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Prediction of an Optimum Biodiesel-Diesel Blended Fuel for Compression Ignition Engine Using GT-Power

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Abstract

This paper describes the development of a turbocharged direct-injection compression ignition (CI) engine model using fluid-dynamic engine simulation codes through a simulating tool known as GT Power. The model was first fueled with diesel, and then with various blends of biodiesel and diesel by allotting suitable parameters to predict an optimum blended fuel. During the optimization, main focus was on the engine performance, combustion, and one of the major regulated gaseous pollutants known as oxides of nitrogen (NO_x). The combustion parameters such as Premix Duration (D_P), Main Duration (D_M), Premix Fraction (F_P), Main Exponent (E_M) and ignition delay (ID) affect the start of injection (SOI) angle, and thus played significant role in the prediction of optimum blended fuel. The SOI angle ranging from 5.2 to 5.7 degree crank angle (DCA) measured before top dead center (TDC) revealed an optimum biodiesel-diesel blend known as B20 (20% biodiesel and 80% diesel by volume). B20 exhibited the minimum possible NO_x emissions, better combustion and acceptable engine performance. Moreover, experiments were performed to validate the simulated results by fueling the engine with B20 fuel and operating it on AC electrical dynamometer. Both the experimental and simulated results were in good agreement revealing maximum deviations of only 3%, 3.4%, 4.2%, and 5.1% for NO_x, maximum combustion pressure (MCP), engine brake power (BP), and brake specific fuel consumption (BSFC), respectively. Meanwhile, a positive correlation was found between MCP and NO_x showing that both the parameters are higher at lower speeds, relative to higher engine speeds.

Key Words: *Diesel engine, biodiesel, exhaust emissions, simulation, performance, GT-Power*

Nomenclature

CI	compression ignition
NO_x	nitrogen oxides
NO	nitric oxide
THC	total hydro carbons
CO	carbon monoxide
PM	particulate matter
D_P	premix duration
D_M	main duration
D_T	tail duration
F_P	premix fraction
F_T	tail fraction
F_M	main fraction
E_P	premix exponent
E_M	main exponent
E_T	tail exponent
WC_P	wiebe premix constant
WC_M	wiebe main constant
WC_T	wiebe tail constant
CE	combustion efficiency
EGR	exhaust gas recirculation
CLD	chemi-luminescent
WOT	wide open throttle
ID	ignition delay
SOI	start of injection
DCA	degree crank angle
TDC	top dead center
MCP	maximum combustion pressure
BP	brake power
BSFC	brake specific fuel consumption
MRPR	maximum rate of pressure rise

1. Introduction

Biodiesel, consisting of alkyl monoester of fatty acids from vegetable oils or animal fats, is gaining considerable attentions as an alternative fuel for CI engine on account of its better physicochemical properties and flexibility to be used either in neat or in blended form. It has the potential to alleviate the pollutants such as total hydrocarbons (THC), carbon monoxide (CO), particulate matter (PM) and smoke [1-3]. NO_x emissions, however, are increased when CI engine is fueled with neat biodiesel owing to improved combustion efficiency caused by higher MCP and temperature [3-5].

NO_x are considered as an important class of regulated pollutants resulted from the reaction of nitrogen with the atomic oxygen [6]. These are, generally, formed during the initial phase of rapid burning when there is a tremendous rise in temperature inside the combustion chamber of engine [7]. Thermal or Zeldovich mechanism based on three reactions produces nitric oxide (NO) in the presence of high temperature burned gases left behind by the flame front, and is given by the following three chemical equations [8]:

$$O + N_2 \leftrightarrow NO + N$$
$$N + O_2 \leftrightarrow NO + O$$
$$N + OH \leftrightarrow NO + H$$

The first reaction in which nitrogen is dissociated by an oxygen atom is an endothermic reaction and is also called controlling reaction because it controls the system. In the second reaction, a nitrogen atom reacts exothermically with an oxygen molecule to give NO and atomic oxygen. The third reaction is also an exothermic reaction in which a nitrogen atom reacts with hydroxide radical to from NO and a hydrogen atom.

In previous research [3, 9], the authors have reported the decrease in CO, THC and smoke, but increase in NO_x emissions from an unmodified CI engine fueled with neat biodiesel. Moreover, the authors have also demonstrated an important technique to control NO_x emissions from CI engine fueled on neat biodiesel [6]. This technique is based on engine modification based on the retardation of SOI angle of a diesel engine fueled with neat biodiesel.

Current work, however, deals with the prediction of an optimum biodiesel-diesel blend to be used as an alternative fuel without any modifications in the engine hardware. But finding of such an optimum biodiesel-diesel blend is not only the time consuming process but also the wastage of resources. Consequently, a simulating tool known as GT-Power [10] is used to predict a fuel blend ratio very similar to commercial diesel in terms of NO_x pollutants and engine performance, but superior in combustion. Finally, the predicted results are verified experimentally by running the engine on a test bench in the control laboratory.

Biodiesel, inheriting oxygen content as shown in Table 2, promotes oxidation rate, and thus combustion process [9]. However, it possesses the lower calorific value (energy density), leading to an important fact that more fuel is required to maintain the same BP of the engine. Consequently, both BSFC and NO_x emissions are increased. Therefore it is imperative for a blend to have just enough oxygen content along with appropriate physicochemical properties to improve the combustion, keeping the NO_x pollutants within acceptable limits. In addition to this, it is also necessary for a fuel blend not to disturb the engine performance factors such as BP and BSFC when used as an alternative to petroleum diesel. This study will help to gain deep insight into the behavior of engine in terms of performance, combustion and NO_x emissions when fueled with a large variety of blends. Investigations of an optimal blend ratio among such a wide range of biodiesel-diesel blends have seldom been reported in the literature. To best of author’s knowledge, prediction of a suitable blend ratio based on the above discussed criteria using GT-Power tool has not been addressed so far.

