INTERNATIONAL JOURNAL OF
ENERGY AND ENVIRONMENT

Volume 4, Issue 2, 2013 pp.231-242
Journal homepage: www.IJEE.IEEFoundation.org

Theoretical modeling of combustion characteristics and performance parameters of biodiesel in DI diesel engine with variable compression ratio

Mohamed F. Al-Dawody, S. K. Bhatti

Department of Mechanical Engineering, Andhra University, India.

Abstract
Increasing of costly and depleting fossil fuels are prompting researchers to use edible as well as non-edible vegetable oils as a promising alternative to petro-diesel fuels. A comprehensive computer code using "Quick basic" language was developed for the diesel engine cycle to study the combustion and performance characteristics of a single cylinder, four stroke, direct injection diesel engine with variable compression ratio. The engine operates on diesel fuel and 20% (mass basis) of biodiesel (derived from soybean oil) blended with diesel. Combustion characteristics such as cylinder pressure, heat release fraction, heat transfer and performance characteristics such as brake power; and brake specific fuel consumption (BSFC) 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. The computed results are validated through the results obtained in the simulation Diesel-rk software.

Keywords: Biodiesel; Combustion parameters; Engine performance; Soybean methyl ester.

1. 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 [1]. 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 [2]. 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,[3]. 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 [4-6].

2. Physical properties of fuels

The properties of the diesel and Soybean methyl ester (SME) biodiesel are necessary as input data for the calculation of combustion parameters and heat release rates. Table 1 presents the properties of Diesel fuel and Biodiesel (SME). 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.

Table 1. Properties of diesel fuel and SME biodiesel [7]

Properties	Diesel	B20%	B100%
Density [kg/m^3]	830	841	876
Viscosity [Pa.s]	0.003	0.00334	0.00463
Flash point [C^o]	55	80	170
Cetane number	48	48.69	51.3
Lower heating value [MJ/kg]	42.5	41.18	36.22

Table 2. Specification of engine [7]

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

3. Theoretical analysis

The present work involves the using of diesel and B20% biodiesel fuels in a diesel engine with variable compression ratio (12-19). The simulation results are validated and compared with the results computed in the simulation software Diesel-rk. In this analysis the molecular formula for diesel and biodiesel are approximate, as $C_{13.77}H_{23.44}$ and $C_{19}H_{35}O_2$ respectively [8, 9]. The combustion model is developed for the C.I engine and suitable for any hydrocarbon fuel and their blends. During the start of combustion, the moles of different species are considered includes O_2, N_2 from the intake air and CO_2 and H_2O from the residual gases. The overall combustion equation considered for the fuel with C-H-O-N is:

$$(1-\lambda).C_{n1}H_{m1} + \lambda.C_{n2}H_{m2}O_Z + X\left[O_2 + 3.76N_2\right] \rightarrow \upsilon_1 CO_2 + \upsilon_2 H_2O + \upsilon_3 N_2 + \upsilon_4 O \quad (1)$$

where: λ mole ratio of biodiesel added, n_1, m_1 number of carbon and hydrogen atoms for diesel fuel respectively, n_2, m_2, z number of carbon, hydrogen and oxygen for biodiesel fuel respectively, υ mole fraction of product species, *X* number of kmoles of oxygen per one kmole of fuel and its equal to:

$$X = \left(\frac{1}{\phi}\right) * \left[n_1(1-\lambda) + n_2\lambda\right] + \frac{\left[m_1(1-\lambda) + m_2\lambda\right]}{4} - 0.5z.\lambda \quad (2)$$

where ϕ equivalence ratio

The total number of reactants and products during the start of combustion as well as every degree crank angle was calculated from the equations:

$$N_r = 1 + X * 4.76 \quad (3)$$

$$N_p = \left(\lambda.n_1 + (1-\lambda).n_2\right) + 0.5 * \left(\lambda.m_1 + (1-\lambda).m_2\right) + 3.76 * X + (\phi - 1) * \left[n_1(1-\lambda) + n_2\lambda\right] + \frac{\left[m_1(1-\lambda) + m_2\lambda\right]}{4} - 0.5z.\lambda \tag{4}$$

