Modelling Combustion Characteristics of a Turbocharged Low Heat Rejection Direct Injection Compression Ignition Engine Fuelled with methyl Ester of Seed Oil of Terminalia Catappa *L*. and its Blends

Fasogbon, S. K. and Odia, M. F.

Thermo-Fluid Research Unit, Department of Mechanical Engineering,
Faculty of Technology, University of Ibadan, Ibadan, Nigeria
**Corresponding Author*

***Abstract*—Modelling and Characterization of combustion characteristics of hydrocarbon fuelled engines have always been left largely at the mercy of experimental means. Meanwhile the experimental means is either cumbersome to set up or costly to achieve. This work therefore modelled mathematically the combustion characteristics of Low Heat Rejection (LHR) direct injection diesel engine running on the methyl ester of seed oil of Terminalia Catappa *L*. and its blends. The choice of LHR engine is occasioned by its superior advantages of improved fuel economy, higher energy in exhaust gases and capability of handling higher viscous fuel. First law of thermodynamics, ANNAND's heat transfer equations and Olikara and Borman fundamental combustion equations were employed to develop the combustion mathematical model for the LHR direct injection diesel engine fuelled with methyl ester of seed oil of Terminalia Catappa *L*. MATLAB was employed to simulate the developed model, and evaluate the impacts of crank angles on the peak temperature, peak pressure, rate of heat transfer and other combustion variables. The results show that for crank angle increase of the engine, there is corresponding cylinder peak pressure decrease by about 0.03 % for diesel fuel and 0 % decrease for blends of methyl ester of seed oil of Terminalia Catappa *L*., cylinder peak temperature increase between 6 to 15 % for the blends and 0 % increase for diesel; and heat transfer increase between 10 to 47 % for the blends and 0 % increase for diesel. The study concludes that the developed combustion model for Low Heat Rejection (LHR) direct injection diesel engines running on the methyl ester of seed oil of Terminalia Catappa *L*. and its blends is sufficient and can be extended to other fuels. Crank angle increase also enhances combustion characteristics and same is improved when percentage composition of methyl ester is increased in the blends.**

***Keywords* – Biodiesel, Terminalia Cattapa Linn Oil, Low Heat rejection, Direct Injection, Turbocharged Engine, Compression Ignition**

I. INTRODUCTION

In recent years, the continuous search for new blends of fuel and better engines with better combustion characteristics and economic viability has led to tonnes of research in the automotive engineering field. The new blends are most times expected to be biodegradable, non-toxic and renewable in nature. Vegetable oil is known to be a possible alternative engine fuel because it burns cleanly, it is renewable, nontoxic, biodegradable and quite environmentally friendly. It is produced from plants such as the tropical African fruit, soybean, peanut, sunflower, cotton, jatropha, coconut etc. Experimental results in the use of these oils show that they have better ignition characteristics; however, they cause serious problems such as carbon deposits build-up, poor durability, high density, high viscosity, poor combustion etc. but some of these problems were rectified by the trans-esterification process [1]. Researchers have trans-esterified various vegetable oils in order to produce different biodiesel blends with the most desirable properties for a particular application. The concept of using a biodiesel as a fuel for diesel engines is relatively not new, Rudolph Diesel first developed the diesel engine in 1885 with the intention of running it on a variety of fuels including vegetable oils, he demonstrated his engine at a Paris exposition in 1900 using peanut oil as the fuel, in 1912 he said this "The use of vegetable oils for engine fuels may seem insignificant today, but such oils may become in the course of time as important as petroleum and the coal tar products of the present" [3].

The emergence of the Low Heat Rejection (LHR) Diesel Engine which has been proven to be a far better variant than just normal diesel engines have risen to a peak as applications have been found in various fields. In this type of engine, heat rejection is suppressed to the engine coolant side with the help

of insulated coatings and the cycle operating temperature is increased. It is one of the energy conservation technique used in diesel engines as it results in low fuel consumption for the same power output, thereby reducing the size of the engine and also aids to eliminate the cooling system of the engine. The engine with its combustion chamber walls are insulated by heat flow resistant coatings such as PSZ (Partially Stabilized Zirconia) of 0.5mm to 1mm in thickness, the coated surfaces also includes the piston top, valves, cylinder head and outer surface of the cylinder liner. The LHR engine can handle the high viscous biodiesel and its blends because of its high operating temperature while the excess energy available in the engine exhaust could be effectively utilized with the help of turbochargers to improve the thermal efficiency of the engine.

