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**Prediction of Performance and Emissions of a Biodiesel Fueled
Lanthanum Zirconate Coated Direct Injection Diesel engine using
Artificial Neural Networks**

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Abstract

Different techniques are being attempted over the years to use low pollution emitting fuels in diesel engines to reduce tail pipe emissions with improved engine efficiency. Especially, Biodiesel fuel, derived from different vegetable oils, animal fat and waste cooking oil has received a great attention in the recent past. Transesterification is a proven simplest process to prepare biodiesel in labs with little infrastructure. Application of thermal barrier coatings (TBC) on the engine components is a seriously perused area of interest with low grade fuels like biodiesel fuels. Artificial neural networks (ANN) are gaining popularity to predict the performance and emissions of diesel engines with fairly accurate results besides the thermodynamic models with considerably less complexity and lower computing time. In the present study, experiments have been conducted on a single cylinder diesel engine whose combustion elements are coated with an experimental thermal barrier coating material made from Lanthanum Zirconate. Biodiesel has been prepared from Pongamia Pinnata oil through transesterification process. A series of experiments are conducted on the engine with and without thermal barrier coating using diesel and biodiesel fuels. Performance and emissions data from the experiments is used to train the network with the load, fuel type and coating being the input layer and the brake specific fuel consumption, brake thermal efficiency, CO, HC and NO_x emissions being the output layer. Results showed that the coating of engine components with lanthanum zirconate TBC resulted in improved engine efficiency with reduced emissions. ANN model is tested for its accuracy to predict the performance and emissions of the engine with the R values of 0.99 for both the training and test data with a mean square error of 0.002 and a mean relative error of 6.8%

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1. Introduction

Energy derived from renewable and alternative fuels is an essential input for economic growth of any country. It is quite essential in the present world's energy scenario to use alternative fuels because of their energy security, environmental concerns, foreign exchange savings and socioeconomic issues [1]. It was recognized even at the early years of invention of internal combustion engines that the alternate fuels are going to play an important role in the future to meet the increased energy demands and to reduce tail pipe emissions, which instigated Dr. Rudolph Diesel to use vegetable oil as fuel in his designs. Even after several processing techniques, biodiesel fuels still face some challenges to be used as diesel fuel replacements. The major drawback of biodiesel usage is its higher viscosity, and lower volatility. Methods of extracting maximum energy out of biodiesel fuel in diesel engines are underway and Low Heat Rejection Engine (LHRE) is one of the areas of interest in the engine development community since the recent past.

Yttria stabilized zirconia, also called partially stabilized zirconia (Y-PSZ) material is believed to be a reliable TBC until now but the failure of the coating at elevated temperatures under continuous thermal shocks as in diesel engines lead to the investigation of new materials for TBC applications. PSZ is limited due to phase transitions and increased sintering of the porous TBC layer above 1200 °C, which leads to catastrophic delamination of the coating. The failure of the PSZ coatings is also attributed to the high concentration of oxygen vacancies which permeates the oxygen through it, leading to the oxidation of the bond coat and sintering of the coating at higher temperatures, which leads to a decrease in porosity and an increase of Young's modulus and, hence, to higher thermally induced stresses [2].