3.1 Volume of cylinder

The cylinder volume at any crank angle is given by [10]:

$$V(\theta) = V_{disp}\left[\frac{\varepsilon}{\varepsilon - 1} - \frac{1 - COS(\theta)}{2} + \frac{L}{S} - 0.5\sqrt{\left(\frac{2L}{S}\right)^2 - SIN^2(\theta)}\right] \tag{5}$$

where V_{disp} displacement volume (m^3), ε compression ratio, *L* connection rod length (m), *S* stroke (m)

3.2 Calculation of specific heat

The specific heat at constant volume and constant pressure for each species is in kJ/kg.K and calculated using the expression given below [9]:

$$Cv(T) = Cp(T) - R \tag{6}$$

$$Cp(T) = b + \frac{c}{T} \tag{7}$$

where *b* and *c* are the coefficients of polynomial equation and R gas constant (kJ/kg.K).

3.3 Pressure and temperature during compression

The initial pressure and temperature at the beginning of the compression process is calculated as follows;

$$P_2 = \left(\frac{V_1}{V_2}\right) \times \left(\frac{T_2}{T_1}\right) \times P_1 \tag{8}$$

$$T_2 = T_1 \frac{R}{\varepsilon^{Cv(T_1)}} \tag{9}$$

3.4 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.

$$H(T) = a + b * T + c * \ln(T) \tag{10}$$

The internal energy for each species and overall internal energy are calculated from the expressions given below [10]:

$$U(T) = a + (b - R) * T + c * \ln(T) \tag{11}$$

$$U(T) = \sum \left(x_i U_i(T)\right) \tag{12}$$

where *a, b, c* are the coefficients of polynomial equation.

3.5 Heat transfer model

The gas-wall heat transfer is found out using Woschni heat transfer model [11].

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

where h_c heat transfer coefficient (w/m2K), A_c convection heat transfer area (m^2), T_g & T_w gas and wall temperature respectively (K^o)
For convection Woschni developed the following empirical correlations for Nusselt number;

$$Nu_s = 0.035 R_e^{0.8} \tag{14}$$

where R_e 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;

$$w = \left[C_1 u_p + C_2 \left(\frac{V_{disp}}{V_{cyl}} \right) . \left(\frac{p(\theta) - p_{motor}(\theta)}{P_{cyl}} \right) \right] . T \tag{17}$$

where C_1 and C_2 are model constant, which specified as
For gas exchange period: C_1=6.18; C_2=0
For compression period: C1=2.28; C_1=0
For the combustion and expansion period: C_1=6.18; C_2=3.24*10^{-3}
u_p average piston speed (m/s), P_{cyl} pressure of cylinder at initial condition (bar).

3.6 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 Q_{in} Total heat supply (kJ/kg).
To find the correct value of T_2, 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 T_2 has been established, otherwise a new value of T is calculated for new internal energy and C_V values.

$$ERR_2 = C_V\left(T_2\right) * N_p \tag{20}$$

Using Newton Raphson method to get;

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

3.7 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 [12]. The Wiebe function is often used as a parameterization of the mass fraction burned and it has the following form;

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

And the burn rate is given by its differential form:

$$\frac{dx_b(\theta)}{d\theta} = \frac{a(m+1)}{\Delta\theta}.\left(\frac{\theta-\theta_{ig}}{\Delta\theta}\right)^m .e^{-a.\left(\frac{\theta-\theta_{ig}}{\Delta\theta}\right)^{m+1}} \tag{23}$$

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_{ig} crank angle at which combustion starts (degrees) and $\Delta\theta$ total combustion duration (degrees).

The absolute value of the heat release rate is given by the fuel mass m_f, the heating value of fuel q_{HV} and combustion efficiency η_c as [12];

$$\frac{dQ_{ch}}{d\theta} = m_f .q_{HV} .\eta_c \frac{dx_b}{d\theta} \tag{24}$$

3.8 Two-zone mean temperature model

A two-zone model is divided into two zones; one containing the unburned gases, and the other containing the burned gases separated by the flame front. Prior to start of combustion (SOC), the unburned zone temperature T_u equals to the single zone temperature. The unburned zone temperature after the start of combustion is then computed assuming adiabatic compression of the unburned charge according to:

$$T_u = T_{SOC}\left(\frac{p}{p_{SOC}}\right)^{\frac{\gamma-1}{\gamma}} \tag{25}$$

where T_{SOC} & P_{SOC} temperature and pressure at the start of combustion respectively.