II. THEORETICAL CONSIDERATIONS

Computer simulation is now becoming a powerful tool for the virtual prediction of fundamental process in engine system as it saves time and it is also quite economical compared to experimental studies. In this work, the computer simulation was carried out using the MATLAB computer program from Mathworks Inc. In this analysis, the molecular formula for diesel and biodiesel are approximated as $C_{10}H_{22}$ and $C_{19}H_{34}O_2$.

A. Fundamental Combustion Equation

The equilibrium constant method proposed by Olikara and Borman (1975) for the gas phase combustion of hydrocarbon fuel is used.

$$C_{a1}H_{b1}O_{c1} + \lambda \times A \times (O_2 + 3.76N_2) \longrightarrow n_1CO_2 + n_2H_2O + n_3N_2 + n_4O_2 + n_5CO + n_6H_2 + n_7H + n_8O + n_9OH + n_{10}NO \quad (1)$$

Where $A = a1 + \left(\frac{b1}{4}\right) - (c1\backslash 2)$

A is the stochiometric air fuel ratio and λ is the excess air ratio

Balancing of the C, H, O and N atom yields

C balance: $a1 = n_1 + n_5$ (2)

H balance: $b1 = 2n_2 + 2n_6 + n_7 + n_9$ (3)

O balance: $c1 + 2\lambda \times A = 2n_1 + n_2 + 2n_4 + n_5 + n_8 + n_9 + n_{10}$ (4)

N balance: $2 \times 3.76 \times \lambda \times A = 2n_3 + n_{10}$ (5)

The following six gas phase equilibrium reactions are considered;

$$\frac{1}{2}H_2 \Leftrightarrow H \quad (6)$$

$$\frac{1}{2}O_2 \Leftrightarrow O \quad (7)$$

$$\frac{1}{2}H_2 + \frac{1}{2}O_2 \Leftrightarrow OH \quad (8)$$

$$\frac{1}{2}N_2 + \frac{1}{2}O_2 \Leftrightarrow NO \quad (9)$$

$$H_2 + \frac{1}{2}O_2 \Leftrightarrow H_2O \quad (10)$$

$$CO + \frac{1}{2}O_2 \Leftrightarrow CO_2 \quad (11)$$

From the equilibrium concentration equations, i.e. where $K_p = K_c(RT)^{\sum v_i}$ (12)

K_p = Equilibrium concentration on the basis of pressure

K_c = Equilibrium concentration on the basis of concentrations

$$K_1 = \frac{n_7}{\sqrt{n_6}} \times \sqrt{P} \quad (13)$$

$$K_2 = \frac{n_8}{\sqrt{n_4}} \times \sqrt{P} \quad (14)$$

$$K_3 = \frac{n_9}{\sqrt{n_6 \times n_4}} \quad (15)$$

$$K_4 = \frac{n_{10}}{\sqrt{n_3 \times n_4}} \quad (16)$$

$$K_5 = \frac{n_2}{n_6 \times \sqrt{n_4}} \times \frac{1}{\sqrt{P}} \quad (17)$$

$$K_6 = \frac{n_1}{n_5 \times \sqrt{n_4}} \times \frac{1}{\sqrt{P}} \quad (18)$$

Olikara and Borman curve fitted the equilibrium constant K_i (i) to JANAF table data for 600 < T < 4000K. The expression is as follows:

$$\log_{10} K_i(T) = A_i \ln\frac{T}{1000} + \frac{B_i}{T} + C_i + D_i + E_iT^2 \quad (19)$$

$$Total\ Moles\ of\ Reactants(TMR) = 1 + \lambda \times A \times 4.76 \quad (20)$$

$$Total\ Moles\ of\ Products(TMP) = a1 + (b1/4) + 3.76 \times A \times \lambda + (\lambda - 1) \times A \quad (21)$$

$$X_{CO_2} = \frac{n_1}{TMP} \quad X_{H_2O} = \frac{n_2}{TMP} \quad X_{N_2} = \frac{n_3}{TMP} \quad X_{O_2} = \frac{n_4}{TMP} \quad (22)$$

$$X_{CO} = \frac{n_5}{TMP} \quad X_{H_2} = \frac{n_6}{TMP} \quad X_H = \frac{n_7}{TMP} \quad X_O = \frac{n_8}{TMP}$$

$$X_{OH} = \frac{n_9}{TMP} \quad X_{NO} = \frac{n_{10}}{TMP} \quad (23)$$

$$V_\theta = V_C + \left[\pi \times \frac{d^2}{4} \times \frac{l}{2}\right] \times \left[1 + S - (S^2 - sin^2\theta)^{1/2} - \cos\theta\right] \quad (24)$$