2. Modeling and Simulations

The engine was modeled using GT Power-software recommended for the design and optimization of both spark ignition as well as CI engines with equal ease. It shortens not only the time involved in design cycle but also cuts down the cost of process. The engine components such as induction and exhaust valves, intake system, cylinder, inter cooler, compressor and turbine of turbocharger are built into the model with the aid of specific tools such as flow-splits, pipes, cylinder, environment, etc. In order to connect these components, connectors such as valves and orifices are used as shown in Fig. 1. The detailed discussions related to the simulation package have been reported in literature [11-12]. A brief introduction, however, is given here:

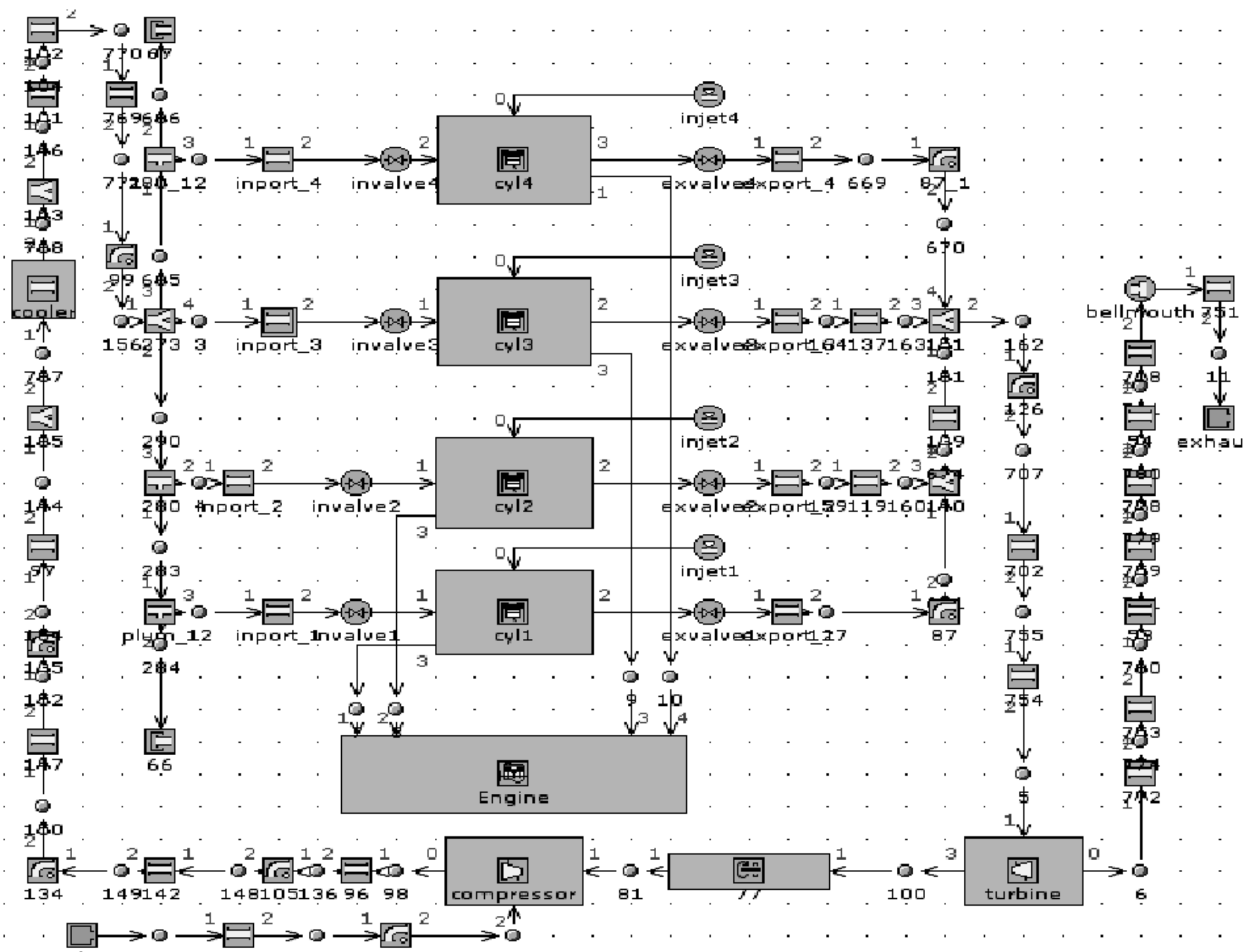

Fig. 1: Modeling of the engine using GT-Power

For the boundary conditions of pressure, temperature, and the mixture compositions of the intake and exhaust system an object ‘Env’ is used. The template ‘pipe’ is used to model the flow through tubes having constant as well as tapered diameters. In order to consider the effects of physical geometries of the pipes, friction multiplier, heat transfer multiplier, and pressure loss coefficients are adjusted in them. The template ‘EngCyliner’ is used for the object ‘cylinder’ designating the attributes of the engine cylinder such as bore, stroke, connecting rod length, compression ratio, heat transfer, combustion model, etc. The engine injection system is modeled using the template ‘InjProfileConn’. The attributes such as number of holes per nozzle, nozzle-hole diameter, etc. are assigned to model an injector. The template ‘EngineCrankTrain’ is used for the modeling of the component ‘Cranktrain or Engine’ wherein the attributes such as number of cylinders, configuration of cylinders, firing order, engine friction and cylinder geometry, etc. are assigned. GT-Power uses the Chen-Flynn model [13] to predict the engine friction. The software provides some combustion models like DI-Weib, Profile Combustion, and DI-Jet which are used for CI engines. It has the potential to consider turbo-charging, gas exchange, combustion, simple and complex heat release models for the turbocharger matching, thermal analysis, engine performance, exhaust emissions, etc.

In current work, in cylinder burn rate (cumulative) was predicted through Direct-Injection Diesel Weib Model (i.e. EngCylCombDIWeib) as follows [10]:

$$\begin{aligned} Combustion(\theta) = \\ &(CE)(F_P)[1-e^{-(WC_P)(\theta-SOI-ID)^{(E_P+1)}}]+ \\ &(CE)(F_M)[1-e^{-(WC_M)(\theta-SOI-ID)^{(E_M+1)}}]+ \\ &(CE)(F_T)[1-e^{-(WC_T)(\theta-SOI-ID)^{(E_T+1)}}] \end{aligned} \quad (1)$$

where 'θ' is the instantaneous crank angle, and WC_P, WC_M, and WC_T are Wiebe premix, Wiebe main, and Wiebe tail constants, respectively. These constants are defined as follows:

$$WC_P = \left[\frac{D_P}{2.302^{1/(E_P+1)} - 0.105^{1/(E_P+1)}}\right]^{-(E_P+1)} \quad (2)$$

$$WC_M = \left[\frac{D_M}{2.302^{1/(E_M+1)} - 0.105^{1/(E_M+1)}}\right]^{-(E_M+1)} \quad (3)$$

$$WC_T = \left[\frac{D_T}{2.302^{1/(E_T+1)} - 0.105^{1/(E_T+1)}}\right]^{-(E_T+1)} \quad (4)$$

In above equations (1–4), constants such as WC_P, WC_M, WC_T and F_M (Main fraction) are the calculated constants, while the inputs are given as:

SOI = start of injection; ID = ignition delay; D_P = premix duration; D_M = main duration; D_T = tail duration; F_P = premix fraction; F_T = tail fraction; E_P = premix exponent; E_M = main exponent; E_T = tail exponent; CE = combustion efficiency or fraction of fuel burned.

