissions by 15% compared to diesel fuel.

Zhenhua Ji et al. [14]. Using a diesel-methyl heptanoate blend with a 20% methyl heptanoate (MH20) ratio as fuel for a diesel engine, the results showed that the spray cone angle was reduced, and the ignition delay was short. However, the soot emission of MH20 was reduced to 4% compared to diesel fuel when injected at low pressure.

S. Sinha et al. [15]. Studied the combustion characteristics of a non-turbocharged diesel engine with diesel and biodiesel fuel derived from rice bran at 10%, 20%, and 100%

biodiesel (B100); the experiment was conducted at 50% load at 1,400 rpm. The results showed that the maximum pressure was low when the mixing ratio increased. In this case, the ignition time of DO was the latest, and the earliest was B100.

Mukesh Kumar and Onkar Singh [16]. Studied the effect of biodiesel fuel on the characteristics of direct fuel injection diesel engines; when blending biodiesel derived from Karanja oil (Indian oak oil) at a ratio of 10 – 50% (K10 – K50), at the ratio of K50, the thermal efficiency decreased sharply, soot increased with the blending ratio. NO_x emissions decreased when the engine operated at a moderate load.

K Winangun et al. [17]. Applied palm oil-derived biodiesel to a single-cylinder direct injection diesel engine, adding hydrogen to the biodiesel fuel. The results showed that the advantage of hydrogen addition was reduced soot emissions, but increased NO emissions. However, the engine performance improved, and other exhaust pollutants were reduced.

SM Javad Yahyaei et al. [18]. Research biodiesel with added hydrogen gas as a fuel for diesel engines using the simulation method on the Converge software. The results showed that adding 12% hydrogen resulted in a 40% reduction in HC and soot emissions. In addition, the ignition delay decreased from 15.20 to 9.40 degrees crank angle rotation (CA) when hydrogen content was added.

M.S. Gad, Ahmed et al. [19]. Using biodiesel (B20) at a ratio of 20% biodiesel combined with nano additives as a fuel mixture for diesel engines. The results showed that the HC content was reduced by up to 36%. The engine operated stably.

Elkelawy, M et al. [20]. Study on prediction and optimization of performance and emissions of a single-cylinder diesel engine using biodiesel derived from waste cooking oil (WCO). The results showed that emissions were reduced at B20 (20% biodiesel), and the performance was improved compared to conventional diesel fuel through optimization of chemical reactions.

As analyzed above, biofuel can be biodiesel or vegetable oil. This study presents a solution to improve the combustion process of diesel mixed with vegetable oil, reducing the amount of toxic gases emitted into the environment and increasing the engine's power and specific fuel consumption rate (SFC).

In Southeast Asian countries, coconut oil is highly productive, abundant, and renewable, and can be used as fuel for diesel engines [21, 22]. However, its high viscosity and density affect the formation of the combustible mixture, making the combustion process of lower quality than that of traditional DO fuel. Therefore, it is necessary to conduct simulation studies to evaluate the engine characteristics when using coconut oil before conducting experiments [23].

Previous studies have shown that when the engine uses vegetable oil, it is necessary to adjust the fuel injection system to improve power and reduce emissions for the engine. Simulation methods using specialized software are highly recommended in current studies on alternative energy for engines and engine improvements. Simulation studies with proven mathematical models will help to initially evaluate the research results, thereby making comments to facilitate experimental orientation. At the same time, allowing easy modification of input conditions and imposing diverse boundary conditions, each sub-process can be studied separately in fuel injection, combustion, and emission formation when studying alternative energy and fuels. In addition, simulation studies will extract relevant information in detail at all stages of the simulation process at different times [23–25].

Among the above scientific works, the works mainly focus on the use of vegetable biodiesel combined with additives as fuel for diesel engines; very few works mention the combustion and emission characteristics of diesel engines when using diesel fuel mixed with pure vegetable oil (not synthesized into biodiesel) and without adding additives. Therefore, the objective of this study is to apply diesel fuel mixed with coconut oil as fuel for diesel engines of fishing vessels, combined with adjusting the injection timing to optimize the combustion process, reduce soot emissions by simulation method on Kiva-3V software, contributing to reducing toxic emissions and encouraging the use of vegetable oil (coconut oil) to produce biofuel.

