Study of Theoretical Modelling of Combustion Characteristics of Biodiesel Fuelled Direct Injection CI Engine – A Review

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Abstract— Increasing of costly and depleting fossil fuels are prompting researchers to use edible as well as no edible vegetable oils as a promising alternative to petro-diesel fuels. Biodiesel are found near about similar properties like diesel. A comprehensive computer code using ”Quick basic” language was developed for the diesel engine cycle to study the combustion characteristics of a single cylinder, four stroke, direct injection diesel engine. The engine operates on diesel fuel and 20% (mass basis) of biodiesel blended with diesel. Combustion characteristics such as cylinder pressure, heat release fraction, heat transfer were analyzed. On the basis of the first law of thermodynamics the properties at each degree crank angle was calculated. Wiebe function is used to calculate the instantaneous heat release rate. A simulated combustion results are found satisfactory with experimental results.

Key words: Biodiesel, Combustion characteristics, Numerical modelling, Simulation

I. INTRODUCTION

The petroleum fuels fulfill our energy needs in industrial development, transportation, agriculture sector and many other basic requirements. These fuel reserves are fast depleting due to excessive usage. Besides combating the limited availability of crude oil, researchers are also dealing with other associated serious problems with petroleum fuel such as increase in pollutant emissions like: CO2, HC, NOx, and SOx. In recent times, biodiesel has received significant attention both as a possible renewable alternative fuel and as an additive to the existing petroleum-based fuels. Biodiesel is a non-toxic, biodegradable and renewable alternative fuel that can be used with no engine modifications. It can be produced from various vegetable oils, waste cooking oils or animal fats. The properties of Biodiesel may change when different feed stocks are used. In general, if the fuel properties of Biodiesel are compared to petroleum diesel fuel, it can be seen that Biodiesel has a higher viscosity, density, and cetane number. But the energy content or net calorific value of Biodiesel is about 10-12 % less than that of conventional diesel fuel on the mass basis. The rapid development of computer technology narrows down the time consumption for engine test through the simulation techniques. The insight of the combustion process is analyzed thoroughly, which enhance the engine power output and consider as the heart of the engine process [3].

The theoretical models used in the case of internal combustion engines can be classified into two main groups: thermodynamic models and fluid dynamic models. Thermodynamic models are mainly based on the first law of thermodynamics and are used to analyze the performance characteristics of engines. Pressure, temperature and other required properties are evaluated with respect to crank angle or time. The engine friction and heat transfer are taken into account using empirical equations obtained from experiments. These models are further classified into two groups namely single-zone models and multi-zone models. On the other hand, multi-zone models are also called computational fluid dynamics models. They are based on the numerical calculation of mass, momentum, energy and species conservation equations in either one, two or three dimensions to follow the propagation of flame or combustion front within the engine combustion chamber. Two zone model consists of one non burning zone which contain pure air and other zone consist of fuel and combustion products called burning zone. First law of thermodynamics and state equations are applied in each of the two zones to yield cylinder temperatures and cylinder pressure histories. Using the two zone combustion model the combustion parameters and the chemical equilibrium composition were determined. Multi-dimensional models need detail information of many phenomena and large computation time.

B. Rajendra Prasath *et al* (2010) carried out the two-zone modeling of diesel / biodiesel blended fuel operated ceramic coated direct injection diesel engine. A comprehensive computer code using ”C” language was developed for compression ignition (C.I) engine cycle and modified in to low heat rejection (LHR) engine through wall heat transfer model. On the basis of first law of thermodynamics the properties at each degree crank angle was calculated. Preparation and reaction rate model was used to calculate the instantaneous heat release rate. The effect of coating on engine heat transfer was analysed using a gas-wall heat transfer calculations and total heat transfer was based on ANNAND’s combined heat transfer model [4].

Mohamed F. Al-Dawody *et al* carried out the theoretical modeling of combustion characteristics and performance parameters of biodiesel in DI diesel engine with variable compression ratio. They observed the different combustion parameters at different compression ratio. The experiment was carried on four stroke, single cylinder diesel engine running on biodiesel (derived from soybean oil) [3].