In order to overcome the disadvantages of PSZ and to meet the requirements of an ideal TBC, it is needed to develop a new candidate material with even lower thermal conductivity, capability to withstand higher operating temperatures, higher sintering-resistance and phase stability at even higher temperature. Among the interesting candidates for TBCs, rare earth zirconates have been investigated, and they have been proved to be significant for the top coating materials [19]. Among these materials, lanthanum zirconate ($\text{La}_2\text{Zr}_2\text{O}_7$, LZ) shows promising thermo-physical properties and has attracted great attention as candidate material for thermal barrier applications [3]. Sintered LZ has a thermal conductivity of 1.56 W/mK which is lower than PSZ (2.5 Wm⁻¹K⁻¹), a cubic pyrochlore structure which is stable up to its melting point (2300°C), and it has been proposed as a promising TBCs material with catalytic activity. The catalytic nature of LZ could be a resource within the engine cylinder to reduce the CO, HC and soot emissions from diesel engines significantly. Higher Thermal expansion coefficient (TEC) is another important parameter that a promising TBC candidate material should possess in order to prevent the failure of the coating because of the thermal expansion mismatch. PSZ is widely known TBC to have higher TEC of 10.5×10^{-6} K⁻¹ and LZ has a TEC of 9.7×10^{-6} K⁻¹ which is lower than the PSZ. But the Young's modulus of the LZ is lower than that of PSZ and this lower value might compensate the effect of lower thermal expansion coefficient on increased thermal stresses [4, 5]. Many researchers have conducted experiments on diesel engines with different thermal barrier coatings. It has also been reported that the application of thermal barrier coating lead to the improvement in the efficiency with reduced tail pipe emissions.

Artificial neural networks (ANNs) have found applications in different areas of science and engineering over the years [27-35]. The ANNs can be used to achieve solutions, since a range of experimental data set will be used to train the network. The network trained with certain range is then used to predict the parameters that have not been used anywhere in the network system.

The insulated engine, referred to as low heat rejection diesel engine, consists of a piston, valves and cylinder head coated with an experimental Lanthanum Zirconate thermal barrier material. Since lanthanum zirconate powders are not commercially available, one has to prepare the material with a grain size that is recommended for different coating techniques. The LZ powder was procured with a grain size of 55 microns which is suitable to be

fed through the powder feeder of the automatic (which can also be operated manually) atmospheric plasma spray system type MP 200 from AMT AG, Switzerland.

2. Experimental Setup and Procedure

The experimental setup consists of a Kirloskar made single cylinder direct injection diesel engine whose specifications are given below in Table.1 is a widely used engine for agricultural activities and water pumping in India. Exhaust gas emissions are measured using a NETEL Made five gas analyzer model NPM-MGA-2 and smoke opacity is measured using NETEL smoke meter model no.NPM-SM-111B. Fuel consumption is measured using a calibrated burette and volume flow rate of air is measured using an air box and U-tube manometer. The engine components viz. piston, cylinder head and valves are coated with Lanthanum zirconate and have been shown in Fig.1. Thermocouples are used to measure the engine coolant inlet and outlet temperatures and exhaust gas temperatures.

An experimental thermal barrier coating material, Lanthanum Zirconate ($\text{La}_2\text{Zr}_2\text{O}_7$, LZ) has been prepared at Star Earth Minerals Private Limited, Mumbai using solid state reaction method on the request of the author. The grain size of the procured powder is as recommended by the plasma spray coating company and coatings are done at Sri Sai Surface coating Technologies, Hyderabad using the atmospheric plasma spray system type MP 200 from AMT AG, Switzerland. The coating process parameters used are given in Table.3 as reported by Hongfei Chen et al. An amount of 500 microns of material has been machined off the surfaces over which the coating is applied to keep the compression ratio of the engine unchanged because of the coating thickness. The bond coat of 150 microns is applied using NiCrAlY (Amdry 962, Sulzer Metco, Ni:69.2%, Cr:21%, Al:9%, Y:0.8% w%) and Lanthanum zirconate top coat with a thickness of 350 microns, maintaining the total coating thickness to 500 microns has been applied over the top surface of the piston, the engine head and over valves faces. The thickness of the coating is measured using Minitest650 from Elektrophysik.