Where $S = \frac{2l_c}{l}$ (25)

d = bore (m); l = stroke length (m); V_C = clearance volume (m^3); θ = Crank angle (degrees); V_θ = Volume at any crank angle (m^3)

$$T_2 = T_1 \times \left(\frac{V_1}{V_2}\right)^{R/C_V(T_1)} \quad (26)$$

$$P_2 = \left(\frac{V_1}{V_2}\right) \times \left(\frac{T_2}{T_1}\right) \times P_1 \quad (27)$$

T_1 = Initial Temperature (K); T_2 = Final Temperature (K); P_1 = Initial Pressure (bar); P_2 = Final Pressure (bar); R = Characteristic gas constant (kJ/kgK); C_v = Specific heat at constant volume (kJ/KgK); V_1 = Initial Volume (m^3); V_2 = Final Volume (m^3)

$$\frac{C_{P,i}}{R} = a_{i1} + a_{i2}T + a_{i3}T^2 + a_{i4}T^3 + a_{i5}T^4 \quad (28)$$

$$\frac{h_i}{RT} = a_{i1} + \frac{a_{i2}}{2}T + \frac{a_{i3}}{3}T^2 + \frac{a_{i4}}{4}T^3 + \frac{a_{i5}}{5}T^4 + \frac{a_{i6}}{T} \quad (29)$$

$$\frac{s_i}{R} = a_{i1}\ln T + a_{i2}T + \frac{a_{i3}}{2}T^2 + \frac{a_{i4}}{3}T^3 + \frac{a_{i5}}{4}T^4 + a_{i7} \quad (30)$$

$$u_i(T) = h_i(T) - RT \quad (31)$$

The work done is calculated from the mean pressure and for each degree crank angle, it is calculated as;

$$dW = \left[\frac{P_1+P_2}{2}\right] \times (V_2 - V_1) \quad (32)$$

The total heat transfer is the sum of the convective heat transfer and radiative heat transfer since an LHR Turbocharged engine operates at elevated temperatures.

Viscosity of air at each temperature change;

$$\mu_{air} = 3.3 \times 10^{-7}(T)^{0.7} \quad (33)$$

Viscosity of combustion gases;

$$\mu_{prod} = \frac{\mu_{air}}{(1+0.027\varphi)} \quad (34)$$

φ = Equivalence Ratio

Reynolds number for each step as viscosity varies;

$$Re = \frac{\rho d V_p}{\mu_{prod}}; \qquad \text{where, } V_p = \frac{2NS}{60} \quad (35)$$

ρ = Density of gas mixture (kg/m^3); V_p = Mean piston speed (m/min)

Thermal conductivity is calculated for each change in viscosity;

$$k = \frac{C_p \mu_{prod}}{0.7} \quad (36)$$

Heat transfer coefficient

$$h_g = 0.26 \times (k/d) \times Re^{0.6} \quad (37)$$

Total heat transfer

These is gotten from the Annand's heat transfer equation and it is given as

$$\frac{dQ}{dT} = ak\frac{Re^b}{d}(T_g - T_w) + c({T_g}^4 - {T_w}^4) \quad (38)$$

Where a = 0.36; b = 0.7 and $c = 3.88 \times 10^{-8}\, kJ/m^2 - sec - K^4$

$\frac{dQ}{dT}$ = Heat Transfer rate (KJ/CA), T_g = Gas Temperature (K), T_w = Wall Temperature (K)

B. Wall Heat Transfer Model

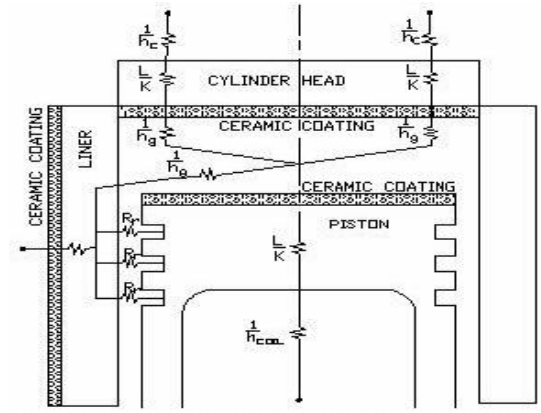

Figure 1. Thermal Network Model

A thermal network model was gottenfrom [20] for the wall heat transfer analysis and it is used to analyse the effect of coating on the engine heat transfer. The model is used to analyse the heat transfer through cylinder to the coolant and thereby finds instantaneous wall temperature. The total resistance offered by the cylinder liner, piston rings, cylinder head, ceramic coating and piston for the heat transfer from cylinder gases to coolant is given by the following equation