II. TRANSESTERIFICATION OF VEGETABLE OIL

B. Rajendra Prasath *et al* (2010) carried out the transesterification of Jatropha seed oil. The vegetable oil was transesterified using methanol in the presence of sodium hydroxide (NaOH) as a catalyst (Figure 1 and 2). The parameter involved in the processing such as catalyst amount, molar ratio of alcohol to oil, reaction temperature and reaction time are optimized.

CH_2OOCR		CH_3OH		CH_3OOCR		CH_2OH
$CHOOCR$	+	CH_3OH	→	CH_3OOCR	+	$CHOH$
CH_2OOCR		CH_3OH		CH_3OOCR		CH_2OH
Triglycerides		Methanol		Methyl Ester		Glycerol

Fig. 1: Transesterification Chemistry Of Vegetable Oil

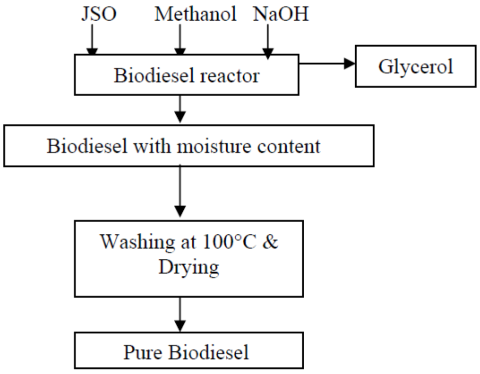

Fig. 2: Transesterification Process Of Vegetable Oil

Known quantity of vegetable oil was taken in a biodiesel reactor. A water-cooled condenser and a thermometer with cork were connected to the side openings. The required amount of catalyst (NaOH) was weighed and dissolved completely in the required amount of methanol by using a stirrer to form sodium methoxide solution. Meanwhile, the oil was warmed by placing the reactor in water bath maintained at the selected temperature. The sodium methoxide solution was added into the oil and stirred vigorously by means of a mechanical stirrer. The required temperature was maintained throughout the reaction time and the reacted mixture was kept in the separating drum. The mixture was allowed to separate and settled down by gravity settling into a clear, golden liquid biodiesel on the top with the light brown glycerol at the bottom. The glycerol was drained off from the separating drum leaving the biodiesel at the top. This pure biodiesel was measured on weight basis and the important fuel and chemical properties were determined. The theoretical analysis was carried out on a naturally aspirated, water-cooled, four stroke, single cylinder, direct injection diesel engine. The specifications of the engine are shown in Table 2 [4].

Properties	Diesel Fuel (DF)	Biodiesel (B100)	20%DF / 80%B100 (B20)
Density @ 15°C(kg/m^3)	830	880	840
Viscosity @ 40°C(cSt)	2.8	4.6	3.15
Flash point (°C)	55	170	80
Cetane number	45	50	46
Lower Heating Value (MJ/kg)	42	36	40.5

Table 1: Properties Of Diesel Fuel, B100 And B20 [4]

Engine Make	Kirloskar AV-1
Engine Type	(4-Stroke, Diesel Engine)
Number of Cylinder	1
Bore × stroke	87.5×110 mm
Cylinder capacity	0.66 L
Compression ratio	Variable (12-19)
Rated power	3.7 kW , 1500 rpm
Dynamometer	Electric AC-generator
Orifice diameter	0.15 mm
Injection pressure	(200-220) bar

Table 2: Specification of Engine [3]

III. Theoretical Considerations

In this analysis the molecular formula for diesel and biodiesel are approximated, as C10H22 and C19H34O2. The combustion model is developed for the C.I engine and suitable for any hydrocarbon fuel and their blends.

A. Calculation of Number of Moles of Reactants and Products:

In this simulation during the start of combustion, the moles of different species are considered includes O2, N2 from intake air and CO2, H2O, N2 and O2 from the residual gases [4]. The overall combustion equation considered for the fuel with C-H-O-N is

$$C_xH_yO_z + \lambda * y_{cc} * (O_2 + 3.773N_2) \rightarrow xCO_2 + (y/2)H_2O + (\lambda - 1)y_{cc}O_2 + \lambda y_{cc} * 3.773N_2 \quad (1)$$

Stoichiometric air fuel ratio AFR $y_{cc} = x + (y/4) - (z/2)$, λ - is excess air factor