Table 1. Specifications of the Test Engine

Manufacturer and Model	Kirloskar, AV 1
Number of Cylinders	One
Bore, mm	80
Stroke, mm	110
Cubic Capacity, CC	553.5
Rated Output, kW	3.68
Compression Ratio	16.5
Type of Injection	Direct
Type of Cooling	Water Cooled
Inj. Opening Pressure, Bar	200
Inj. Timing, °BTDC	23
Rated Speed, RPM	1500

Table 2. Fuel properties of B100 and B20

Property	PME (B100)	B20
Density @ 30 Deg C, g/cm ³	0.891	0.842
Viscosity @40 Deg C, Cst	4.08	3.63
Calorific Value, kj/kg	36540	41063
Flash Point, °C	174	157
Fire point, °C	178	160
Cetane Number	56	52

Table 3. Coating parameters for the Plasma Spray

Parameter	Value
Arc current intensity (A)	660
Primary gas (Ar) flow rate, slpm	30
Secondary gas (H_2)flow rate, slpm	15
Spray distance, (mm)	130
Powder flow rate, (g/min)	40



Fig. 1. LZ coated piston, valves and cylinder head

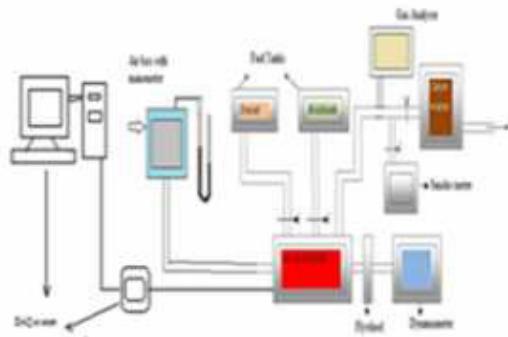


Fig. 2. Schematic Diagram of Experimental Setup

Biodiesel has been prepared using Pongamia Pinnata oil through transesterification process. B20 is a blend of 20 volume percent biodiesel and 80 volume percent diesel and is prepared just before the commencement of experiment to avoid possible separation of the blend. Experiments were conducted initially on the standard engine i.e. without applying coating to the engine parts at standard injector opening pressure of 19.5-20 MPa (200-205 bar) and injection timing of 23° BTDC using diesel, B20 and B100 as fuels. Then the engine is assembled with the parts which are coated with Lanthanum Zirconate TBC thus making it an LHR engine and above set of experiments are repeated for LHR engine using diesel, B20 and B100 for comparison. Fuel properties of pongamia biodiesel (B100) and B20 fuels are presented in Table 2.

3. Results and Discussions

Results obtained out of the experiments are discussed here. The effect of LZ TBC on the diesel engine with different fuels is analyzed. It is observed from the test results that the TBC has a significant role on performance and emissions of the engine. When run using biofuels, an improvement in the performance and reduction in the emissions is observed with LHR operation.

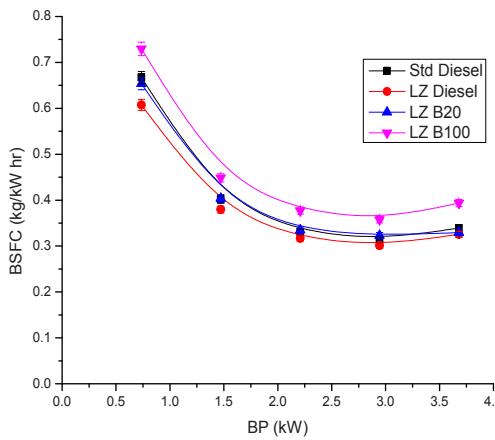


Fig.3 Variation of BSFC with brake power with LZ LHR engine compared to standard operation

Figure 3 presents the effect of TBC on the brake specific fuel consumption with respect to brake power. It can be observed from the figure that the BSFC of the LHR engine is lower with diesel and B20 fuels compared to the

standard diesel fuel operation and a little higher for B100 fuel. It is believed that the increased in-cylinder temperatures because of the insulation have helped to increase the rate of vaporization and burning of fuel, which in turn might have resulted in consuming less fuel to develop same amount of power. BSFC of the LZ diesel operation is found to be 0.325 kg/kWhr which is 4.16% lower compared to the standard diesel operation of 0.339 kg/kWhr. BSFC of LZ B20 is observed to be 0.329 kg/kWhr which is 2.9% lower compared to the standard diesel operation at full load of the engine. BSFC of LZ B100 is 0.393 kg/kWhr and is 13% higher compared to the standard diesel operation and it is about 9.5% lower compared to the standard B100 operation. The insulation applied over various combustion elements of the engine is believed to have played a major role in retaining heat losses to the coolant and to increase the cylinder gas temperatures which contributed to the higher vaporization rates of biodiesel fuels extracting maximum energy out of combustion from biodiesel fuels.