For the estimation of heat transfer in engine cylinder, the Woschni correlation [14] was used. In this model, the average gas velocity and heat transfer rate were increased with the increasing piston speed during the induction, compression and exhaust strokes of the engine. In case of turbocharger, the performance maps such as pressure ratios, rpm of the turbocharger shaft, air-mass flow rates and efficiencies required for the compressor and turbine were used as per data provided by the manufacturer.

The temperature and pressure were set equal to 295 K and 0.975 bar as the environment conditions (i.e. boundary conditions). The component "injector" was set as 'diesel (B00)' for the initial prediction of the model, and then subsequently B05, B10, B15, B20, B25, B30, and B50 for 5%, 10%, 15%, 20%, 25%, 30%, and 50% of biodiesel-diesel blends as per requirement.

Thus the fuel was specified on the basis of allotted attributes like density, viscosity, lower heating value, number of hydrogen, nitrogen, oxygen, and carbon atoms per molecule, etc. In compressor and turbine, standard models were selected in which pressure flags for the inlet and outlet conditions were 'total'. Efficiency pressure ratios were kept as 'same-as-map', and both of the efficiency as well as mass multipliers were set equal to 1. Moreover, reference temperature and pressure were 290 K, and 1.013 bar respectively, while maximum pressure ratio was set equal to 2.9. Maximum speed of the turbine was considered as 130000 rpm, as per manufacturer recommendations. The initial speed of the turbocharger shaft and mass moment of inertia about the axis of rotation were 100000 rpm and 1.211×10^{-5} kg.m^2, respectively.

2.1 Solution Procedure:

For the simulation, the factors which directly affect the in-cylinder pressure during the premix and main intervals were given due considerations. At first, the intake air was exhibiting higher pressure and temperature which were not showing any significant variations in the presence of intercooler. Consequently, it was necessary to correctly predict the heat transfer in the intercooler consisting of many thin tubes. Thus, the heat of exhaust pipe and its effect on the intake air pressure were investigated. This was, no doubt, a difficult task involving a large number of simulating steps and trials.

Initially, the model did not reveal much difference in the performance behavior when the only heat of exhaust pipe was considered, and hence heat exchange through the intercooler was natural. However, the D_p pressure was significantly dropped with the introduction of a large number of intercooler tubes, say 105. Further, the intake air pressure and temperature both were fallen from their initial readings indicating that the rate of heat transfer from the cooler was low at the beginning. Thus, the tubes of intercooler were increased to 125 (in steps), without varying the other parameters such as ID, SOI, D_M and D_P angles. After simulations, it was found that among a number of combustion parameters, heat exchange coefficient and D_M angle played a dominant role in the heat transfer. Further, the D_p angle was also varied from 4 to 9° in steps to investigate its impact on the combustions, performance and NO_x emissions, treating the other parameters as constants. Similarly, ID and SOI angles were also altered step by step to know their influence on the combustion model.

During the prediction of an optimum fuel blend ratio, a series of simulations were made using different values of D_P, D_M, F_P, E_M and ID in steps along with appropriate fuel attributes without changing the SOI angle.

3. Experimental Section

The engine used for the validation of the simulated results is a 4 cylinder inline diesel engine (Made in China) without exhaust gas recirculation (EGR) or any other pollutant control after-treatment units. The significant features of the engine are shown in Table 1. The engine was operated on a test bench in the control laboratory by coupling it through an AC Power electrical dynamometer, specified as $Dynas_3$ HT350 (Made in Germany). The schematic diagram of the test unit is given in Fig. 2.

Table 1: Engine Specifications

Parameter	Feature/Size
Engine Type	Diesel, 4-stroke, 4-cylinders in line
Fuel metering system	Direct injection with mechanical system
Air intake system	Turbocharged, inter-cooled
Valves	2 valves per cylinder
Capacity (cc)	4752
Bore (mm)	110
Stroke (mm)	125
Compression Ratio	16.8:1
Nozzle hole diameter (mm)	0.23
Number of nozzle holes	6
Max. Power (kW@r/min)	117@2300
Max. Torque (Nm@r/min)	580@1400

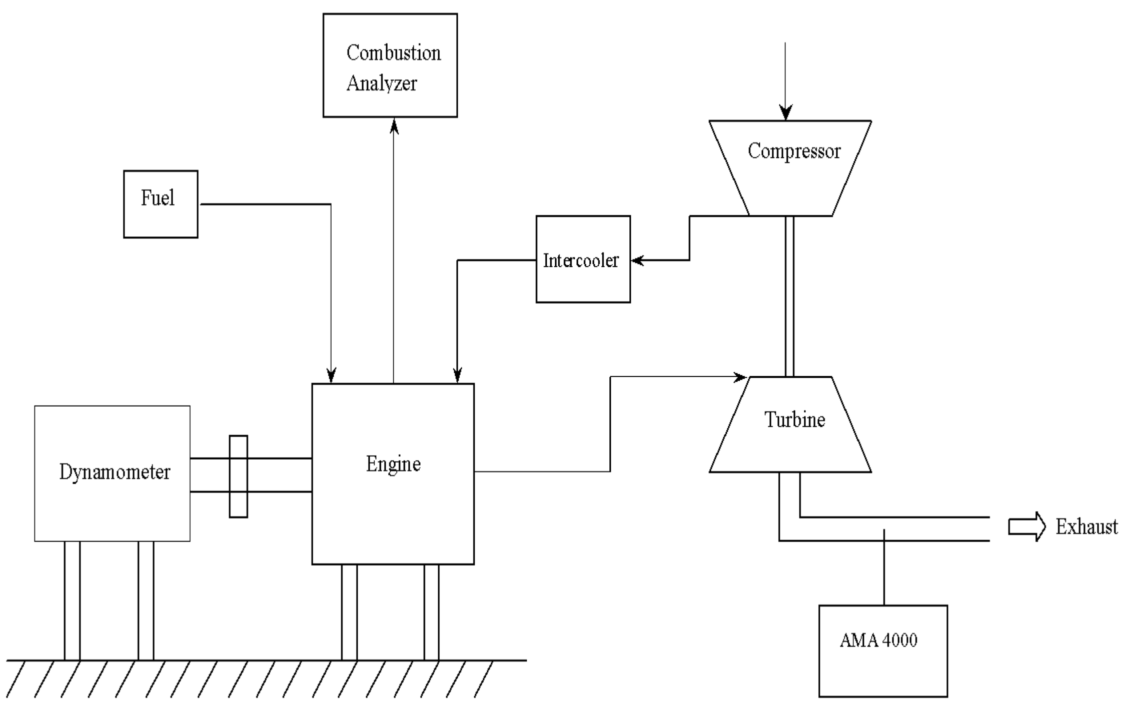

Fig. 2: Experimental setup.

