STUDY ON THE EFFECT OF BIOFUEL PROPERTIES ON SOOT EMISSIONS OF HIGH-SPEED DIESEL ENGINES USING THE SIMULATION METHOD

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Abstract - Biofuels have more oxygen and less sulfur and carbon content than traditional diesel fuel, so soot emissions will be reduced when used for engines. Biofuels can be original vegetable oils, vegetable oils, or animal fats converted into biodiesel. Biofuels are environmentally friendly and renewable, so they are encouraged to be utilized. This study used a mixture of diesel-coconut oil and biodiesel B10 produced from animal fats as fuel for high-speed diesel engines. The simulation results using Kiva-3V software for the Yanmar 4-cylinder diesel engine show that the mixture of diesel-coconut oil (C10) at the ratio of 10% coconut oil and 90% diesel oil gives soot emissions (1.72x10-4g) close to biodiesel B10 fuel (10% biodiesel B100) at 1.63x10-4g and both lower than diesel fuel (2.08x10-4g). The research findings provide a foundation for correctly adjusting the diesel engine's fuel injection system when utilizing biofuel.

Key words - Diesel engine; biodiesel; coconut oil; soot; Kiva-3V

1. Introduction

In the trend of industrial development, the demand for fuel and petroleum products for internal combustion engines has increased significantly, leading to many problems that need to be solved. For example, fuel is increasingly depleted, and environmental pollution due to engine emissions is increasing, leading to many negative consequences affecting human health and social development. Many measures and technological solutions have been proposed and applied worldwide to enhance energy security and mitigate environmental impacts [1].

Biofuels derived from vegetable oils and animal fats have great potential as an alternative to traditional fuels. In addition to their function as an additive to enhance oxygen in combustion, biofuels are also a renewable fuel source. A favorable characteristic of biofuels is that they are easy to blend with traditional fuels without the need for complex equipment. Biofuels can be pure vegetable oils or vegetable oils and animal fats, produced into biodiesel [2].

Vegetable oils mainly concentrate on plants with a relatively high oil content, such as soybean oil, rapeseed oil in Europe, sunflower oil in the US, coconut oil, palm oil, and jatropha oil in Asia [2-4]. Vegetable oils have a high viscosity, so they need to be heated when used in engines. However, the advantage of vegetable oil is that it does not need to go through the refining stage to form biodiesel, saving costs [4-5].

Biodiesel has properties similar to DO fuel, but it is produced from vegetable oil, animal fat, or waste cooking oil. With more than 3,260 km of coastline and the Mekong Delta, Vietnam has a superior advantage in excess fish fat products compared to many countries worldwide. It is a rich and renewable source of raw materials for domestic Biodiesel production, positively reducing environmental pollution and socio-economic development [6].

Based on the theory of the working cycle of diesel engines, when using traditional fuels as well as biofuels, the factors that directly affect the performance indicators include [7-8]:

- Fuel type*;
- Fuel injection system**;
- Combustion chamber type***;
- Gas exchange system****.

When using a mixture of diesel-coconut oil or biodiesel, it is possible to affect (*) the fuel's physical and chemical properties and (**) the fuel injection system to optimize the diesel engine's economic and environmental indicators while keeping the engine's structural elements intact.

From the above analysis, it can be seen that when using fuel with changing physical and chemical properties, the fuel spray structure will change as follows [8-9]:

- Break - up length;
- Spray penetration;
- Spray cone angle.

The above factors all affect the combustion mixture formation process, including soot formation and soot oxidation, leading to changes in diesel engines' soot emissions.

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 [9].

Among them, soot is a significant pollutant in diesel engine exhaust. It exists in the form of solid particles, causing harm to the environment and human health. The formation of soot in a diffusion flame depends primarily on the fuel. The higher the carbon content of the fuel, the greater the soot concentration [9]. The diesel fuel-coconut oil blending and biodiesel from animal fat (biofuel) have a low carbon content, low sulfur content, and much oxygen, so it limits the formation of soot, which is an advantage compared to diesel fuel.

For diesel engines, the Multi-Zone combustion model based on the empirical law of the gas drawn into the fuel jet and the fuel distribution in the spray to calculate the average temperature in each zone and, from there calculate the soot has allowed the construction of multidimensional simulation programs such as the open source CFD code Kiva-3V, Open Foam to calculate the soot content with popular two-step models of soot formation and soot oxidation such as Tesner - Magnussen model; Hiroyasu and the 8-step soot formation model of Kazakov and Foster [9-10]. According to these models, after the soot is formed, it will be oxidized at a high temperature; the soot oxidation process depends mainly on the soot concentration and the turbulence kinetic energy of the flame and combustion temperature [10].