$$R_t = \frac{1}{h_g 2\pi r_1 l} + \frac{1}{2\pi h_{co} r_3 l} + \frac{\log(r_2/r_1)}{2\pi k_1 l_1} + \frac{\log(r_3/r_4)}{2\pi k_c l_c} + 3\frac{\log(r_5/r_9)}{2\pi k_r l_r} + \frac{\log(r_7/r_8)}{2\pi k_s l_s} + \frac{t_p}{2\pi k_p {r_7}^2} \quad (39)$$

Heat transfer to the wall is given by;

$$Q_w = \frac{T_g - T_{co}}{R_t} \quad (40)$$

Wall temperature is then given by;

$$T_w = T_g - \frac{Q_w}{h_g 2\pi r_1 l} \quad (41)$$

$$M_f = C_d A_n \sqrt{2\rho_f}\Delta P\left(\frac{\Delta\theta}{360N}\right) \quad (42)$$

C_d = Coefficient of discharge of injector nozzle; A_n = Cross sectional area of nozzle (m^2);

ΔP = Pressure drop across the nozzle (bar); $\Delta\theta$ = Fuel Injection Period (degrees); N = Engine speed (rpm)

From the first law of thermodynamics, the energy balance is given by;

$$E(T_2) = E(T_1) - dW - dQ + dM_f Q_{vs} \quad (43)$$

If the correct value of T_2 has been established, both sides of the above equation should be equal, we then arrange the equation as follows;

$$F(E) = E(T_2) - E(T_1) - dW - dQ + dM_f Q_{vs} \quad (44)$$

To then calculate T2,

$$E(T_2) = C_v(T_2) \times TMP \quad (45)$$

$$P_r = KM_f^{(1-x)} M_u^{\,x} P_{O_2}^{\,L} \quad (46)$$

$$K = 0.085N^{0.414} M_f^{\,1.414} \Delta\theta_f^{\,-1.414} h^{-1.414} d_n^{\,-3.644} \quad (47)$$

x = 0.667, L = 0.4

M_u = Mass of fuel unprepared (g/CA); n = No. of nozzle holes; d_n = Diameter of nozzle (m);

P_{O_2} = Partial pressure of oxygen (bar)

$$R_r = \frac{K' P_{O_2}}{N\sqrt{T}} e^{\frac{-act}{T}} \int (P_r - R_r) d\theta \quad (48)$$

$$K' = Reaction\ rate\ constant \left(87 \times \frac{10^{10}\sqrt{K}}{bar}\right)$$

act = Activation energy for the total species

$$T_u = T_{soc} \left[\frac{P}{P_{soc}}\right]^{\frac{n-1}{n}} \quad (49)$$

T_u = Unburned zone temperature (K); T_{soc} = Temperature at the start of combustion (K)

P_{soc} = Pressure at the start of combustion (bar); n = specific heat ratio

$$T_b = \frac{T-(1-x_b)T_u}{x_b} \quad (50)$$

$$Heat = \left(\frac{\gamma}{\gamma-1}\right) \times dW + \left(\frac{V1+V2}{2}\right) \times (P2 - P1) \quad (51)$$

C. Engine Specifications

The following are the technical details of the engine taken intoconsideration for simulation.