In current study, biodiesel produced from waste cooking oil was provided by a well reputed laboratory situated in Beijing city (China). The petroleum diesel was purchased from a local fuel pump. The important properties of the both fuels are given in Table 2.

Table 2: Properties of Biodiesel and diesel fuels

Characteristics	Biodiesel	Diesel	Test Method*
Cetane index	60.1	52	GB/T 386-91
Sulfur content (mg/L)	25	264	SH/T 0253-92
Lower heating value (MJ/kg)	37.3	42.8	GB/T 384
Viscosity at 20 ºC (mm^2/s)	8.067	4.0	GB/T 265
Density (g/cm^3)	0.886	0.841	SH/T 0604
Carbon content (%)	76.83	87	SH/T 0656-98
Hydrogen content (%)	11.91	13	SH/T 0656-98
Oxygen content (%)	11.33	0	Element analysis

*Chinese standard

In order to measure the air flow and fuel consumption of the engine, Sensy-flow P (ABB Inc.) and PLU-4000 (Pier Berg) were used, respectively. The engine exhaust temperature was measured by using thermocouple (k-series), whereas the coolant and engine oil temperatures were sensed through sensors PT-100.

The engine was connected to the dynamometer through torque flange so that the torque, speed and throttle position can be measured by using the software (Automation System STARS Rev. 1.5). For the sensing of varying combustion pressures inside the cylinder and the top dead center (TDC) signal for the crank angle, piezo-electric sensors 6125B and 2613A (kistler) were used, respectively. Further, the TDC pulse of the crankshaft optical encoder and the signal output of the amplifier were known with the help of combustion analyzer Dewetron (DEWE-5000), and the data was finally analyzed using the software package (FlexProTM). The NO_x emissions were detected through chemi-luminescent detector (CLD) using an analytical package (AMA4000, Austria).

4. Results and Discussion

4.1 Optimum Blended Fuel

Figure 3 presents the trends of MCP, while Fig. 4 and Fig. 5 show the respective variations in NO_x emissions and SOI angles for various fuel blends simulated at different engine speeds. Figures 6 and 7, on the other hand, show the corresponding engine behavior in terms of brake power and BSFC. It is clear that SOI angle first increases with the increase in biodiesel percentage up to B20, and then gets decreased particularly from B25 to B50. This leads to an important finding that B20 is the maximum possible blended ratio, with minimum possible NO_x and acceptable performance. Thus, the model predicts 2.8% and 3.5% increase in NO_x and BSFC respectively, while only 3% decrease in brake power with B20. At this fuel blended level, SOI angle fluctuates from 5.2 to 5.7 DCA at different engine speeds. Although B25 shows almost similar trend in terms of SOI angle NO_x emissions during most of the speed modes, both combustion and performance results are not in favor of B25 to be considered as an optimum fuel.

The increasing and decreasing trends of SOI angle with the increase in biodiesel percentage are attributed mainly to Premix and Main durations, Premix fractions, Main exponents, and ID along with other parameters such as viscosity, density, bulk modulus, etc. of the fuels specified to the model. However, the influence of Tail duration, Tail fraction and Tail exponent on the model was nominal.

It is quite understandable that SOI angle is increased with increasing biodiesel percentage because higher viscosity of biodiesel plays an important role in the diminution of fuel losses during the injection and in the faster development of pressure [15]. Moreover, relative to commercial diesel higher density and less compressibility of biodiesel also help in the quicker growing of pressure in the injection system, with the consequence of earlier fuel-injection [9]. This earlier injection causes the increase in SOI angle to provide the required calorific value, and hence desired brake power of the engine.