Figure.4 shows the variation of Brake thermal efficiency with brake power for different fuels with LZ coating compared to the standard diesel operation. LZ LHR engine has shown improved efficiency especially with biodiesel fuels compared to the standard operation. BTE of LZ diesel and B20 are observed to be 25.33%, 25.34% which are 4% and 8.55% higher compared to standard diesel fuel operation. LZ B100 is found to be 2.55% lower than the standard diesel operation and it is 10.7% higher than the standard B100 operation at full load. This may be attributed to the lower amount of energy consumption required to generate same amount of power specifically with biodiesel fuels making use of higher gas temperatures along with the characteristic advantage of 10% molecular oxygen in biodiesel fuels resulting in improved brake thermal efficiencies with LZ coating.

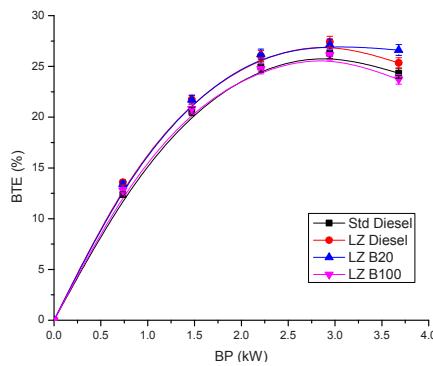


Fig.4 Variation of Brake thermal efficiency with brake power with and without coating

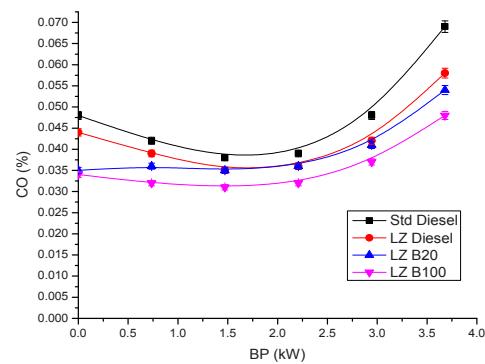


Fig.5 Variation of CO emissions with brake power with and without coating

Variation of CO emissions with and without coating using different fuels is presented figure 5. Formation of CO emissions is multistep process in diesel engines and is majorly dependent of prevailing cylinder temperatures and pressures. CO emissions are high at low and full loads owing to the fact that the maximum amount of heat generated from the combustion of fuel is lost to the walls of the cylinder depriving the fuel sufficient temperature to get oxidized resulting in incomplete combustion at low loads and continues pumping of higher amounts of fuel by the governor to overcome the load effects on the engine results in incomplete combustion forming CO emissions. It has been observed that the LZ coated engine operation has generated lower CO emissions with all fuels compared to the standard diesel operation. Presence of molecular oxygen in the biodiesel fuel makes the combustion complete resulting in lower CO emissions. The results showed that the LZ coated diesel operation produced about 18% lower CO emissions compared to the standard diesel operation. And it is 27.7% and 43.75% lower with LZ B20 and B100 operation than the standard diesel operation at full load.

Variation of HC emissions are shown in figure.6 using different fuels with and without LZ coating. Like CO emissions, HC emissions are also temperature dependent and the formation kinetics are quite complex. Quenching of fuel particles on cylinder walls, crevice and sac volume fuel particles are major sources of HC emissions in

diesel engines. Higher gas temperatures can oxidize the fuel particles in the later phases of combustion which remained in the cylinder without burning. The LHR concept is very attractive in this regard to increase the gas temperatures and to oxidize the unburnt hydrocarbons. The LZ coated engine operation with diesel, B20 and B100 are observed to have emitted 11.68%, 40.98% and 62.26% lower HC emissions at full load than the standard diesel operation respectively.