Biofuels with high oxygen and low sulfur content are advantageous in reducing soot formation. However, too high viscosity and great density can affect the formation of the combustible mixture. It will lower the combustion temperature, reducing the oxidation of soot.

Based on that, the objective of studying the influence of biofuel properties on soot emissions is to determine the appropriate adjustment of engine operating mode and recommend adjusting injection parameters to create an effective combustion mixture formation process, improve combustion efficiency, and optimize soot emissions when the engine uses biofuel with different properties.

2. Materials and Methods

2.1. Materials

The fuel used includes diesel fuel (DO: 100% diesel oil), a mixture of diesel-coconut oil (C10: 10% coconut oil, 90% diesel oil), and biodiesel produced from animal fat (B10: 10% biodiesel B100, 90% diesel oil). The fuel specifications were determined at QUATEST 3 in Vietnam and presented in Table 1. The engine used in this study is a Yanmar 4che high-speed diesel engine; the specifications are shown in Table 2.

Table 1. *Basic fuel specifications*

Fuel properties	DO	B10	C10
Density (g/cm³)	0.8360 at 40^0C	0.8389 at 40^0C	0.8372 at 80^0C
Cetane number (CN)	52.1	52.5	53
Kinematic viscosity (medium mm²/s)	2.419 at 40^0C	2.848 at 40^0C	3.267 at 80^0C
Calorific value (Kcal/kg)	10915	10845	10675

Table 2. *Yanmar 4che diesel engine specifications*

Parameters	Value
Chamber type/Number of cylinders (-)	Unified/4
Cylinder diameter x piston stroke (mm)	105x125
Power (Hp/rpm)	70/2,300
Compression ratio (-)	16.4
Number of nozzle holes x diameter x spray direction (deg)	4 x 0.32 x 140
Injection timing (^{0}BTDC)	18
Injection pressure (kg/cm²)	210
Rod length (mm)	215
IVO (^{0}BTDC)	16
IVC (^{0}ABDC)	52
EVO (^{0}BBDC)	52
EVC (^{0}ATDC)	16

2.2. Simulation Research

Using Kiva–3V software to simulate the combustion and emission process of diesel engines, Kiva–3V software was developed by Los Alamos National Laboratory (LANL) of the US, specializing in simulating the combustion process and emission formation [11].

The basis of simulation:

Conservation equations, turbulence models, combustion computational models, heat transfer, and emissions are the basis of an engine's combustion simulation and emissions [12-15].

Mass conservation equation:

$$\frac{\partial \rho_m}{\partial t}+\frac{\partial(\rho_m u_i)}{\partial x_i}=\frac{\partial}{\partial x_i}\left(\rho D\frac{\partial(\rho_m/\rho)}{\partial x_i}\right)+\dot{\rho}_m^s+\dot{\rho}_m^c \quad (1)$$

In there:

$\rho=\sum_m \rho_m$ - Total density of the component masses (g/cm³);

$\dot{\rho}^s=\sum_m \dot{\rho}_m^s$ - The condition of total source mass when spraying (g);

$\sum_m \dot{\rho}_m^c=0$ - Constraint conditions on mass sources due to combustion (g).

Conservation of momentum equation:

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

With $j = 1,2,3$

Energy conservation equation:

$$\rho c_p\left(\frac{\partial T}{\partial t}+\frac{\partial T}{\partial x_i}\right)=k\frac{\partial^2 T}{\partial x_i^2}+\frac{\partial}{\partial x_i}\left(\rho D\sum_m h_m\frac{\partial(\rho_m/\rho)}{\partial x_i}\right) + A_0\rho\varepsilon+\dot{Q}^s+\dot{Q}^c \quad (3)$$

In the above equations, t - time (s), x_i - coordinates (m), p - pressure (N/m²), ρ_m - density of substance m (g/m³); u_i, u_j - velocity of fluid element (m/s), T - temperature (K), t_{ij} - components of stress tensor (N/m²), h - static enthalpy (J/kg), A_0 and $1/\alpha^2$ - coefficients to improve the calculation efficiency of flows with small Mach numbers.

The soot emission calculation model used is the 8-step model of Kazakov and Foster [16].