On that basis, the simulation study results will determine the appropriate injection timing of diesel-vegetable oil blends to reduce emissions, especially soot, while increasing engine power, thereby reducing specific fuel consumption. Simulation studies before experimental studies will help reduce time and cost during experimental studies.

2. Materials and Methods

2.1. Materials

Diesel fuel (DO) and a diesel-coconut oil blend (B15: 15% coconut oil and 85% diesel).

The fuel specifications were tested at QUATEST 3, Vietnam (**Tables 1** and **2**).

Table 1. Chemical Composition of Coconut Oil and Diesel Oil.

Chemical Composition	Coconut Oil	Diesel Oil
Carbon (%)	72.00	86.60
Hydrogen (%)	12.00	13.40
Oxygen (%)	16.00	0.00
C/H ratio (-)	6.00	6.46

Table 2. Properties of B15 Fuel and DO.

Fuel	Viscosity (mm^2 s^{-1})	Cetane Number (CN)	Density (g cm^{-3})	Flashpoint (°C)	Calorific Value (kcal kg^{-1})
DO	3.25 at 40°C	50	0.8360	Min 60	10,478
B15	3.65 at 80°C	52	0.8420	75	10,650

This study uses a Yanmar 4CHE diesel engine, which is also the main engine for fishing vessels. The engine specifications are presented in **Table 3**.

Table 3. Yanmar 4CHE Diesel Engine Specifications.

Parameters	Value
Chamber type/Number of cylinders (-)	Unified/4
Cylinder diameter ×piston stroke (mm)	105 ×125
Power (Hp/rpm)	70/2,300
Compression ratio (-)	16.4
Number of nozzle holes ×diameter ×spray direction (deg)	4 ×0.32 ×140
Injection timing (°BTDC)	18
Injection pressure (kg cm^{-2})	210
Rod length (mm)	215
IVO (°BTDC)	16
IVC (°ABDC)	52
EVO (°BBDC)	52
EVC (°ATDC)	16

2.2. Simulation Research

The basis of the simulation is based on chemical equations describing the combustion process, emission formation, and computational models of the engine combustion and emission processes combined with energy conservation equations.

The balanced equation completely oxidizes a generic fuel molecule $C_xH_yS_z$ into carbon dioxide CO_2, water H_2O, and sulfur dioxide SO_2 as follows [26].

$$C_xH_yS_z + [(y/2) + z]O_2 \rightarrow xCO_2 + \frac{y}{2}H_2O + zSO_2 + Q_{ex} \quad (1)$$

$$S + O_2 \rightarrow SO_2 \quad (2)$$

$$2SO_2 + O_2 \rightarrow 2SO_3 \quad (3)$$

Where the heat Q_{ex} released during combustion corresponds to the fuel-specific calorific value.

In this study, NO_x and soot are the two emission components of interest.

NO_x is formed during fuel combustion in the presence of nitrogen (N_2). According to the main chemical reactions that produce NO, NO_x formation is mainly due to the oxidation of N_2 [26].

$$O + N_2 \Leftrightarrow NO + N \quad (4)$$

$$N + O_2 \Leftrightarrow NO + O \quad (5)$$

$$N + OH \Leftrightarrow NO + H \quad (6)$$

$$NO + O_2 \Leftrightarrow 2NO \quad (7)$$

Soot is formed by the developing PR (Precursor radical particles). However, the amount of soot formed is partially oxidized at high temperatures. The equation describing the formation and oxidation of soot is (8), (9) [26].

$$PR \rightarrow C_{soot} \quad (8)$$

$$C_{soot} + O_2 \rightarrow C_{soot-2} + 2CO \quad (9)$$

Application Kiva-3V software. That is specialized computational fluid dynamics software for calculating and simulating internal combustion engines. The basis of simulation calculation is the following equations [27, 28]:

Mass conservation equation:

$$\frac{\partial \rho_m}{\partial t} + \frac{\partial(\rho_m u_i)}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\rho D \frac{\partial(\rho_m/\rho)}{\partial x_i}\right) + \dot{\rho}_m^s + \dot{\rho}_m^c \quad (10)$$