The energy balance between single-zone and two-zone model yields:

$$\left(m_b + m_u\right)Cv.T = m_b Cv_b T_b + m_u Cv_u T_u \tag{26}$$

Assuming $Cv = Cv_b = Cv_u$ a calorically perfect gas, end up in

$$T = \frac{m_b T_b + m_u T_u}{m_b + m_u} = x_b T_b + (1 - x_b).T_u \tag{27}$$

where the single zone temperature T which is found from the equation of state can be used as the mass weighted mean temperature of the two zones [12].
From equation (26) we can calculate the burned zone temperature;

$$T_b = \frac{T - (1 - x_b)T_u}{x_b} \tag{28}$$

4. Diesel-rk simulation software

The software Diesel-rk is intended for the calculation and optimization of internal combustion engines. It has advanced RK-model of mixture formation and combustion in a diesel engine, and also the tool for multi parameter optimization [13]. Same operating conditions and fuel properties with engine specifications were used as input data to the software. The details of the computed results are mentioned in [7, 14].

5. Results and discussions

In this study combustion parameter like cylinder pressure, peak cylinder pressure, combustion zone temperature, ignition delay and heat release are discussed. Performance parameters like brake power, and brake specific fuel consumption are discussed with variable compression ratio from 12 to 19, constant engine speed 1500 rpm and 20^{o} BTDC injection timing.

5.1 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. 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 [14]. 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 [7].

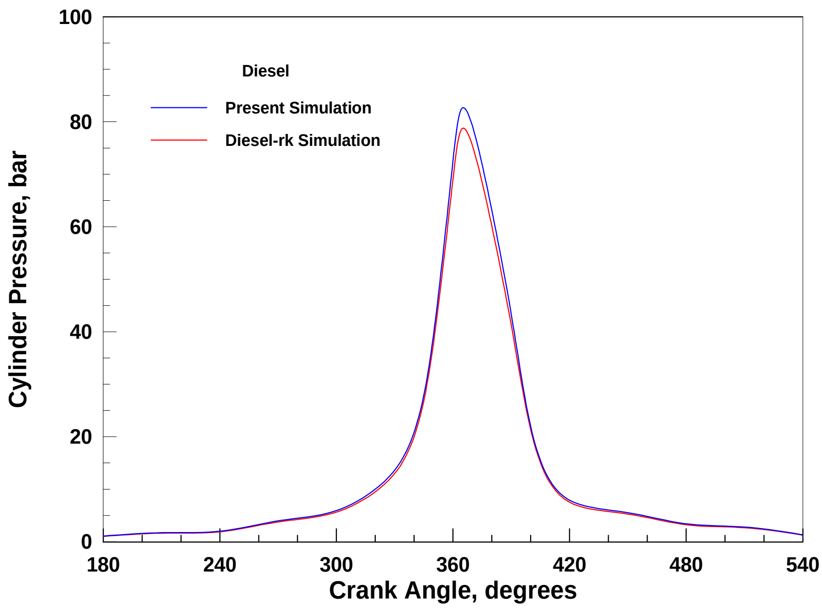

Figure 1. Variation of cylinder pressure with crank angle for diesel

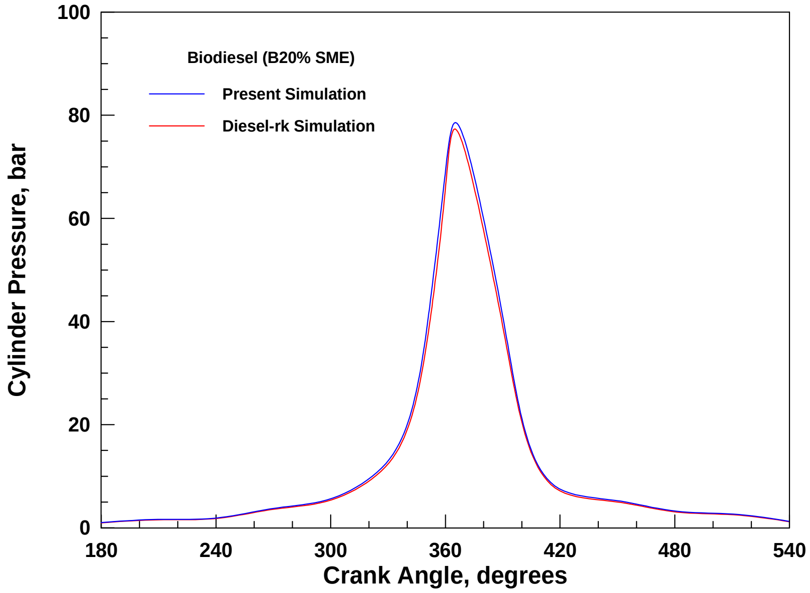

Figure 2. Variation of cylinder pressure with crank angle for B20% SME

5.2 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 [15, 16]. Thus, the peak temperature of biodiesel-fueled engine is higher than that of diesel fueled engine by 1.5 %. The results of both fuels are verified with the results computed in Diesel-rk at the same operating conditions.