According to this model, under high-temperature conditions during the combustion process, primary particles and Acetylene C_2H_2 are produced from fuel pyrolysis. The calculation basis of the model is based on the hypothesis that Precursor Radical particles, abbreviated as PR, develop and form soot.

Eight equations representing the formation and oxidation of soot are presented in Table 3.

Table 3. *Steps of soot formation, oxidation, and reaction rates*

(i) Fuel pyrolysis

$$RH \xrightarrow{r_1} \frac{m}{2} PR$$

Reaction rate

$$r_1 = \frac{m}{2} 0.7\times 10^{12} \exp\left(\frac{-502,400}{RT}\right)\left[RH_g\right]$$

(ii) Fuel pyrolysis

$$RH \xrightarrow{r_2} \frac{m}{2} C_2H_2$$

Reaction rate

$$r_2 = \frac{m}{2} 2.0\times 10^{8} \exp\left(\frac{-205,200}{RT}\right)\left[RH_g\right]$$

(iii) Fuel pyrolysis

$$PR \xrightarrow{r_3} C_{soot}$$

Reaction rate

$$r_3 = 1.0\times 10^{12} \exp\left(\frac{-167,500}{RT}\right)\left[PR\right]\left[O_2\right]$$

(iv) Fuel pyrolysis

$$C_{soot} + C_2H_2 \xrightarrow{r_4} C_{soot+2} + H_2$$

Reaction rate

$$r_4 = 6.0\times 10^{13} \exp\left(\frac{-209,000}{RT}\right)\left[C_2H_2\right]\left[O_2\right]$$

(v) Fuel pyrolysis

$$xC_{soot} \xrightarrow{r_5} yC_{soot}$$

Reaction rate

$$r_5 = 1.0\times 10^{10} \exp\left(\frac{-209,000}{RT}\right)\left[PR\right]$$

(vi) Fuel pyrolysis

$$PR + O_2 \xrightarrow{r_6} Combustion\ products$$

Reaction rate

$$r_6 = 4.2\times 10^{4} \exp\left(\frac{-50,200}{RT}\right)\left[C_2H_2\right]S_P^{0.5},$$

$$S_P = \pi D_P^2 N_P$$

(vii) Fuel pyrolysis

$$C_2H_2 + O_2 \xrightarrow{r_7} 2CO + H_2$$

Reaction rate

$$r_7 = S_P\left[x\frac{K_A P_{O_2}}{1+K_Z P_{O_2}} + (1-x)K_B P_{O_2}\right],$$

$$x = \left(1+\frac{K_T}{K_B P_{O_2}}\right)^{-1}$$

(viii) Fuel pyrolysis

$$C_{soot} + O_2 \xrightarrow{r_8} C_{soot-2} + 2CO$$

Reaction rate

$$r_8 = 1.05\times 10^{-7}\times T^{-0.5}\times f_v^{1/6}\times N_P^{11/6}$$

First, fuel is pyrolyzed, and then the primary soot particles develop into soot. At that time, Acetylene adds carbon molecules to the surface of the soot atoms to create new atoms of larger size, and this new soot atom also combines with itself to continue to grow in size. Due to the high temperature and presence of oxygen during combustion, the Acetylene base particles and soot atoms are oxidized. The soot emission after the exhaust valve is the difference between the amount of soot formed and the amount of soot oxidized in the combustion chamber.

In the table above, f_v - soot particle volume (cm^3); K_A, K_B, K_T, K_Z - soot oxidation reaction rate constants (-), S_P - soot particle surface area (cm^2), N_p - particle density (g/cm^3), D_P - soot particle diameter (cm), P_{O2} - oxygen partial pressure (kPa), r_i - i-th reaction rate (g/cm^3s).

The combustion chamber mesh model of the Yanmar 4che 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. Simulation modes are shown in Table 4.