Momentum conservation equation:

$$\frac{\partial(\rho u_j)}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i u_j - \tau_{ij}) = -\frac{1}{\alpha^2}\frac{\partial p}{\partial x_j} + \rho F_j^s + \rho g_j - A_0 \frac{2}{3}\frac{\partial(\rho k)}{\partial x_i}, \text{ with } j = 1, 2, 3 \quad (11)$$

Conservation of energy equation:

$$\rho c_p\left(\frac{\partial T}{\partial t}+\frac{\partial T}{\partial x_i}\right)=k\frac{\partial^2 T}{\partial x_i^2}+\frac{\partial}{\partial x_i}\left(\rho D\sum_m h_m\frac{\partial(\rho_m/\rho)}{\partial x_i}\right)+A_0\rho\epsilon+\dot{Q}^s+\dot{Q}^c \quad (12)$$

In the above equations, $\rho=\sum_m \rho_m$: the total density of the component masses entering the observation space due to the displacement of the fluid flow (g/cm^3); $\dot{\rho}^s=\sum_m \dot{\rho}_m^s$: condition of total source mass when spraying (g); $\sum_m \dot{\rho}_m^c=0$: constraint conditions on mass sources due to fire (g); t: time (s); x_i: coordinates (m); p: pressure (N/m^2); ρ_m: density of substance m (g/cm^3); u_i, u_j: velocity of fluid element (m/s); T: temperature (K); t_{ij}: components of stress tensor (N/m^2); h: static enthalpy (J/kg); A_0 and $1/\alpha^2$: parameters to improve computational efficiency for flows with small Mach numbers.

To calculate the simulation of the combustion process. The Kiva-3V software uses Kong S. Z et al.'s Shell combustion model[29]. The Shell combustion model is as follows:

$$RH+O_2\xrightarrow{k_q}2R^* \quad (13)$$

$$R^*\xrightarrow{k_p}R^*+P+Heat \quad (14)$$

$$R^*\xrightarrow{f_1k_p}R^*+B \quad (15)$$

$$R^*\xrightarrow{f_4k_p}R^*+Q \quad (16)$$

$$R^*+Q\xrightarrow{f_2k_p}R^*+B \quad (17)$$

$$B\xrightarrow{k_p}2R^* \quad (18)$$

$$R^*\xrightarrow{f_3k_p}\text{Termination} \quad (19)$$

$$R^*\xrightarrow{k_t}\text{Termination} \quad (20)$$

Where R^*: general base Hydrocarbon; Q: unstable intermediate substances; B: branching substance; P: combustion products (CO, CO_2, H_2O). Rate of formation of substances:

$$\frac{d[R^*]}{dt}=2k_q[RH][O_2]+2k_b[B]-f_3k_p[R^*]-k_t[R^*]^2 \quad (21)$$

$$\frac{d[B]}{dt}=f_1k_p[R^*]+f_2k_p[R^*][Q]-k_p[B] \quad (22)$$

$$\frac{d[Q]}{dt}=f_4k_p[R^*]-f_2k_p[R^*][Q] \quad (23)$$

$$\frac{d[O_2]}{dt}=-pk_p[R^*] \quad (24)$$

$$\frac{d[RH]}{dt}=\frac{[O_2]-[O_2]_{t=0}}{p.m}+[RH]_{(t=0)} \quad (25)$$

Where $p=(n(2-\gamma)+m)/2m$, n and m are the fuel's Carbon and Hydrogen indices, $\gamma=0.67$ is the CO/CO_2 ratio in the model.

The equation determines the coefficients of the rate of formation of substances and model coefficients in the Shell model:

$$f_1=A_{f_1}\exp(-E_{f_1}/RT)[O_2]^{x1}[RH]^{y1} \quad (26)$$

$$f_2=A_{f_2}\exp(-E_{f_2}/RT) \quad (27)$$

$$f_3=A_{f_3}\exp(-E_{f_3}/RT)[O_2]^{x3}[RH]^{y3} \quad (28)$$

$$f_4=A_{f_4}\exp(-E_{f_4}/RT)[O_2]^{x4}[RH]^{y4} \quad (29)$$

$$k_i=A_i\exp(-E_i/RT)\text{, with i = 1,2,3,q,b,t} \quad (30)$$

$$k_p=[1/k_1[O_2]+1/k_2+1/k_3[RH]]^{-1} \quad (31)$$

The turbulence model used is the RNG k-ε model of Han et al.[30]. The calculation model for soot formation and soot oxidation is simulated following the 8-step model of Kazakov et al.[31]. The NO_x formation model is calculated using the Y. B. Zel'Dovic mechanism[32].