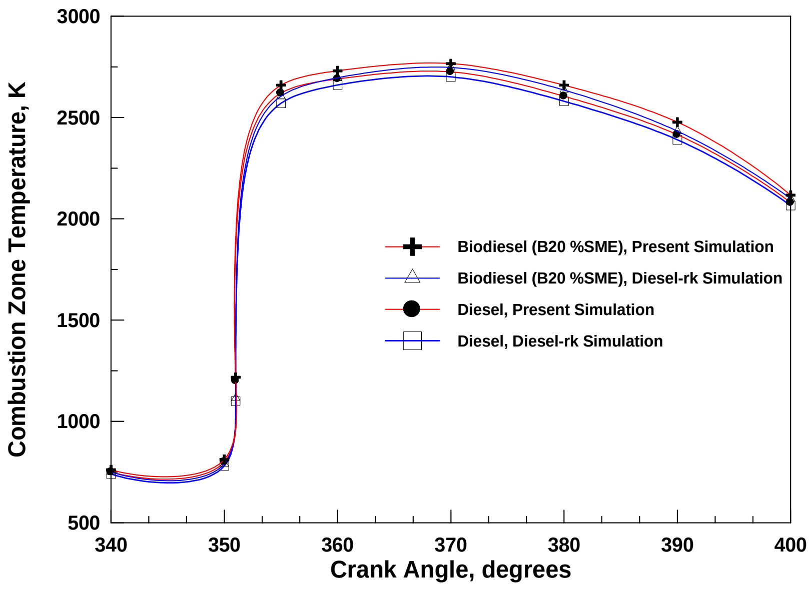

Figure 3. Combustion zone temperature for diesel and SME biodiesel

5.3 Heat release rate

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 behavior like the computed results in Diesel-rk software.

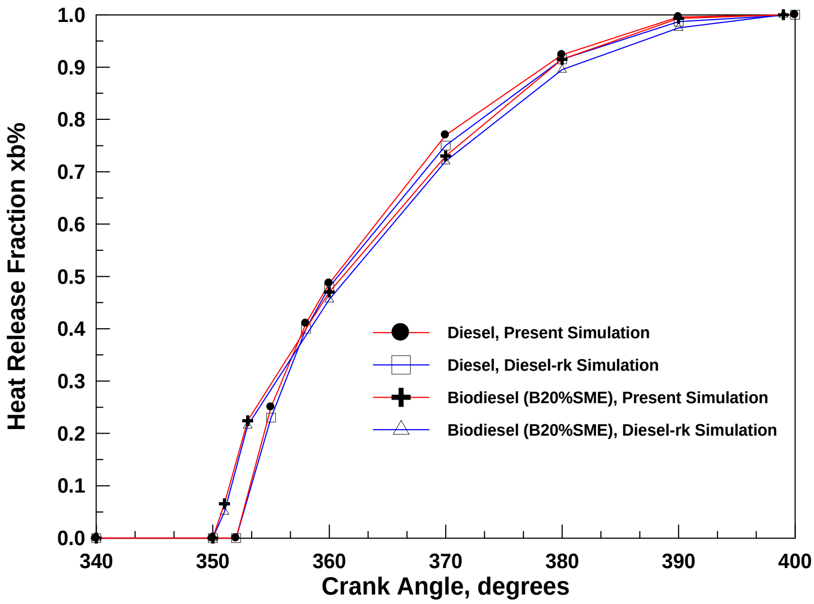

Figure 4. Fraction of heat release for diesel and biodiesel

5.4 Parametric study

The results of combustion characteristics and performance parameters are presented with variable compression ratio started from 12 up to19 for both diesel and B20 % biodiesel respectively.