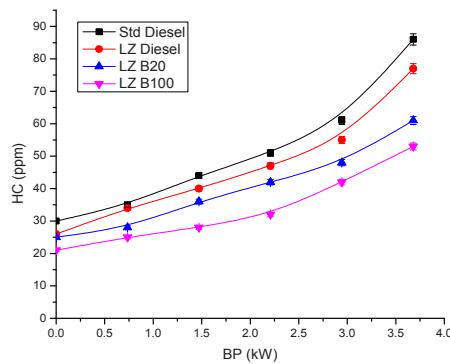


Fig. 6 Variation of HC emissions with and without LZ coating using different fuels

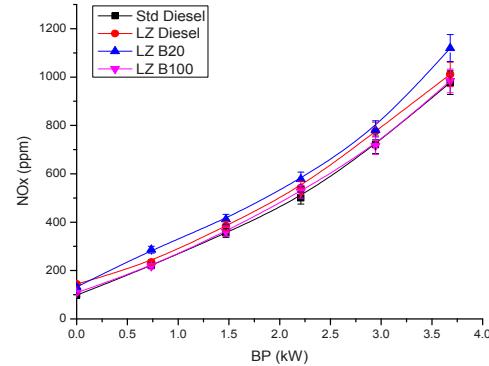


Fig. 7 Variation of NO_x emissions with and without coating using different fuels

Figure 7 presents the effect of LZ TBC on NO_x emissions of the engine using different fuels. The NO_x emissions are mostly temperature dependent in internal combustion engines and hence the rise in gas temperature results in increase in NO_x emissions. The higher NO_x emissions from the LHR engine compared to the standard engine are attributed to the primarily to the higher combustion chamber temperature and partly to the reduced ignition delay. Similar trends of increased NO_x emissions are reported in literature [14, 18, 20]. It has been observed in the study that the fuels B20 and B100 produced higher NO_x emissions with LZ coating in the order of about 9% and 12% respectively than the LZ diesel operation. This may be attributed to the presence of molecular oxygen content in the biofuels, which could help increasing the combustion temperature and another reason being denser fuels that the higher fuel delivery to meet the power generation requirement as the load increase would increase the NO_x emissions. It is also believed that the higher bulk modulus of biofuels would result in approximately one degree advanced injection of fuel than the actual timing contributing to increased gas temperatures. An increase of 3.5%, 12% and 15% in NO_x emissions has been observed than the standard diesel operation respectively.

4. Prediction of performance and emissions using ANN model

Back propagation (BP) learning algorithm, which gained popularity in science and engineering applications has been used in the present study. This network has one input layer, one hidden layer and one output layer. Input data sets and corresponding target sets are required to train and test the neural networks. To develop an ANN model, the available experimental data set has been divided into two sets, one to be used for training of the network (80% of the data), and the remaining was used to verify the generalization capability of the network [28]. Haykin [32] has presented the mathematical background of the ANN, training and testing procedures. Input and output pairs are presented to the network and weights are adjusted to minimize the error between the network output and actual value. Once training is completed, predictions from a new set of data may be done using the already trained network. The input parameters are engine load, fuel type and type of coating, and the output parameters are brake specific fuel consumption, brake thermal efficiency, CO, HC and NO_x emissions.

The Neural Networks Toolbox of MATLAB 8 was used to develop the network. The Tangent-sigmoid transfer function was used in the hidden layer (first layer) and output layer (second layer). Number of inputs of system determines the neuron number in the input layer of the network and its number of outputs determines the neuron number in the output layer of the network. Thus, input layer of network has three neurons and the output layer has five neurons. Six neurons were used in hidden layer. Neural network requires the range of both the input and output values to be between 0.1 and 0.9 for increased accuracy of prediction. The following formula is used to adjust the range of input and output data to be in between 0.1 and 0.9.