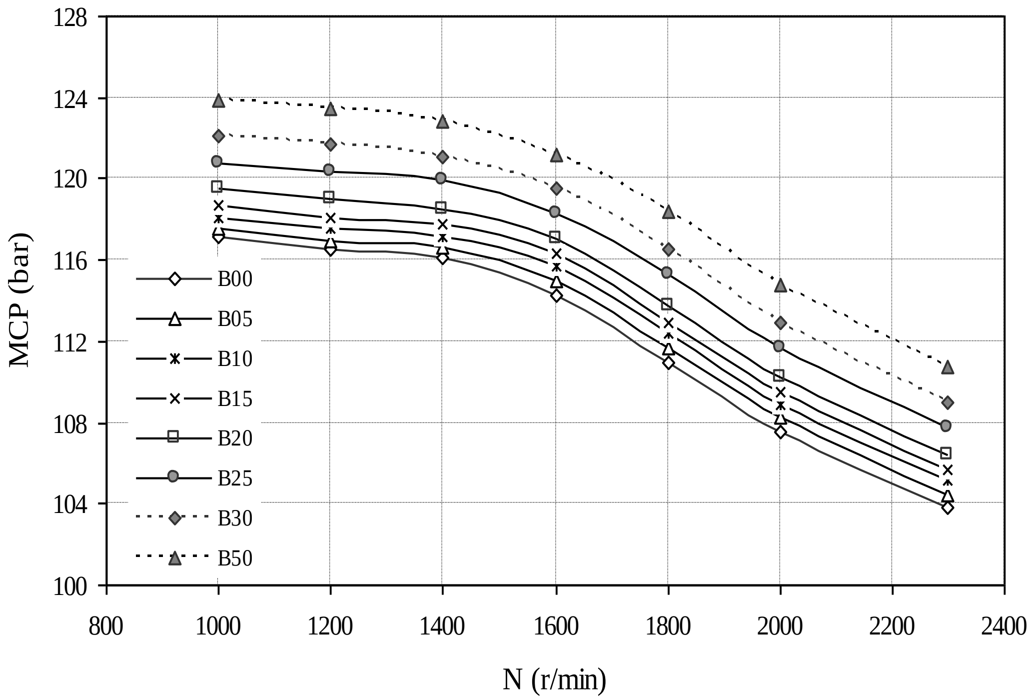

Fig.3 Trends of MCP at different speed modes for various fuel

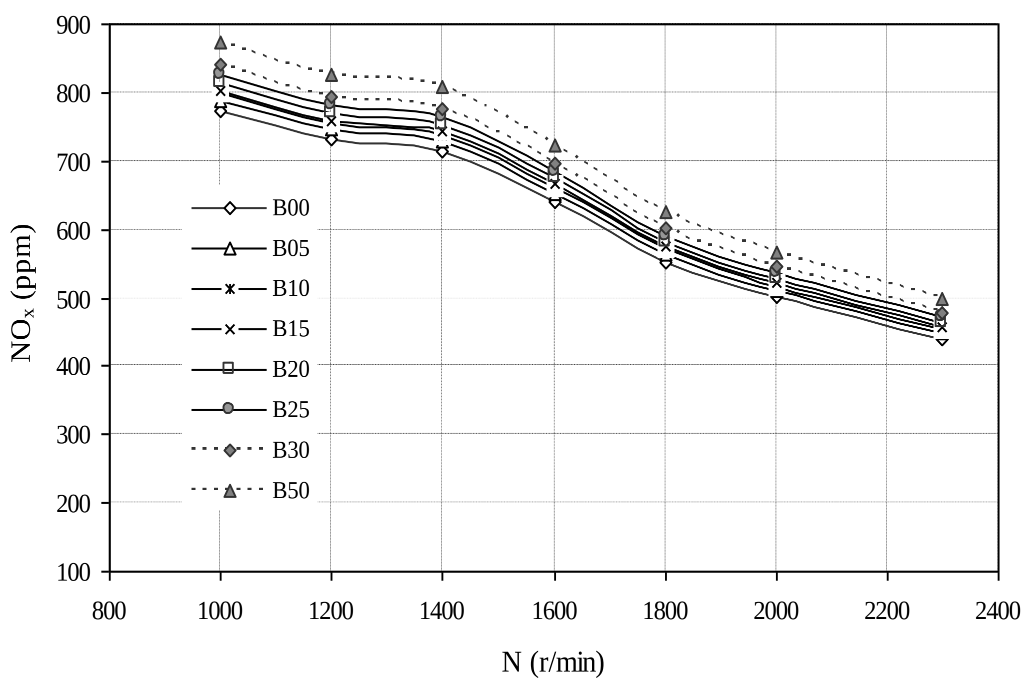

Fig.4 NO_x emissions at different speed modes for various biodiesel-diesel blends.