5.4.1 Maximum pressure

The effect of compression ratio on the maximum pressure for both diesel and biodiesel is present in Figure 5. It can be observed that maximum pressure increase with the increase in compression ratio due to increase in the rate of heat release. The maximum pressure for diesel is higher than the maximum pressure of biodiesel by 1.76%, while it's come up with 1.47% in the results of Diesel-rk.

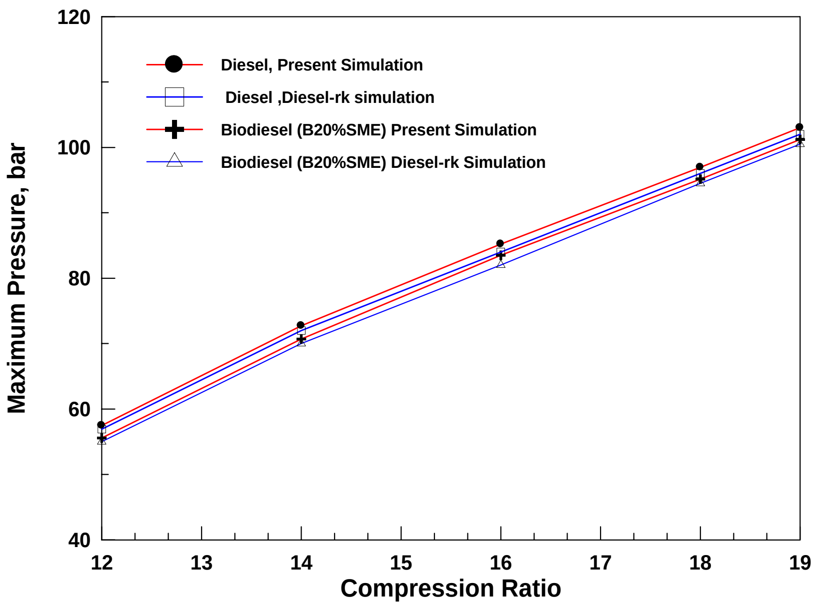

Figure 5. Effect of compression ratio on the maximum pressure

5.4.2 Ignition delay

The delay period can be defined as the time difference between the start of combustion and start of injection. The physical and chemical properties of the fuels will affect the ignition delay period, and researchers have stressed that chemical properties are much more important than physical properties [17].

The ignition quality of a fuel is usually characterized by its cetane number. A higher cetane number generally means shorter ignition delay. So blends of SME biodiesel cause shorter ignition delay which causes earlier start of combustion, and less energy released in premixed phase. The same results were reported by [18]. It can be observed from Figure 6 that ignition delay for B20% SME is lower than diesel fuel by 17.6%, while 18% is detected in the results of Diesel-rk [7].

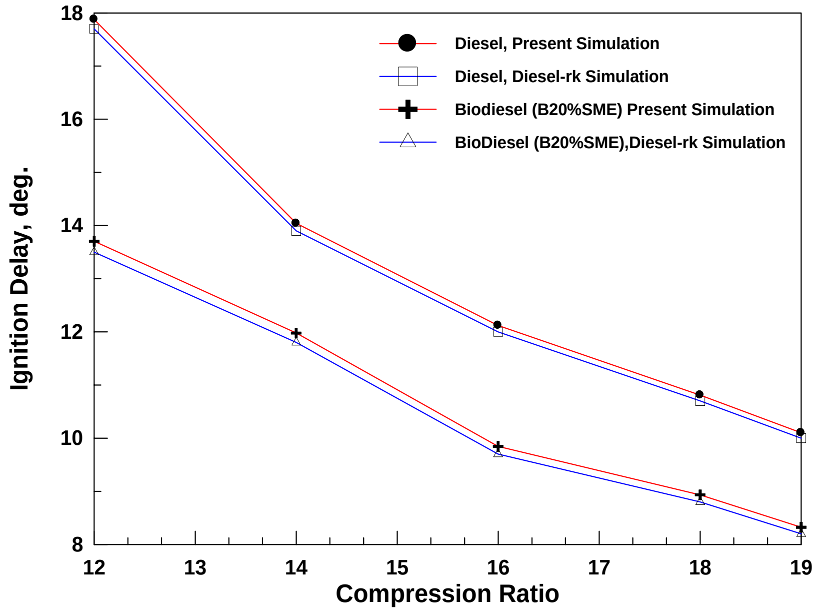

Figure 6. Effect of compression ratio on ignition delay

5.4.3 Total heat transfer

The Woschni heat transfer model was used to predict the engine heat transfer. The variation of the engine heat transfer rate with variable compression ratio is shown in Figure 7.