Table 2.3: Engine Specifications

Variable			Description
1.	Type	:	4 cylinder, 4 stroke, water Cooled Turbocharged DI Diesel engine.
2.	Bore	:	111.1 mm
3.	Stroke	:	127.0 mm
4.	Connecting rod length	:	251.0 mm
5.	Displacement volume	:	$4913.36*10^3$ mm^3
6.	Clearance volume	:	$81.89*10^3$ mm^3
7.	Nominal Compression ratio	:	16:1
8.	Rated speed	:	1500 rpm
9.	Rated power output	:	55.2 kW @ 1500 rpm
10.	BSFC @ full load	:	265 g/kW-hr
11.	Fuel injection pressure	:	210 bar
12.	Lubricating oil	:	SAE 40
13.	Nozzle hole diameter	:	0.26 mm
14.	No. of nozzle holes	:	3
15.	Cone angle of spray	:	17.5^0

D. Properties of Fuels

Table 2.4: Fuel Properties

PROPERTIES	DIESEL	B20	B40	B60	B80	B100
Density @ 20 ^oC (kg/m3)	830	843	852	863	874	888
Viscosity @ 40 ^oC (mm^2/s)	2.8	2.7	3.2	3.7	4.0	4.31
Flash point @ 40 ^oC	55	65	77	89	108	145.3
Lower Heating Value (MJ/kg)	42	39.26	38.54	38.00	37.41	36.97

III. RESULTS AND DISCUSSIONS

After the development of the computer program using the mathematical modelling for combustion characteristics for LHR turbocharged engine operated with diesel and various biodiesel blends, the following synthesized results were obtained and analysed. Tests were conducted in the LHR turbocharged engine using diesel and various biodiesel blends. The following combustion performance were studied and compared.

A. Comparison of Cylinder Pressure

Figure 2 show the comparison of cylinder pressure with crank angle for various blend ratio. The results show that the cylinder peak pressure decreases by about 0.03% for LHR turbocharged engine operated with diesel but stays nearly the same for the other biodiesel blends. The simulation results show that as the blend ratio increases, the cylinder peak pressure decreases for LHR turbocharged engine due to higher molecular mass and the reduced atomization of biodiesel during the fuel injection process. It also decreases due to higher heat retainment inside the cylinder leading to higher wall temperature. The higher wall temperature increases the specific volume of air charge entry during suction stroke and decreases the volumetric efficiency and finally decreases the peak cylinder pressure.

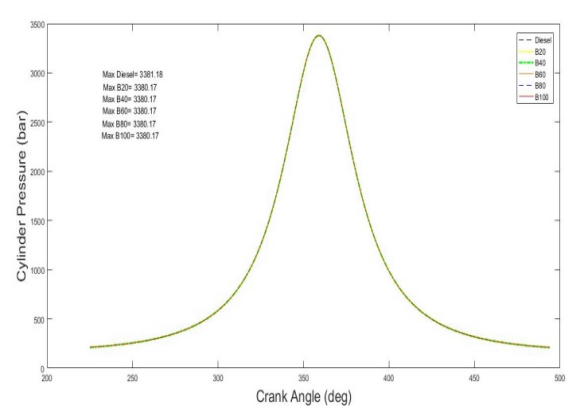

Fig 2: Comparison of all Cylinder Pressure with Crank Angle for LHR turbocharged engine operated with diesel and the different biodiesel blends.

B. Comparison of Cylinder Temperature

Figure 3 show the comparison of cylinder temperature with crank angle for various blend ratio. The results show that the cylinder peak temperature increases by about 7.0%, 9.16%, 14.45%, 14.70% for LHR turbocharged engine operated with B40, B60, B80 and B100 when compared with diesel but reduces by 6.17% for B20. As the oxygen content of the biodiesel blends increases, the temperature increases as the fuel burns more cleanly and less toxic residue is formed. The higher density and Low Heating Value(LHV) of the fuels also play their parts in the temperature distribution of the fuel. The higher rate of heat transfer affects the temperature as the LHR turbocharged engine withholds more heat thereby allowing the more viscous biodiesels burn more.

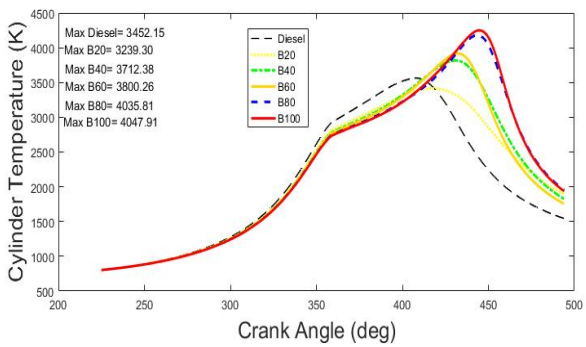

Fig 3: Comparison of all Cylinder Temperature with Crank Angle for LHR turbocharged engine operated with diesel and the different biodiesel blends.