$$\frac{\text{value} - \text{min}}{\text{max} - \text{min}} * (\text{high} - \text{low}) + \text{low} \quad (1)$$

This equation is a widely used method for unification of test and target data [33, 34]. Where, minimum is the minimum value of the data set, maximum is the maximum value of the data set, high is the maximum normalized data which equals to 0.9, and low is the minimum normalized data which equals to 0.1. Weight and bias values of the network are updated according to Levenberg–Marquardt (TrainLM) optimization algorithm by the back propagation training function. The performance index of TrainLM algorithm is the mean squared error (MSE) [35] and it is formulated as given below:

$$\text{MSE} = \frac{1}{N} \sum_{i=1}^N (y_i - y_k)^2 \quad (2)$$

Where, y_i is the predicted value of the i th pattern, y_k is the target value of the i th pattern and N is the number of pattern.

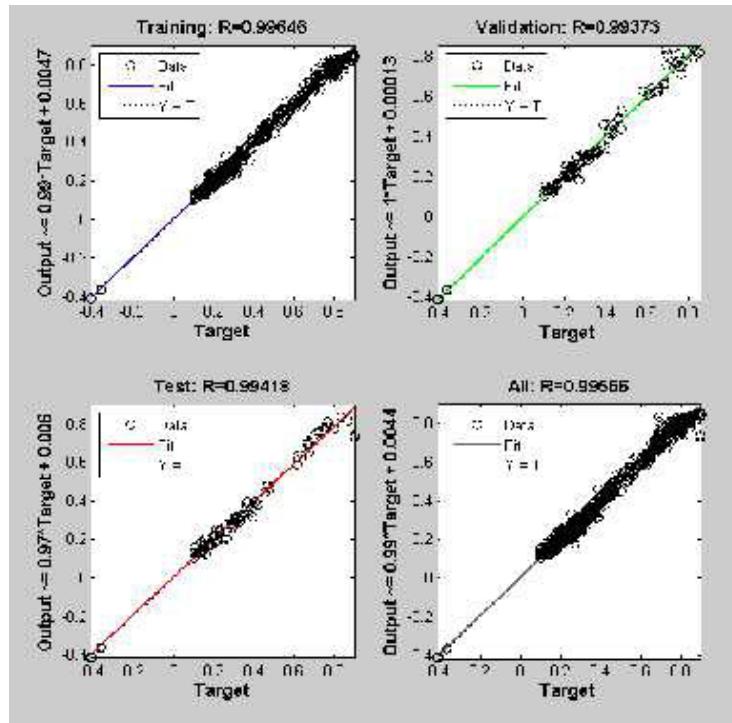


Fig.8 R values of training, validation and test data

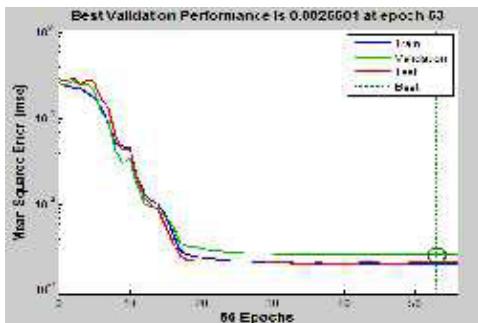


Fig.9. Snapshot of mean square error plot

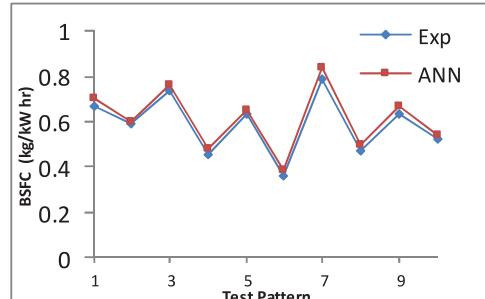


Fig.10. Comparison of experimental BSFC values with ANN predicted values

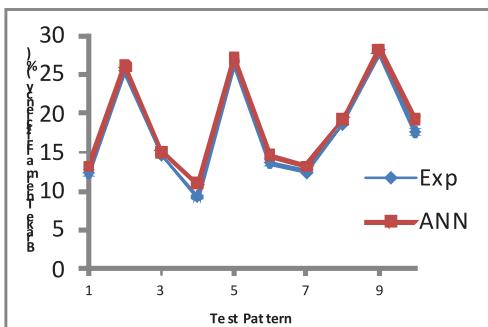


Fig.11 Comparison of experimental BTE with ANN BTE

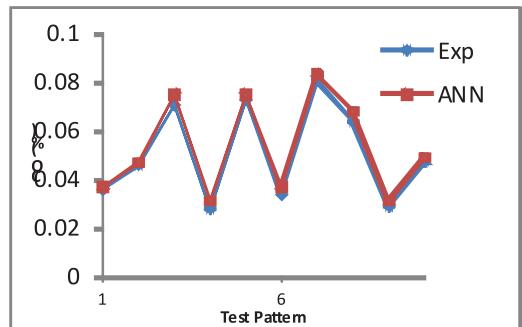


Fig.12 Comparison of experimental CO emission with ANN CO emissions

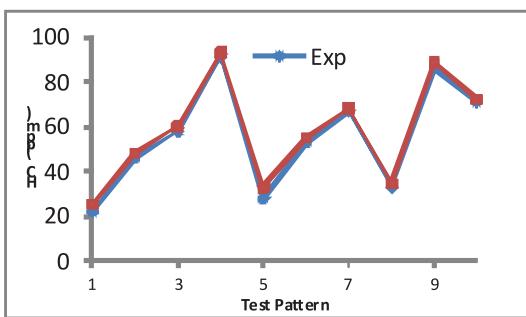
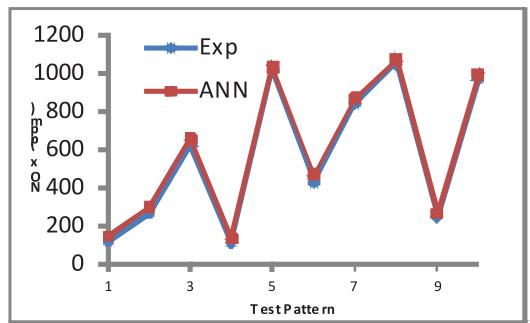


Fig.13 Comparison of experimental HC with ANN HC emissions

Fig.14 Comparison of experimental NO_x with predicted NO_x

5. Conclusions