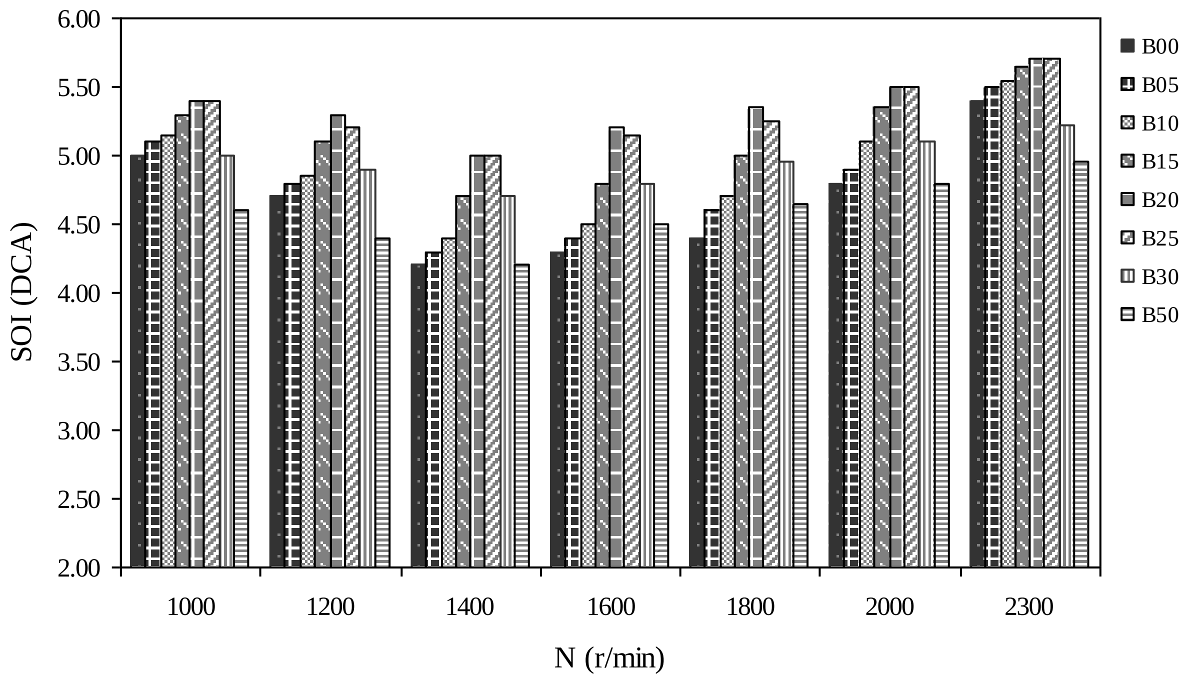

Fig. 5: **Simulated results of SOI angle for various fuel blends.**

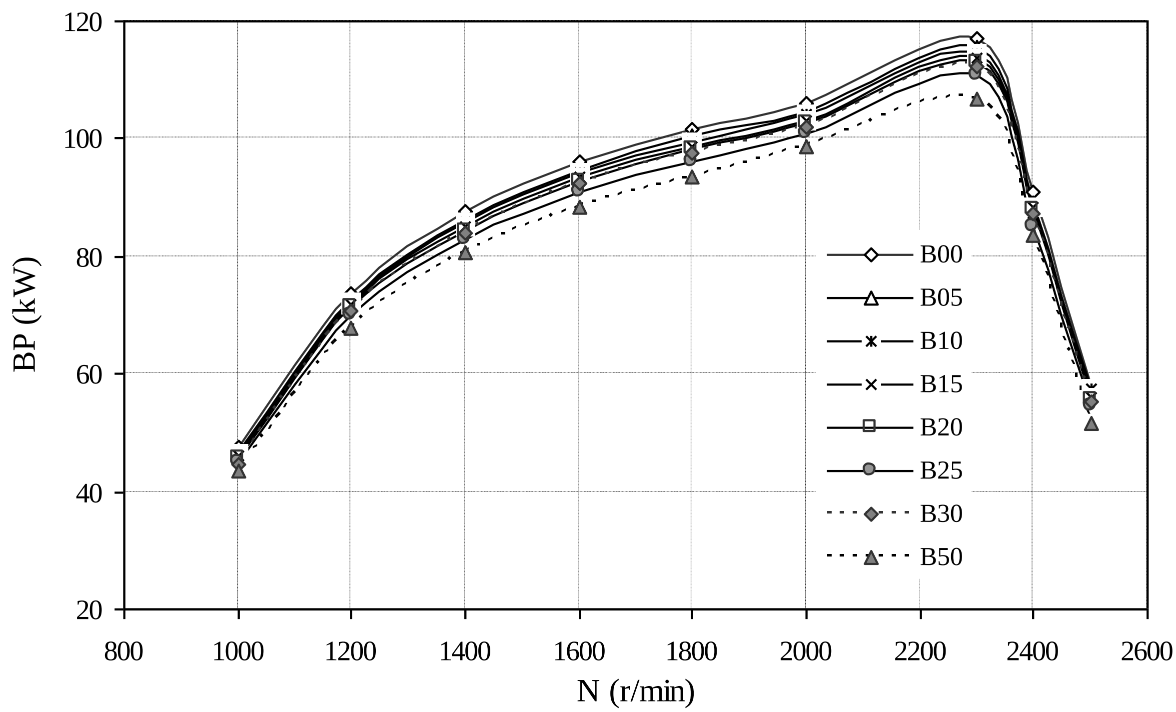

Fig. 6: **Variations of Brake Power for various fuel blends.**

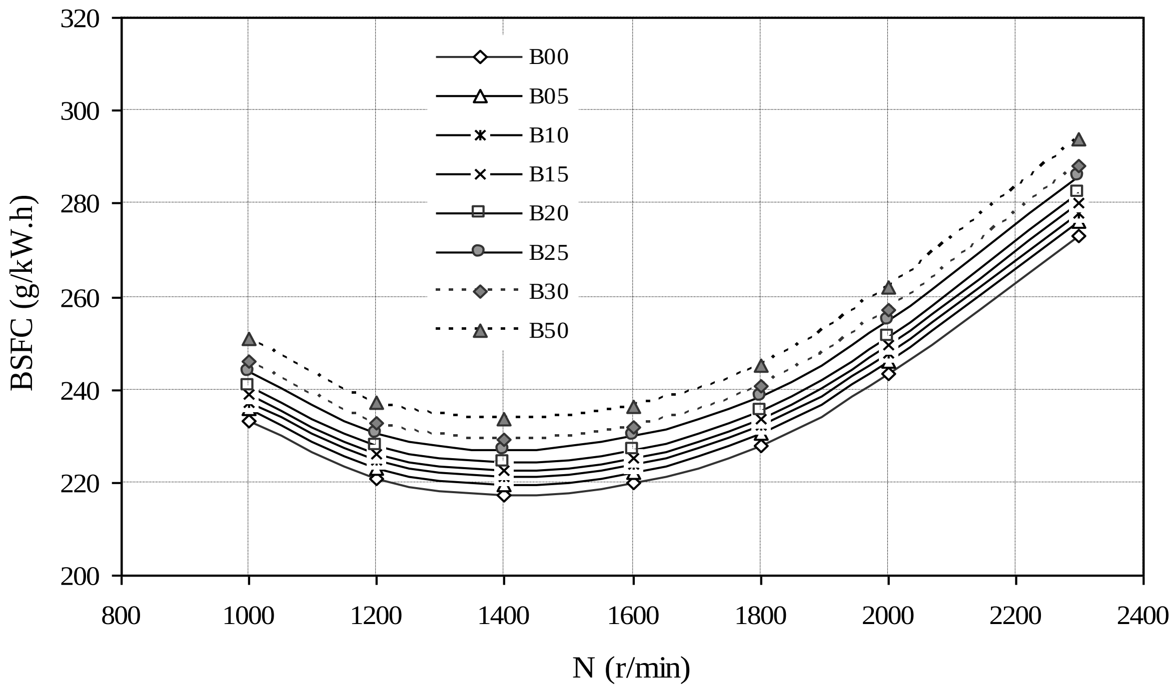

Fig. 7: **Simulated results of BSFC at different speeds for various fuel blends.**

The decreasing trend of SOI angle for B25 or higher blends, on the other hand, are due to efforts made to keep BP, BSFC and NO_x as closer to diesel as possible by playing with the above discussed combustion parameters. It has been reported that premix duration plays a dominant role in the higher levels of heat release rate with the consequent higher gas temperatures, and thus affects the combustion process of the engine [16]. Therefore, the model exhibits decrease in SOI angle for the higher fuel blend ratios.

It is pertinent to note that BP of the engine attains its maximum value at 2300 r/min for all the discussed blended fuels as shown in Fig. 6. This maximum BP, however, shows an obvious decrease at 2400 r/min or higher speed levels of the engine. Although simulations were also performed between 2300 and 2400 r/min, the results were not showing the clear decreasing trends for all the blend ratios discussed in the study.

4.2 Experimental Validation of the Model

The engine model was validated by operating the CI engine on B20 fuel without any modification to the engine. Parameters such as MCP, NO_x, BP, and BSFC were measured at 7 different engine speeds ranging from 1000 r/min to 2300 r/min with wide open throttle (WOT). It is obvious from Fig. 8 -11 that the simulated and experimental results are in good agreement except some modes during which maximum deviations of 3%, 3.4%, 4.2%, and 5.1% in NO_x, MCP, BP, and BSFC respectively, are revealed. Further to this, the results also show under-prediction as well as over-prediction in the trends of MCP, NO_x and BP at some of the modes.

The deviations in experimental and simulated results are due to the fact that engine was designed on the basis of diesel fuel with specific SOI angle, thus turbine and compressor maps for the blended fuels may be the possible causes of inaccuracy. The accuracy of modeling for this turbocharged alternatively fueled engine can further be improved if a sufficient data of turbine and compressor maps is available from the manufacturer. However, unfortunately, no such data could be accessed owing to company proprietorship and some other reasons.