Total number of reactants and products during the start of combustion as well every degree crank angle was calculated from the equations;

$$tmr = 1 + \lambda * y_{cc} * 4.773 \quad (2)$$

$$tmp = x + (y/4) + 3.773 * \lambda * y_{cc} + (\lambda - 1) * y_{cc} \quad (3)$$

B. Volume at Any Crank Angle:

Volume at any crank angle is calculated from this equation [3];

$$V = Vdisp\left[\frac{r}{r-1} - \frac{1-\cos\theta}{2} + \frac{L}{S} - 0.5\sqrt{\left(\frac{2L}{S}\right)^2 - \sin^2\theta}\right] \quad (4)$$

Where *Vdisp* - displacement volume (m3), r - compression ratio, *L* - connection rod length (m), *S* - stroke (m)

C. Calculation of Specific Heat:

Specific heat at constant volume and constant pressure for each species is calculated using the expression given below [4];

$$C_v(T) = (B - \bar{R}) + \frac{C}{T} \quad (5)$$

$$C_p(T) = B + \frac{C}{T} \quad (6)$$

Where A, B and C are the coefficients of the polynomial equation

D. Initial Pressure and Temperature during Start of Compression:

Initial pressure and temperature at the beginning of the compression process is calculated as follows [8];

$$P_2 = \left(\frac{V_1}{V_2}\right) * \left(\frac{T_2}{T_1}\right) * P_1 \quad (7)$$

$$T_2 = T_1 * \left(\frac{V_1}{V_2}\right)^{\frac{R}{C_V(T_1)}} \quad (8)$$

E. Calculation of Enthalpy and Internal Energy:

Enthalpy of each species is calculated from the expression given below which is used to calculate the peak flame temperature of the cyclic process [4];

$$H(T) = A + B * T + C * \ln(T) \quad (9)$$

The internal energy for each species and overall internal energy are calculated from the expressions given below

$$U(T) = A + (B - \bar{R}) * T + C * \ln(T) \quad (10)$$

$$U(T) = \sum(x_i U(T)) \quad (11)$$

Where A, B and C are the coefficients of the polynomial equation.

F. Work Done:

Work done in each crank angle is calculated from [8];

$$dW = \left(\frac{P_1+P_2}{2}\right)(V_2 - V_1) \tag{12}$$

G. Heat Transfer Model:

The gas-wall heat transfer is found out using Woschni heat transfer model [3].

$$\frac{dQ_{ht}}{dt} = h_c A_c (T_g - T_w) \tag{13}$$

Where *hc* heat transfer coefficient (w/m2K), *Ac* convection heat transfer area (m2), *Tg* & *Tw* gas and wall temperature respectively (K)

For convection Woschni developed the following empirical correlations for Nusselt number;

$$N_{u_s} = 0.035 R_e^{\,0.8} \tag{14}$$

Where *Re* is Reynolds number which is given by;

$$R_e = \frac{\rho w B}{\mu_p} \tag{15}$$

Where *B* cylinder bore (m), μ_p kinematic viscosity (Pa.s)

The above correlation can be rewritten;

$$h_c = 3.26 B^{-0.2} T^{-0.55} P^{0.8} w^{0.8} \tag{16}$$

During the compression process, Woschni argued that the average gas velocity should be proportional to the mean piston speed. During combustion and expansion processes he attempted to account directly for the gas velocities induced by the change in density that results from combustion. The following expression is used;

$$w = \left[C_1 v_p + C_2 \left(\frac{V_{disp}}{V_{cyl}}\right) * \left(\frac{P(\theta) - P_{motor}(\theta)}{P_{cyl}}\right)\right] \tag{17}$$

Where C1 and C2 are model constant, which specified as

- For gas exchange period: C1=6.18; C2=0
- For compression period: C1=2.28; C1=0
- For the combustion and expansion period: C1=6.18; C2=3.24*10-3

v_p- average piston speed (m/s), *Pcyl* - pressure of cylinder at initial condition (bar).

H. Energy Equation:

According to the first law of thermodynamics the energy balance equation is given by:

$$U(T_2) = U(T_1) - dW - dQ_{ht} + dm_f Q_{in} \tag{18}$$

Where *Qin* - Total heat supply (kJ/kg).