Experiments are conducted on a single cylinder direct injection diesel engine using an experimental thermal barrier coating material made from Lanthanum Zirconate. Biodiesel made from pongamia oil (B100) and B20 are used as fuels at standard injector opening pressure and fuel injection timing. It has been observed from the experimental observations that the Lanthanum zirconate coated engine has shown an improvement in BSFC in the order of 4.16% lower with LZ diesel operation compared to the standard diesel operation. 2.9% lower BSFC is

observed with LZ B20 operation compared to the standard diesel operation and LZ B100 has shown a BSFC value of 9.5% lower compared to that of standard B100 operation. CO emissions of the coated engine are observed to be 18% lower with diesel, 27.7% with B20 and 43.75% with B100 operation compared to the standard diesel operation. HC emissions are also observed to be low with all fuels with coating compared to that of standard diesel operation and a slight increase of 3.5%, 12% and 15% NO_x emissions are observed with coated engine using diesel, B20 and B100 respectively.

A back propagation (BP) neural network model with a 3–6–5 (number of input layer–hidden layer–output layer neurons) configuration was developed to predict specific fuel consumption, brake thermal efficiency, emissions of CO, HC and NO_x of a diesel engine. The results were in agreement less than 6.8% average relative error with those obtained experimentally. This new approach could be considered as an alternative and practical technique to evaluate the engine parameters. ANNs are feasible for the prediction of engine parameters because of its ability to learn and generalize a wide range of experimental conditions. This makes ANN a powerful tool for solving complicated engineering problems.

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