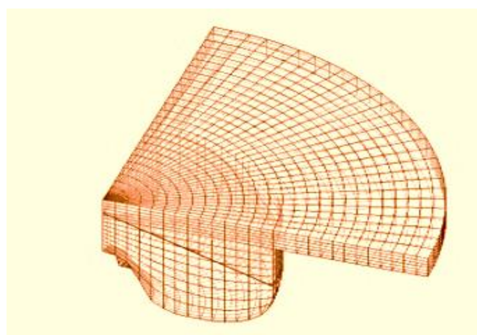


Figure 1. *Combustion chamber mesh model of Yanmar 4che diesel engine*

Table 4. *Simulation modes*

Parameters	Unit	Values
The engine load	%	60
The engine speed	rpm	1,800
Injection pressures	Kg/cm^2	210
Injection timing	^{0}BTDC	18

3. Results and Discussion

Figure 2 shows the variation of combustion pressure of biofuel compared to diesel fuel, in which the combustion pressure of DO fuel is the largest because DO fuel has the highest calorific value (Table 1), followed by the combustion pressure of B10 fuel (10% biodiesel B100) and the lowest combustion pressure is C10 fuel (10% coconut oil). The high viscosity of C10 fuel affects the injection process, forming a poorer combustion mixture than DO and B10 fuels and causing low combustion pressure; the maximum combustion pressure values are shown in Table 5.

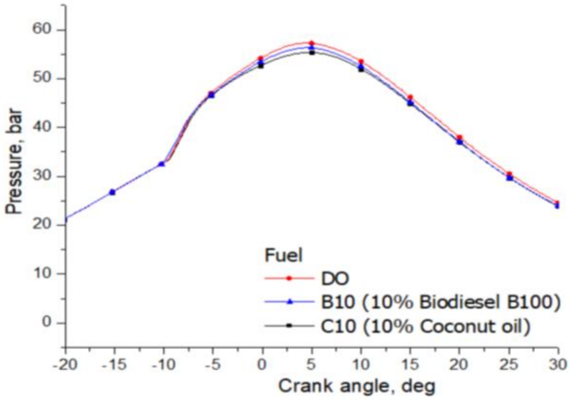


Figure 2. *Variation of combustion pressure of fuels*

Table 5. *Maximum combustion pressure values of fuels*

Fuels	Maximum combustion pressure (bar)
DO	57.4862
B10 (10% Biodiesel B100)	57.2378
C10 (10% Coconut oil)	55.3562

Figure 3 shows that the combustion temperature law of biodiesel fuel B10 from animal fat appears to burn first and has the highest combustion temperature; this is due to the high oxygen concentration contained in the fuel; for fuel C10, although the oxygen concentration is high, due to the high viscosity, the formation of the combustible mixture is poorer, leading to low combustion temperature. The soot oxidation process will decrease when the combustion temperature is low, leading to increased soot emissions. The maximum combustion temperature values are shown in Table 6.

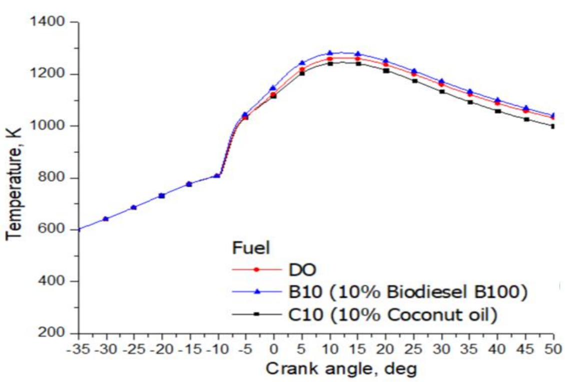


Figure 3. *Variation of combustion temperature of fuels*

Table 6. *Maximum combustion temperature values of fuels*

Fuels	Maximum combustion temperature (K)
DO	1259.26
B10 (10% Biodiesel B100)	1362.72
C10 (10% Coconut oil)	1242.47

Figure 4 shows the soot emissions of different fuels. Biofuels all have much lower soot emissions than DO fuels. B10 fuel has the lowest emissions because it contains a lot of oxygen, low carbon and sulfur content, and has a high combustion temperature (Figure 3), which increases the soot oxidation process. C10 fuel also has properties similar to those of B10 fuel. However, the formation of a combustible mixture is poorer and has a low combustion temperature, leading to higher soot emissions than B10 fuel. The maximum soot emission values are shown in Table 7.