The spray simulation model is estimated using equations (35) and (36)[33]:

Basic and semi-experimental experiments on the relationship of spray parameters to jet parameters, such as cone angle, breakup length, spray penetration depth, and average fuel particle diameter, are often performed with quasi-steady spray and are considered one of the conditions to evaluate the conical spray structure of diesel engines. Thus, they serve as a basis for adjusting the injection system[33].

The development time of the penetration depth s of the spray jet includes stage 1 at the nozzle tip (t = 0, injector opening), and stage 2 is the final stage and is calculated at the time when the liquid coming out of the nozzle starts to break up, creating a spray cone angle. The spray jet was formed and developed in the combustion chamber. During this time, the growth of s is linear with t. The time from the start of injection to the stage of breaking up the spray beam is the breakup time (t_b). The breakup time depends on the injection pressure, fuel density, nozzle diameter, and flow expansion coefficient[33].

According to Hiroyasu and Arai, M[33]:

$$t_b = 15.8C_d^{-1}\left(2\rho_g \cdot \Delta p\right)^{-1/2} \cdot \left(\rho_1 \cdot d_h\right) \quad (32)$$

In which the nozzle flow expansion coefficient:

$$C_d = \dot{m}_{inj} \cdot A_h^{-1} \cdot \left(2\rho_1 \cdot \Delta p\right)^{-1/2} \quad (33)$$

Fuel flow injection rate:

$$\dot{m}_{inj} = A_h \cdot v_1 \cdot \rho_1 \quad (34)$$

Before the breakup $0 < t < t_b$:

$$s = 0.39\left(2\Delta p/\rho_1\right)^{1/2} \cdot t \quad (35)$$

After the breakup $\geq t_b$:

$$s = 2.95\left(\Delta p/\rho_g\right)^{0.25}\left(d_h \cdot t\right)^{0.5} \quad (36)$$

Some other empirical formulas are also proposed. In which the penetration depth of the spray and the spray parameters are expressed through formula (13)[34]:

$$s(\varphi) = \left(\left(|\varphi - \varphi_{inj}| \cdot d_h \cdot v_1\right)/\left(2^{1/2}a_u \cdot 6n\right)\right)^{1/2} \quad (37)$$

In the above formulas, n: engine speed (rpm); φ: crankshaft rotation angle (deg); φ_{inj}: crankshaft rotation angle reflecting fuel injection timing (deg); a_u: vortex coefficient in the injection jet (-), a_u depends on the pressure in the cylinder at the time of fuel injection; A_h: cross-sectional area of the injection hole (mm^2); d_h: injection hole diameter (mm); ρ_l: fuel density (g/cm^3); ρ_g: air density (g/cm^3); v_l: fuel injection velocity (m/s); $\Delta p = (p_{inj} - p_c)$, p_{inj}: fuel injection pressure; p_c: the pressure of the end of compression stroke (bar).

Formulas (35), (36), and (37) show that changing the fuel injection timing changes the gas pressure in the engine combustion chamber, leading to a change in the penetration depths of the spray and affecting the formation of the combustible mixture.

Combustion simulation mesh model:

The combustion chamber mesh model of the 4CHE Yanmar diesel engine was established based on its size. Because the nozzle has four jet holes and is symmetrical, the simulation mesh model is performed in the space of ¼ of the combustion chamber (corresponding to 90-degree angles) to reduce the number and calculation time, as shown in **Figure 1**.

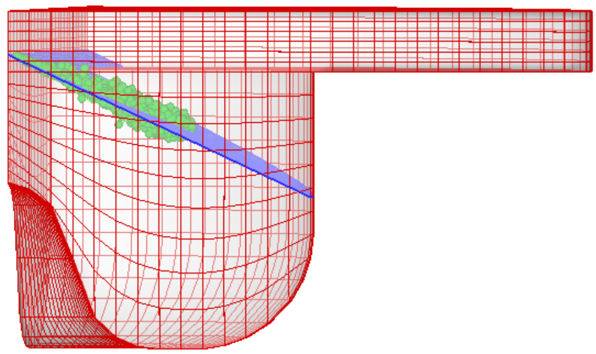

Figure 1. Combustion Chamber Mesh Model of 4CHE Yanmar Diesel Engine.