It can be seen that as compression ratio increased, the heat transfer rate increased due to increase in the cylinder pressure and temperature hence more heat rejected through cylinder walls. The heat transfer for B20% SME is higher that of diesel fuel by 2%, hence higher brake thermal efficiency expected for diesel fuel.

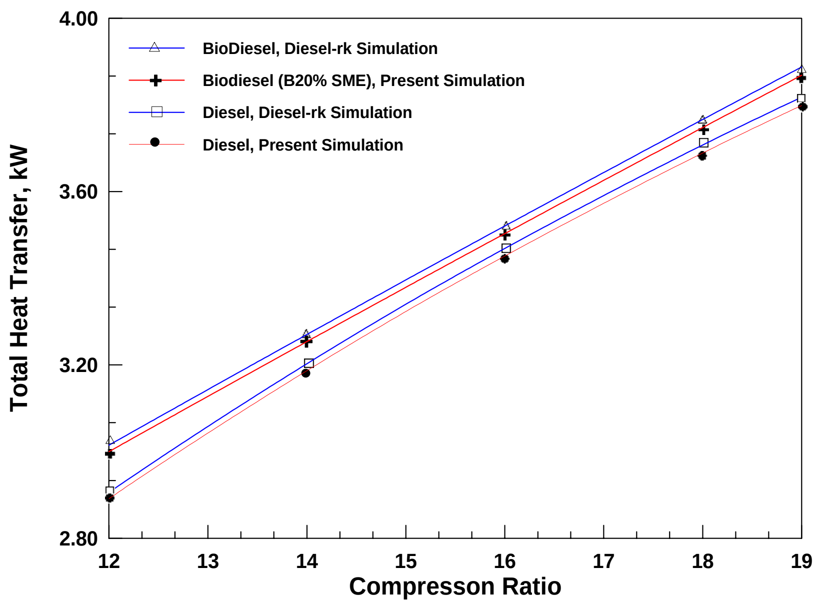

Figure 7. Effect of compression ratio on the heat transfer rate

5.4.4 Brake power and brake specific fuel consumption (BSFC)

The variation of brake power & BSFC with pure diesel and 20% SME biodiesel with different compression ratios are presented in Figures 8, 9 respectively, as the compression ratio increasing there is a decrease in the engine power due to an increase in the load and thermal stresses on the engine, which causes an increase in the BSFC. The engine power for B20% SME was less than that of pure diesel by 3 %. This is due to lower heating value of biodiesel fuel compared to diesel fuel.

On the other hand the BSFC, in general, was found to increase with the increasing proportion of biodiesel in the fuels. BSFC for all SME blending fuels is higher than pure diesel fuel by 12% because of the presence of oxygen in its molecule. The increase in BSFC is due to higher density and lower heating value, since the methyl esters have heating values that are about 12.4% less than pure diesel. These results are similar to those of Monyem A. [19] & Canakci M. [20] & Mustafa Canakci and Jon H. Van Gerpen [21]. The simulation results are validated with the Diesel-rk results.