To find the correct value of T2, both sides of the above equation should be balanced. So the above equation is rearranged as shown below;

$$ERR_1 = U(T_2) - U(T_1) - dW - dQ_{ht} + dm_f Q_{in} \tag{19}$$

If the numerical value of *ERR*1 is less than the accuracy required, then the correct value of *T2* has been established, otherwise a new value of *T* is calculated for new internal energy and *CV* values.

$$ERR_2 = C_v(T_2) * N_p \tag{20}$$

Using Newton Raphson method to get;

$$(T_2)_n = (T_2)_{n-1} - \frac{ERR_1}{ERR_2} \tag{21}$$

I. Combustion Model:

The combustion of fuel and air is a very complex process, and would require extensive modeling to fully capture. In this work Wiebe function is used which some time is spelled Wiebe function to simulate the combustion process. The Wiebe function is often used as a parameterization of the mass fraction burned and it has the following form [3];

$$x_b(\theta) = 1 - e^{-a\left(\frac{\theta-\theta_{ing}}{\Delta\theta}\right)^{m+1}} \tag{22}$$

And the burn rate is given by its differential form:

$$\frac{dx_{b(\theta)}}{d\theta} = \frac{a(m+1)}{\Delta\theta} * \left(\frac{\theta-\theta_{ing}}{\Delta\theta}\right)^{m} * e^{\left(\frac{\theta-\theta_{ing}}{\Delta\theta}\right)^{m+1}} \tag{23}$$

Where *a* is a parameter which characterizes the completeness of combustion and its equal to 6.908, *m* is a parameter characterizing the rate of combustion. The small value of *m* means a high rate at the beginning of combustion, while a large value of *m* means a high rate by the end of combustion, θ_{ing} crank angle at which combustion starts (degrees) and $\Delta\theta$ total combustion duration (degrees).

IV. RESULTS AND DISCUSSIONS

In this study combustion parameter like cylinder pressure, peak cylinder pressure, combustion zone temperature, ignition delay and heat release are discussed. The readings are taken at constant engine speed 1500 rpm.

A. Cylinder Pressure:

In a CI engine the cylinder pressure dependent on the fuel-burning rate during the premixed burning phase. The high cylinder pressure ensures the better combustion and heat release. Mohamed F. Al-Dawody and S. K. Bhatti (2013) carried out theoretical analysis on a naturally aspirated, water-cooled, four stroke, single cylinder, direct injection diesel engine fuelled with Soybean methyl ester at different compression ratio. The software Diesel-rk is intended for the calculation and optimization of internal combustion engines.

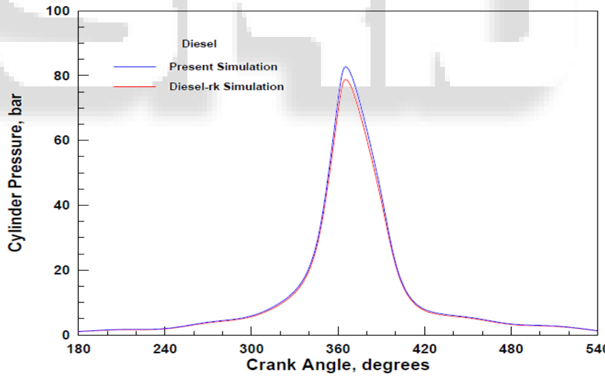

Fig. 1: Variation of Cylinder Pressure With Crank Angle For Diesel

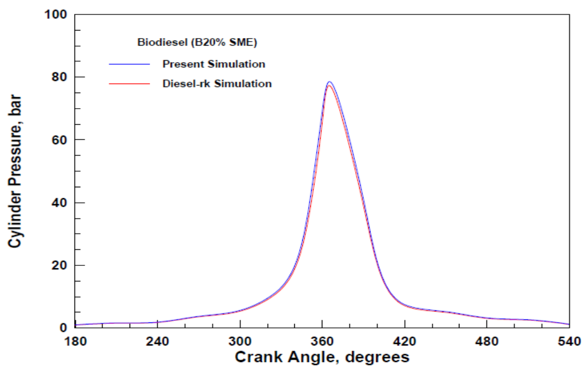

Fig. 2: Variation of Cylinder Pressure with Crank Angle for B20% SME

Figures 1, 2 show the typical pressure variation with respect to crank angle for diesel and biodiesel respectively as compared diesel-rk Simulation. It can be seen that cylinder pressure for biodiesel is lower than that of diesel by 5% due to the reduction in the heat supply for the blended fuel. It is noted that the maximum pressure obtained for biodiesel is closer to TDC than diesel fuel. The pressure of cylinder for both diesel and biodiesel comes into agreement with the results obtained by Diesel-rk software.