The parameters used in the simulation include **Tables 1, 2, 3,** and **4**.

Table 4. Simulation Mode.

Parameters	Unit	Values
The engine load	%	80
The engine speed	rpm	1,800
Injection pressures	Kg cm^{-2}	210
Injection timing	°BTDC	18; 19; 20; 21; 22; 23

3. Results and Discussion

The graph in **Figure 2** shows the simulation results of combustion temperature in the combustion chamber of the 4CHE Yanmar diesel engine using B15 mixture compared to DO fuel. Injection timing decreases (18 °BTDC), reducing combustion temperature. When the injection timing increases (from 19 to 23 °BTDC), the injection time is earlier, causing the combustion delay to be longer and the combustion temperature to increase. The highest B15 fuel combustion temperature is at an injection timing of 23 °BTDC.

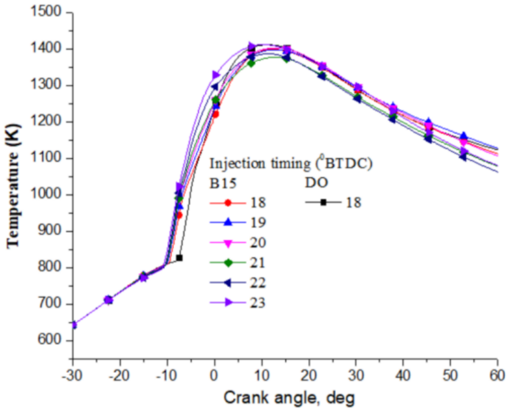

Figure 2. Combustion Temperature of B15 and DO Fuel.

Figure 3 shows the combustion pressure of B15 fuel compared to DO fuel. When the combustion delay increases, the combustion occurs intensely, causing the combustion pressure to grow. However, fuel injection is too early, and the main combustion phase occurs before the top dead center when the combustion chamber volume is still sizeable (from 22 to 23 °BTDC), affecting the engine power.

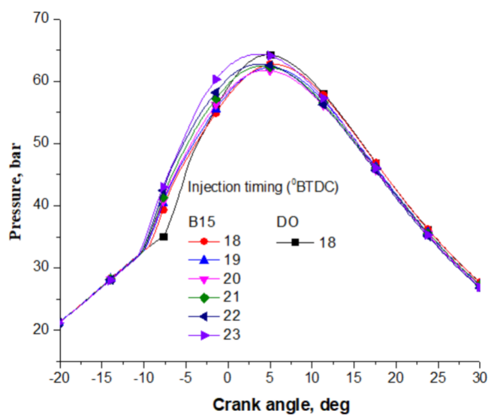

Figure 3. Combustion Pressure of B15 and DO Fuel.

The probability of particle collisions in a dense spray is very high. These collisions result in changes in particle velocity and size. Small particles thus disintegrate into smaller particles, which can also combine to form larger particles called coalescing particles.

In the thin mixture far from the nozzle, the main factors affecting fuel decomposition and evaporation are the conditions of the combustion chamber, such as temperature, pressure, density, and gas flow (turbulence, swirl), in which the fuel injection timing is a factor that directly affects the above conditions and affects the spray structure and the formation of the combustible mixture.

When the fuel spray structure (spray penetration) develops evenly in the combustion chamber space, it forms a better combustion mixture, increasing combustion temperature and pressure. The analysis results in **Figures 2** and **3** are consistent with the simulation image of the B15 fuel spray penetration when increasing the injection timing from 18 to 20 °BTDC compared to DO fuel in **Figure 4**.

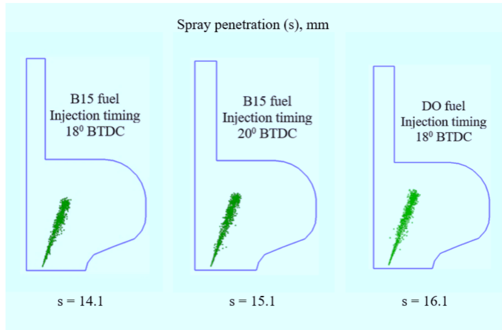

Figure 4. Comparison of B15 and DO Fuel Spray Penetration After Injection (3 deg Crank Angle).