C. Comparison of Rate of Heat Transfer

Figure 4 show the comparison of rate of heat transfer with crank angle for various blend ratio. The results show that the rate of heat transfer increases by about 10.55%, 31.43%, 41.72%, 46.81% for LHR turbocharged engine operated with B40, B60, B80 and B100 when compared with diesel but reduces by 24.13% for B20. In LHR turbocharged engine the heat transfer to the coolant decreases due to insulation thickness, which ultimately increases the cylinder wall temperature. As the fuel then burns more because of the higher heat retainment rate, the heat transfer increases.

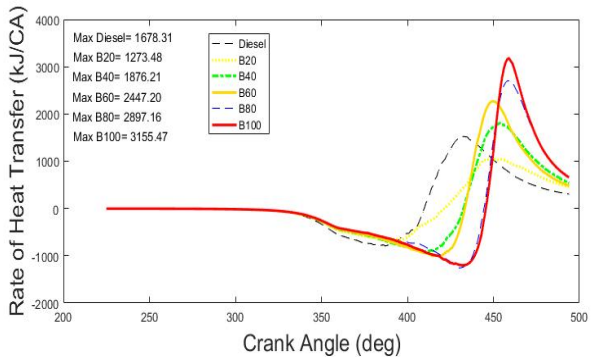

Fig 4: Comparison of all Rates of Heat Transfer with Crank Angle for LHR turbocharged engine operated with diesel and the different biodiesel blends.

D. Comparison of Work Done

Figure 5 show the comparison of work done with crank angle for various blend ratio. The results show that the work done decreases by about 0.023% for LHR turbocharged engine operated with diesel but stays nearly the same for the other biodiesel blends. The reduction in work done in the case of LHR turbocharged engine might be due to the high operating temperature falling beyond the operating limits leading to in-cylinder pressure reduction. The reduction is quite minimal for the diesel to biodiesel blends and stays the same for the biodiesel blends due to the fact that the work done is calculated from the pressure and volume of the cylinder, the temperature distribution has minimal effect.

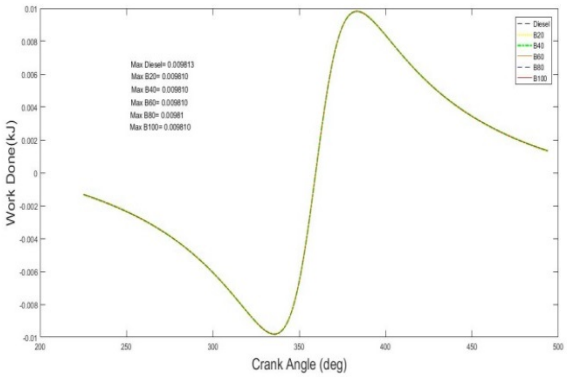

Fig 5: Comparison of Work Done with Crank Angle for LHR turbocharged engine operated with diesel and the different biodiesel blends.

E. Comparison of Net Heat Release Rate

Figure 6 show the comparison of the net heat release rate with crank angle for various blend ratio. The results show that the net heat release rate decreases by about 0.034% for LHR turbocharged engine operated with diesel but stays nearly the same for the other biodiesel blends. The net heat release rate reduces for the biodiesel blends and increases for diesel. It is a function of the work done and the diesel has a higher work done than the biodiesel blends.

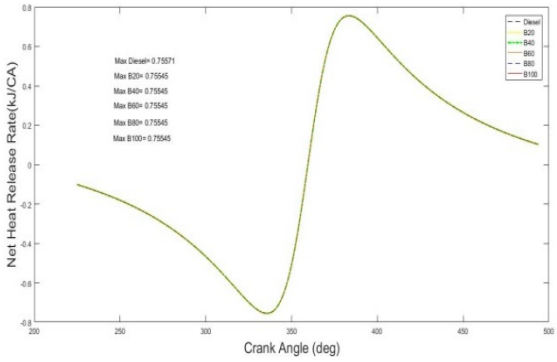

Fig 6: Comparison of Net Heat Release Rate with Crank Angle for LHR turbocharged engine operated with diesel and the different biodiesel blends.

IV. CONCLUSIONS

A detailed analysis of LHR turbocharged engine operated with diesel and biodiesel blends were done. The model was developed in such a way that it can be used for any biodiesel and its blends. The modelling results show that the temperature and the rate of heat transfer increased with the increase of the oxygen content of the biodiesels while the pressure decreased due to higher molecular mass and the reduced atomization of biodiesel during the fuel injection process. The reduced pressure also affected the work done and the net heat release rate.

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