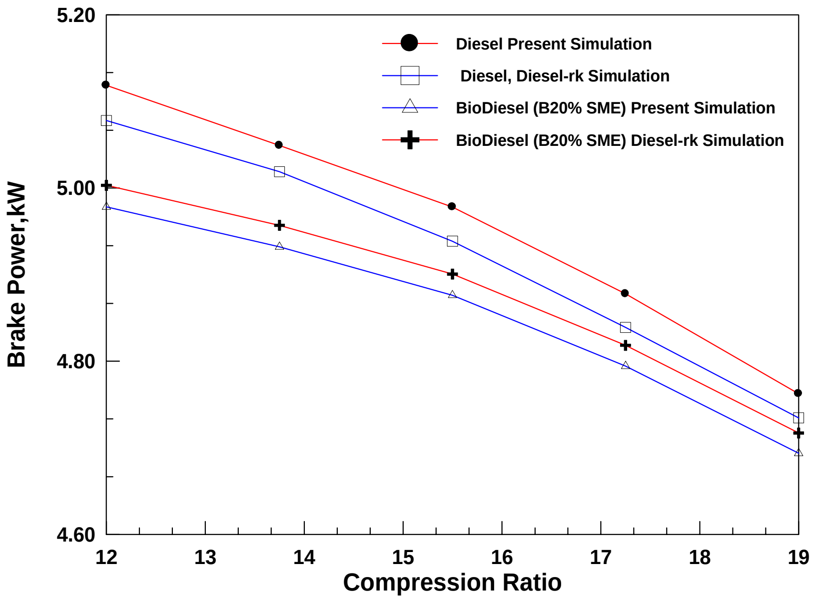

Figure 8. Effect of compression ratio on the brake power

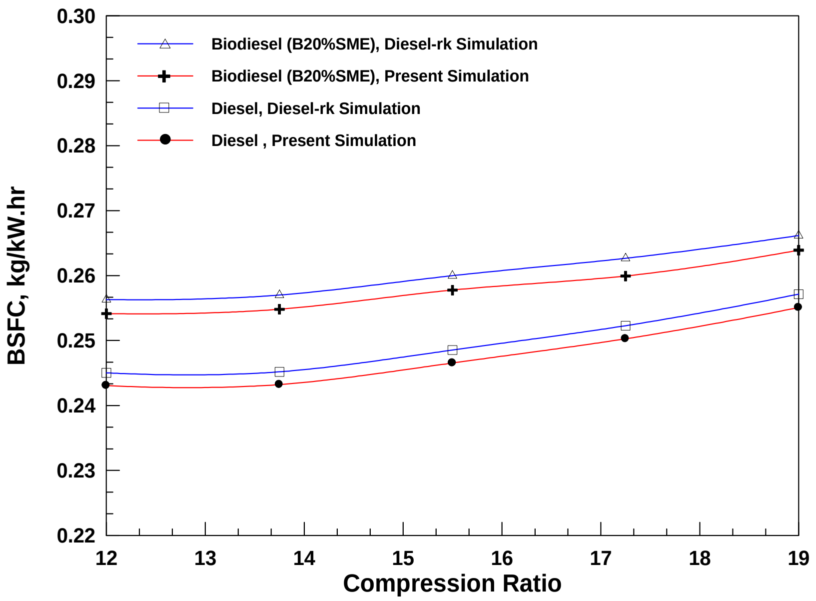

Figure 9. Effect of compression ratio on the BSFC

6. Conclusion

A mathematical model was developed using a Quick basic computer program for analyzing the combustion and performance characteristics in DI diesel engine with variable compression ratio. The equation of combustion has 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 obtained by Diesel-rk software 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) SME showed approximately the same results for diesel fuel so that it is a suitable alternative fuel for diesel. Biodiesel B20 % had an earlier start of combustion, slower combustion rate. The early start of combustion was caused by the earlier start of injection and shorter ignition delay. Using the B20% SME was found to reduce the brake power by 3%, and increase BSFC by 2% as compared to pure diesel fuel. This is due to the lower heating value of biodiesel compared to diesel fuel. In addition higher overall cylinder temperatures were found for B20% biodiesel compared to diesel fuel, which is one of the reasons for higher NOx emissions.