Figure 5 shows the evolution of NO_x emissions according to injection timing. When the injection timing is early (injection timing away from the top dead center of the piston), the fuel jet enters the combustion chamber early, which increases the combustion delay time, leading to the combustion process being intense, and the combustion temperature increases. In addition, B15 fuel has a large amount of oxygen, so when combustion at high temperatures, the amount of NO_x will increase. Because NO_x is a combination of oxygen and nitrogen at high temperatures. In general, NO_x emissions increase when the injection timing is early. The highest NO_x emission is at injection timing 22–23 °BTDC.

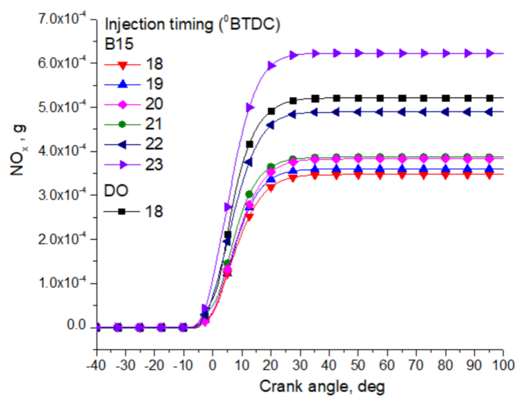

Figure 5. NO_x Emissions of B15 and DO Fuel.

Figure 6 shows the soot emissions according to the injection timing of B15 fuel. Increasing the injection timing increases the combustion temperature, which makes the oxidation process occur better, causing the amount of soot emitted to decrease, resulting in a decrease in soot after the exhaust valve. However, when the injection timing is increased too early (the fuel jet enters the combustion chamber too early), the air vortex in the combustion chamber is low, affecting the formation of an uneven combustion mixture, leading to a large amount of soot formation, because the amount of soot emitted after the exhaust valve is the difference between the amount of soot formed and oxidized. The highest soot emission is at injection timing 22–23 °BTDC.

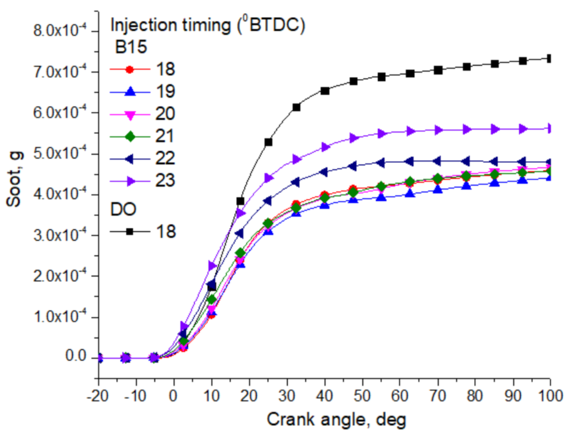

Figure 6. Soot Emissions of B15 and DO Fuel.

Figures 7 and **8** show the engine's power and fuel consumption values when using B15 fuel compared to traditional DO fuel. The results show that when the injection timing is increased from 18 to 19 and 20 °BTDC, the power increases, which is consistent with the increase in combustion pressure (**Figure 3**). However, increasing the injection timing too early causes the combustion process to occur early (21–23 °BTDC), which causes mechanical work loss and reduces engine power. The specific fuel consumption (SFC) will increase when the power decreases, as shown in **Figure 8**.

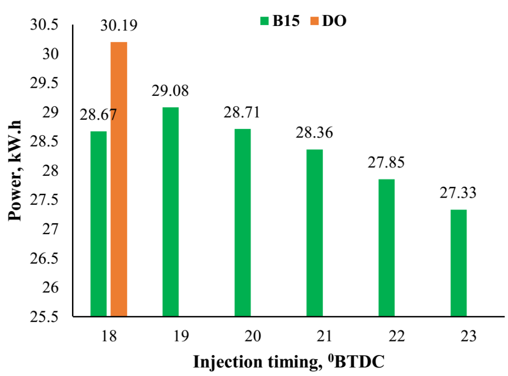

Figure 7. Simulation of Engine Power when Changing Fuel Injection Timing.