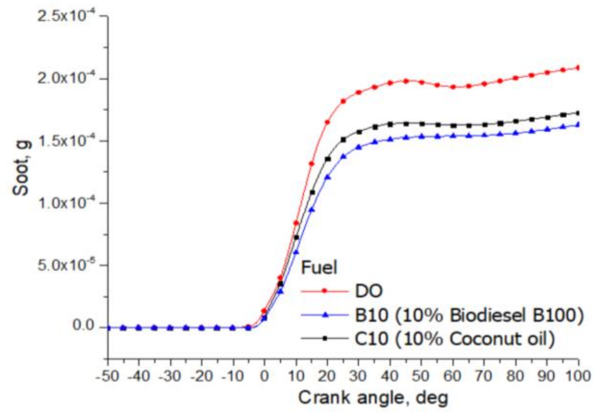
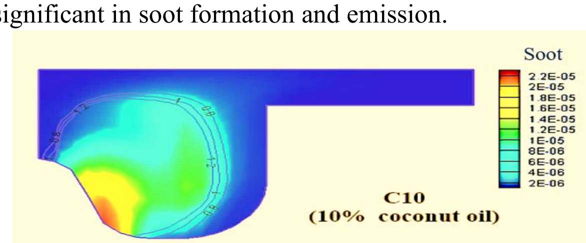


Figure 4. *Soot emissions of fuels*

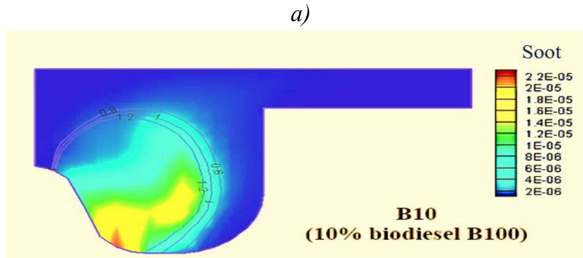
Table 7. *Maximum soot emissions of fuels*

Fuels	Maximum soot emissions (g)
DO	2.08×10^{-4}
B10 (10% Biodiesel B100)	1.63×10^{-4}
C10 (10% Coconut oil)	1.72×10^{-4}

Figure 5 shows the formation of soot from biofuel in the combustion chamber of the engine, in which the case of C10 fuel shows that the soot formation area is concentrated in a region and has a high concentration, it is due to the great viscosity of C10 fuel, affecting the injection process, leading to the formation of a less homogeneous air-fuel mixture. In the case of B10 fuel, the soot formation is dispersed. It has a low concentration, which shows that the combustion mixture formation process of B10 fuel is more homogeneous, limiting soot formation. These factors demonstrate that the influence of biofuel properties such as viscosity and density is very significant in soot formation and emission.



a)



b)

Figure 5. *Soot formation of fuel in the combustion chamber*

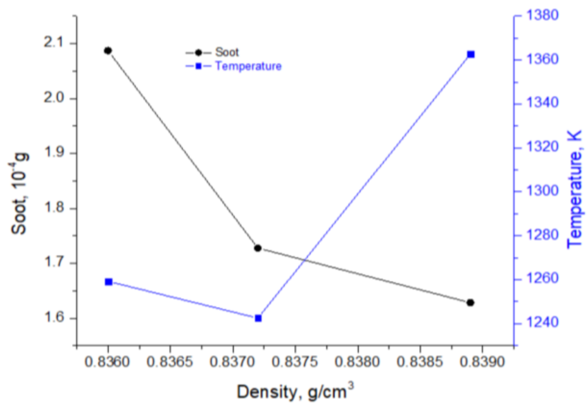


Figure 6. *Soot emission rule according to combustion temperature and density*

Figure 6 shows the soot emission law of fuel samples when changing fuel properties. As the combustion temperature increases, soot emission decreases, which shows that the simulation results are consistent with the actual law. Because the combustion temperature increases, the soot combustion process will increase, causing the amount of soot emission to decrease.

4. Conclusion

Based on the simulation, the research results evaluated the influence of fuel properties on soot emissions. In which B10 fuel (10% Biodiesel B100) has low viscosity, the formation of a homogeneous combustion mixture and high combustion temperature reduces soot emissions (1.63×10^{-4}g). C10 fuel (10% Coconut oil) has a high viscosity, forming a less homogeneous combustion mixture, and a low combustion temperature reduces soot oxidation. Soot emissions increase (1.72×10^{-4}g) compared to B10 fuel.

When using the fuel has a high viscosity, the injection parameters, including injection pressure and injection timing, can be adjusted to create a spray suitable for the combustion chamber space and increase the time to form the combustible mixture, achieving high homogeneity, the combustion process has a high temperature, leading to an increase in the soot oxidation rate and consequently will optimize soot emissions. The simulation results show that adjusting the injection parameters (injection pressure and injection timing increased compared to traditional diesel fuel) is a recommendation to improve diesel engines' economic and environmental indicators when applying high-viscosity biofuels, such as C10 fuel (10% Coconut oil).

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