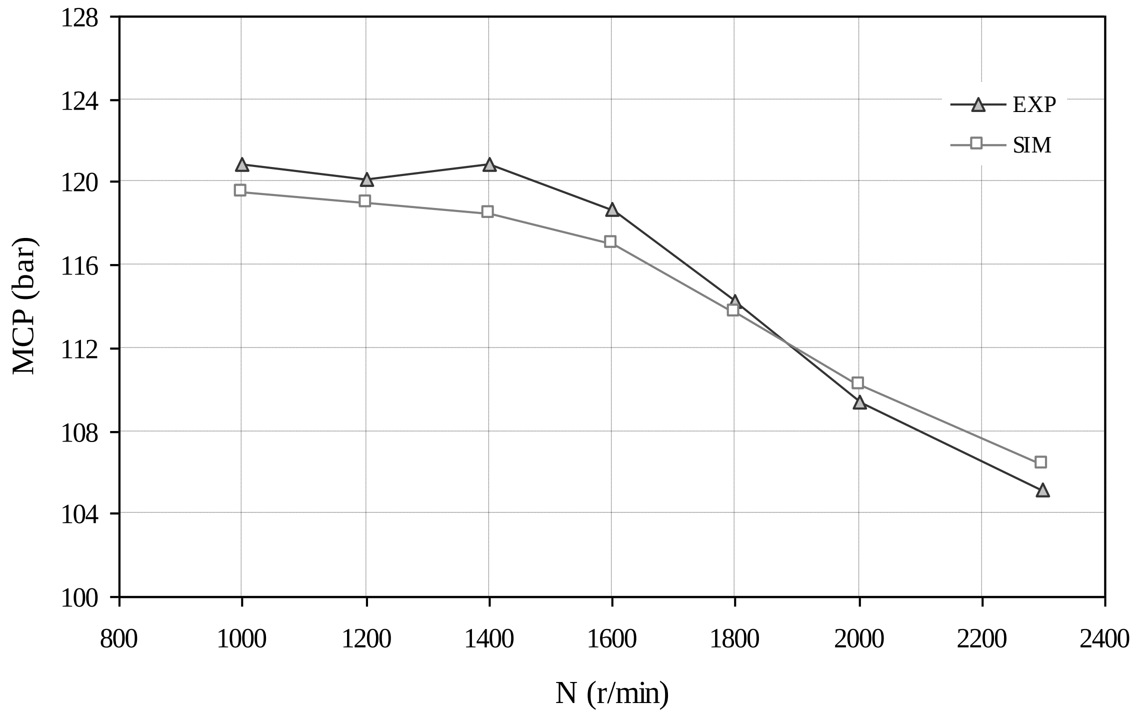

Fig. 8 Comparison of experimental and simulated results for MCP using B20 fuel

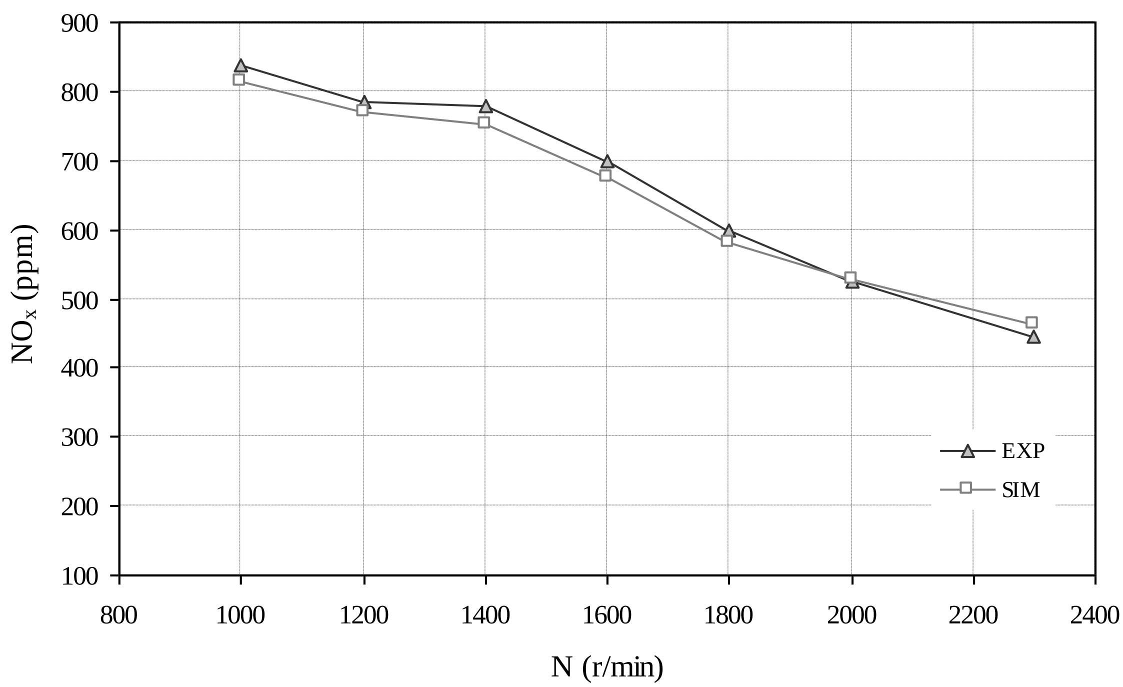

Fig. 9 Comparison of experimental and simulated results for NO_x emissions using B20 fuel

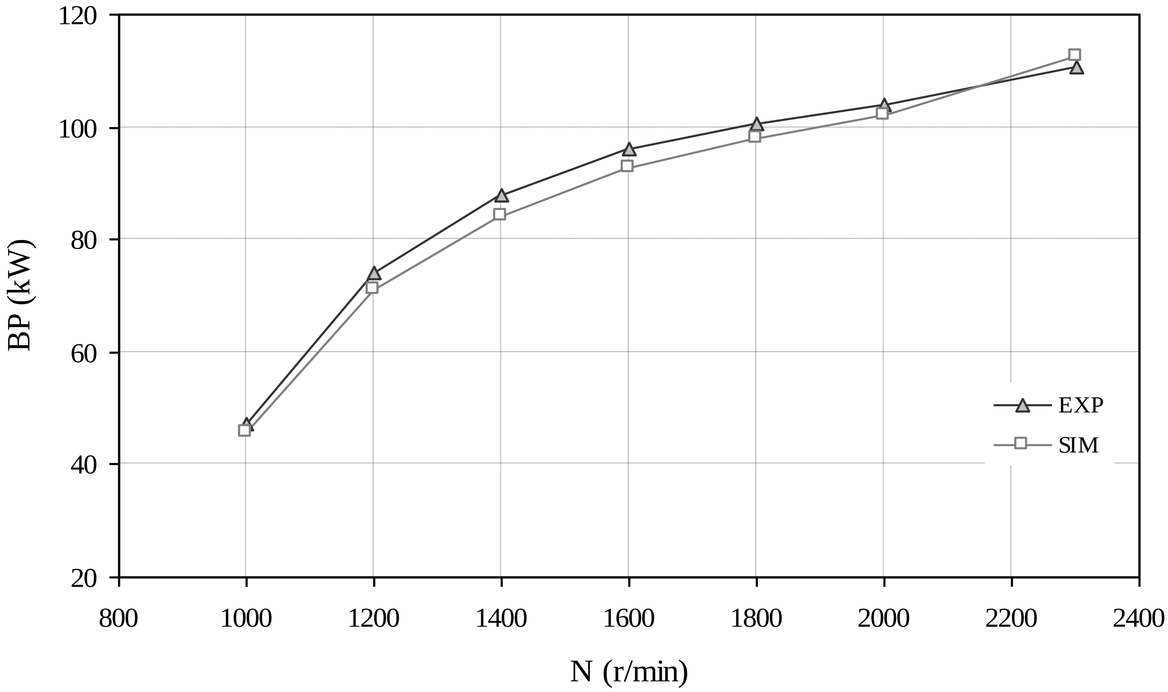

Fig. 10 Comparison of experimental and simulated results for Brake Power using B20 fuel