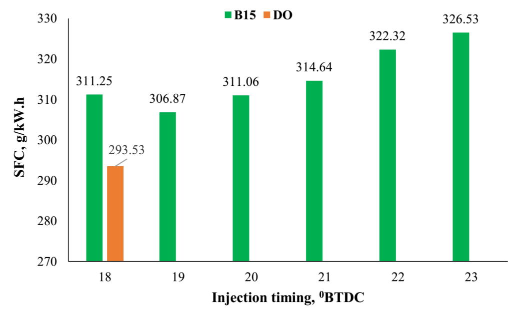

Figure 8. Simulation of the Engine's Specific Fuel Consumption When Changing the Fuel Injection Timing.

Figure 9 shows the maximum soot emission values of B15 fuel according to injection timing compared to DO fuel. Demonstrates that late injection timing (18 °BTDC) and too early injection timing (21 to 23 °BTDC) cause increased emissions.

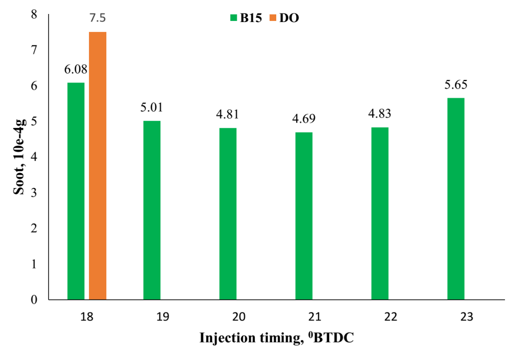

Figure 9. Simulation of Maximum Engine Soot Emissions When Changing the Fuel Injection Timing.

In particular, spray-wall interaction may occur when the injection timing is increased too early (early injection). At that time, the spray-wall interaction develops and forms a thin film, significantly affecting combustion efficiency, leading to changes in economic indicators and negatively impacting engine pollutants. This factor shows that soot increases when the injection timing is increased at 21–23 °BTDC.

The results in **Figure 10** show that NO_x emissions increase with increasing injection timing (early injection) because the NO formation reaction has a much slower rate than the hydrocarbon combustion reaction. The rate of N_2 oxidation reaction and the amount of NO formed highly depend on temperature. The NO concentration also relies heavily on the oxygen concentration, participating in the response. When the injection timing increased, the combustion delay time increased, leading to a rise in the combustion temperature, combined with the high oxygen concentration of B15 fuel, leading to an increase in the NO concentration in the combustion products.

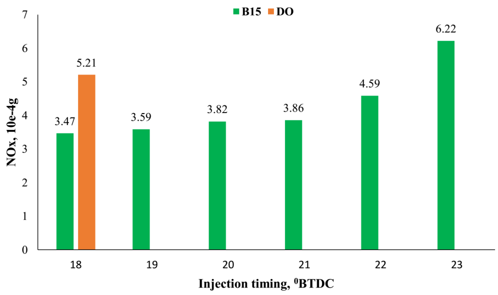

Figure 10. Simulation of Maximum Engine NO_x Emissions When Changing the Fuel Injection Timing.

4. Conclusions

Research on using diesel-coconut oil blends as fuel for fishing vessel diesel engines is one solution to reducing toxic emissions from diesel engines. In addition, coconut oil does not need to be synthesized into biodiesel, and the process of blending diesel with coconut oil does not require additives. This is a great advantage and necessary to encourage the use of vegetable oils to produce biofuels.

A study has applied CFD software Kiva-3V to simulate the combustion process of diesel fuel mixed with vegetable oil (B15) with changes in injection timing. Research has evaluated the spray characteristics and the formation of the combustion mixture, and the power, specific fuel consumption, and soot and NO_x emissions of B15 fuel are determined. In particular, increasing the B15 fuel injection timing by about 1–2 degrees of crankshaft rotation angle before the top dead center (19–20 °BTDC) compared to DO fuel injection timing (18 °BTDC), the power of the 4CHE Yanmar diesel engine increases, fuel consumption decreases, and soot emissions decrease more than when not adjusted. The results of simulation research before experimental research will help reduce time and cost in the experimental study and contribute to expanding research on biofuels of different origins before applying biofuels as fuel for diesel engines to reduce environmental pollution.

Author Contributions

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The authors agree to share their research data upon request.

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Conflicts of Interest

The authors declare no conflict of interest.

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