References

[1] Sunil Kumar, A. Chaube S.Kumar “Experimental evaluation of C.I. engine performance using diesel blended with Jatropha biodiesel”, international journal of energy and environment volume 3, issue 3, 2012 pp.471-484.
[2] B. Gokalp, E. Buyukkaya, H.S. Soyhan, ‘Performance and emissions of a diesel tractor engine fueled with marine diesel and soybean methyl ester’, International journal of biomass and bioenergy, (2011), 3575-3583.
[3] Cengiz Oner and Sehmus Altun, “Biodiesel production from inedible animal tallow and an experimental investigation of its use as alternative fuel in a direct injection diesel engine”, journal of applied energy, 2009.
[4] B.Rajendra P.Tamilporai, Mohd.F.Shabir, “Simulation and Analysis of Combustion Performance and Emission Characteristics of Biodiesel Fueled Low Heat Rejection Direct Injection Diesel Engine”, SAE Paper No. 2007-32-0094.
[5] Mohd.F.Shabir, Tamilporai P., and Rajendra Prasath, ‘Analysis of Combustion, Performance and Emission Characteristics of Turbocharged LHR Extended Expansion DI Diesel Engine’, International Journal of Mechanical Systems Science and Engineering, Vol. 2, No. 2, pp. 126-137, 2010.
[6] V. Ganesan, “Computer simulation of compression ignition engines”, University Press (India) Ltd.; 2000.
[7] Mohamed F. Al-Dawody, S.K. Bhatti, Effect of soybean oil biofuel blending on the performance and emissions of diesel engine using diesel-rk software, International journal of engineering science and technology, 4539-4555, (2011).
[8] A.S. Ramadhas_, S. Jayaraj, C. Muraleedharan, “Theoretical modeling and experimental studies on biodiesel-fueled engine”, Renewable Energy 31, 1813–1826. 2006.
[9] B. Rajendra, P. Tamil ,Mohd. F. Shabir,’ Two-zone modeling of diesel/biodiesel blended fuel operated ceramic coated direct injection diesel engine’, International journal of energy and environment, volume 1, Issue 6, pp.1039-1056, 2010.
[10] J.B. Heywood, “Internal combustion engines fundamentals”,Tata McGraw Hill Book Company; 1989.
[11] Woschni, G., "A Universally Applicable Equation for the Instantaneous Heat Transfer Coefficient in the Internal Combustion Engine", SAE Paper No.670931, 1967.
[12] Marcus K.,’ A specific heat ratio model and compression ratio estimation’, Linkoping studies in science and technology, thesis no.1104, 2004.
[13] Http://www.diesel-rk.bmstu.ru.
[14] Mohamed F. Al-Dawody, S.K. Bhatti, ‘Simulation and optimazation study for the reduction of Nox emissions of diesel engine working with soybean oil biofuel blendings using diesel-rk software’,27th national convention of chemical engineering, September 30 - October 01, 2011.
[15] A. N. Ozsezen, M. Canakci, ‘Determination of performance and combustion characteristics of a dieselengine fueled with canola and waste palm oil methyl esters’, Int. journal of Energy Conversion and Management, volume.52, 108-116, (2011).

[16] D.Tamilvendhan “performance, emission and combustion characteristics of a methyl ester sunflower oil eucalyptus oil in a single cylinder air cooled and direct injection diesel engine”, International Journal of Engineering Science and Technology, Vol. 3 No. 3 March 2011.
[17] V.Ganesan,’Internal combustion Engines’, published by Tata McGraw hill education private limited, 2007.
[18] W. Yuan, A. Hansen, ‘Computational investigation of the effect of biodiesel fuel properties on diesel engine NOx emissions’, Int J Agric & Biol Eng, June,2009.
[19] Monyem, A.“The effect of biodiesel oxidation on engine performance and emissions”. Ph.D. Dissertation, Department of Mechanical Engineering, Iowa State University, Ames, IA, 1998.
[20] Canakci M. ‘Combustion characteristics of a turbocharged DI compression ignition engine fueled with petroleum diesel fuels and biodiesel’’. Bioresour Technol;98:1167–75.,2007.
[21] Mustafa Canakci and Jon H. Van Gerpen, “Comparison of Engine Performance and Emissions for Petroleum Diesel Fuel, Yellow Grease Biodiesel, and Soybean Oil Biodiesel”, Presented as Paper No. 016050 at the 2001 ASAE California, USA July 30-August 1, 2001.

Mohamed F. Al-Dawody is currently working as Research Scholar, Department of Mechanical Engineering, College of Engineering (A), Andhra University, Visakhapatnam, A.P. India He has completed M.Sc in (Power Mechanic) from University of Babylon, Iraq in the year 2006 and B.Sc in (Mechanic) from university of Babylon, Iraq in the year 2002. His research interest in energy and thermal engineering with special interest on alternative fuels and renewable energy. Currently he is doing his research in the field of using biodiesel blending in diesel engine. He has published 12 papers in International / National Journals and Conferences.
E-mail address: rukia612010@gmail.com, Tel: +91-8179439404

S. K. Bhatti is presently working as Professor in the Department of Mechanical Engineering, College of Engineering (A), Andhra University, Visakhapatnam, A.P., India. She has completed her PhD in Heat Transfer and energy systems from Andhra University, India. Her research interest in Energy and Thermal Engineering. She contributed more than 30 papers in International / National Journals and Conferences.
E-mail address: sukhvinder_bhatti@yahoo.com, Tel:+91-9848312427