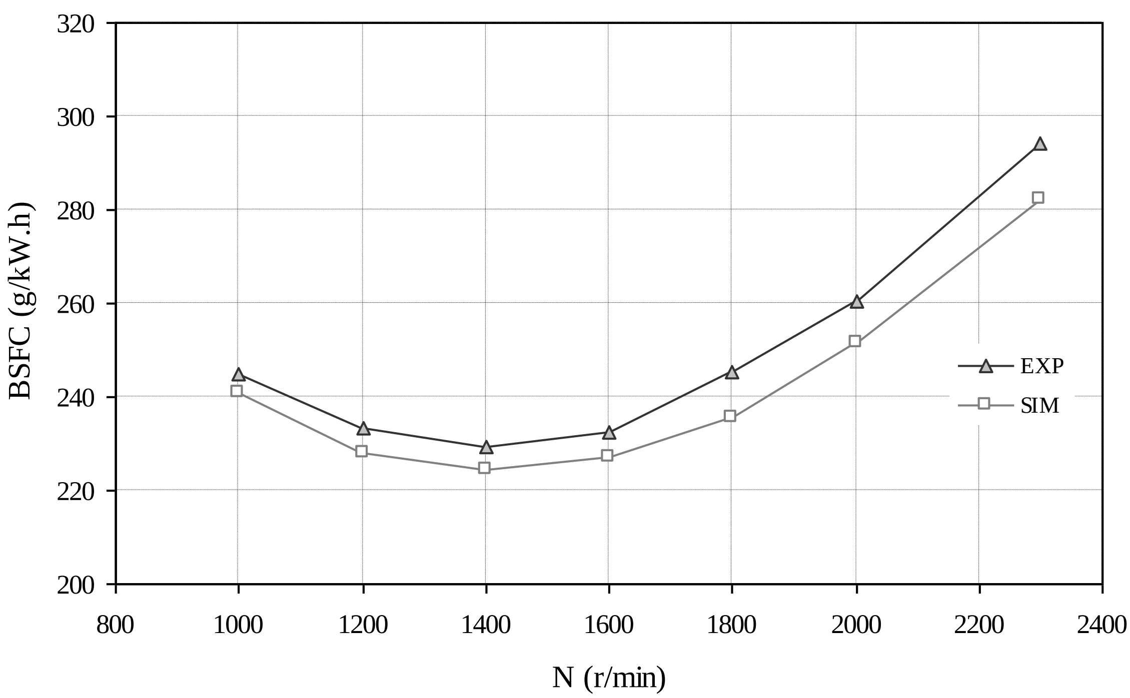

Fig. 11 Comparison of experimental and simulated results for BSFC using B20 fuel

It is worthwhile to note from both simulated and experimental results that there is a positive correlation between MCP and NO_x emissions. The modes during which MCP are higher, NO_x are higher too during the same, and vice versa. Moreover, both MCP and NO_x are decreased with the increase in engine speed.

The possible reason for the increase in NO_x emissions at elevated MCP is more complete combustion owing to the decrease in maximum rate of pressure rise (MRPR) and ID of the fuel. MRPR is defined as the load applied on the cylinder head during the combustion process, while ID is defined as an interval (time or crank angle) between SOI and the actual burning of fuel. Authors have already demonstrated in their previous studies [9, 17] that both MRPR and ID are increased with the increase in engine speed.

At relatively lower engine speeds ranging from 1000 to 1600 r/min, ID remains lower providing an opportunity to all the injected fuel to be burned completely without any endothermic reaction. During the endothermic or negative heat release process, however, burning of fuel is suppressed on account of piling up of the combustible mixtures caused by longer ID. The rate of oxidation of fuel is, therefore, increased in case of shorter ID which also improves the oxidation of NO to NO_2 and thus accounts for higher NO_x emissions. During the longer ID periods, on the other hand, more air-fuel mixtures are developed in the combustion chamber of the engine causing larger premixed burn peaks with the consequent larger premixed combustion amounts indicating relatively weak combustion areas [3, 17]. Further, the decrease in MCP or NO_x at higher speed levels is attributed to the reduction in combustion temperature caused by the turbulence and heat losses to the walls of combustion chamber [9].

5. Conclusions

The main thrust of the current study is to predict an optimum biodiesel-diesel blended fuel suitable to be used as an alternative fuel to an unmodified CI engine without much disturbance to engine performance and combustion together with minimum possible NO_x emissions. For this, one dimensional simulation tool GT-Power was used to model a medium duty turbocharged diesel engine. The model was first set to diesel and then to different blend ratios one by one by assigning the corresponding attributes to specified components. Following are the key findings of the study:

- The model was greatly influenced by the parameters such as D_P, D_M, D_T, and E_M and ID.
- The simulation results revealed that B20 is an optimum biodiesel-diesel blend exhibiting only 2.8% and 3.5% increase in NO_x and BSFC respectively, as compared to diesel.
- BP of the engine was decreased only to 3% in case of B20, relative to its counterpart.
- The experimental validation of the modeling results further endorsed that B20 is an optimal prediction of a blend ratio among the other blends on the basis of criteria set for this purpose.
- Some under-predictions as well as over-predictions were also found during the comparison of the simulated and experimental results.
- However, the deviations in the results were limited to only 3%, 3.4%, 4.2%, and 5.1% in the case of MCP, NO_x, BP, and BSFC, respectively.
- A positive correlation was found between MCP and NO_x emissions revealing that both remain higher at relatively lower speeds of the engine.
- Both MCP and NO_x were decreased with the increase in speed owing to decrease in combustion temperature.

6. Acknowledgements

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