B. Zonal Combustion Temperature:

Figure 3 explains the comparison between combustion zone temperature with crank angle for diesel and biodiesel with respect to the diesel-rk results respectively. The presence of oxygen in the biodiesel makes complete combustion of fuel thereby producing more CO2 and hence more heat is released from the gases. Thus, the peak temperature of biodiesel-fueled engine is higher than that of diesel fuelled engine by 1.5 %. The results of both fuels are verified with the results computed in Diesel-rk at the same operating conditions.

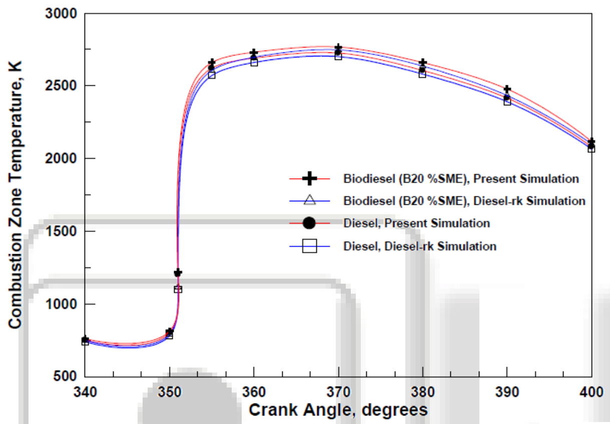

Fig. 3: Combustion Zone Temperature for Diesel And SME Biodiesel

C. Heat Release Rate:

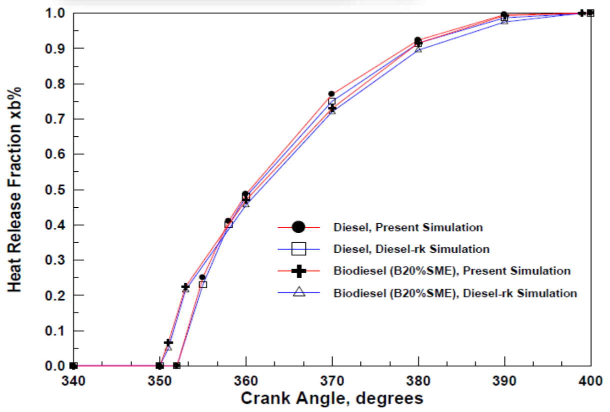

Fig. 4: Fraction Of Heat Release For Diesel And Biodiesel

Figure 4 presents the computed heat release fraction for diesel fuel and B20% SME. It is evident from this figure that biodiesel blend had an earlier start of combustion, but slower combustion rate. The early start of combustion was caused by the earlier start of injection and shorter ignition delay; and the slower premixed combustion rate due to less energy released in premixed phase and also probably the lower volatility of biodiesel. In the diffusion combustion phases, the SME biodiesel fuels had rapid combustion as at this point most of fuels get vaporized. Both fuels come in the same behaviour like the computed results in Diesel-rk software.

V. CONCLUSION

The overall analysis show that the mathematical model can be developed using Quick basic computer program for analyzing the combustion and performance characteristics in DI diesel engine. It has been seen that the equation of combustion can been developed in such way that it can be used for characterizing any hydrocarbon fuels and their blends. This model predicted the engine performance characteristics in close approximation to that of simulation results hence, the developed mathematical model is suitable for the prediction of the combustion and performance characteristics of the C.I engine and further work is required for modeling engine emissions. The combustion and performance results for B20% (by mass) showed approximately the same results for diesel fuel so that it is a suitable alternative fuel for diesel. Higher heat release rate and peak pressure is obtained with diesel than biodiesel. This is because of lower heating value and higher viscosity.

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