A Method for Pre-Calibration of DI Diesel Engine Emissions and Performance Using Neural Network and Multi-Objective Genetic Algorithm

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ABSTRACT: Diesel engine emission standards are being more stringent as it gains more publicity in industry and transportation. Hence, designers have to suggest new controlling strategies which result in small amounts of emissions and a reasonable fuel economy. To achieve such a target, multi-objective optimization methodology is a good approach inasmuch as several types of objective are minimized or maximized simultaneously. In this paper, this technique is implemented on a closed cycle two-zone combustion model of a DI (direct injection) diesel engine. The main outputs of this model are the quantity of NOx, soot (which are the two main emissions in diesel engines) and engine performance. The optimization goal is to minimize NOx and soot while maximizing engine performance. Fuel injection parameters are selected as design variables. A neural network model of the engine is developed as an alternative for the complicated and time-consuming combustion model in a wide range of engine operation. Finally design variables are optimized using an evolutionary genetic algorithm, called NSGA-II.

KEY WORDS: Diesel engine, Emission, Multi-objective, Neural network, NSGA-II, Performance.

INTRODUCTION
Public concern about environment is increasing in consequence of daily growth of diesel engine usage in industry and transportation. Air pollution problems, global warming, greenhouse effects and acid rain would cause serious problems at a global scale. These effects are mainly related to emissions of nitrogen oxides (NOx), particulate matter (PM) and unburned hydrocarbons (HC). On the other hand, depletion of fossil fuel
resources has enormously duplicated global concerns about the future fuel reservoirs. Hence, the allowable limits of exhaust emissions are being reduced and stringent emission standards are being legislated. In order to comply with these regulations, the diesel engine industry has undergone a great technological development in the last few years, creating a high number of new strategies such as electronic control, new injection systems allowing higher pressures, different injection events, etc [1-3].

As a result, the problem of optimization of the engine management in order to simultaneously comply with emission regulations and fuel economy requirements has become a difficult task, especially due to the increased number of degrees of freedom in the engine operating parameters. This optimization process is carried out during the development of a new engine, and is usually known as engine pre calibration. Although calibrations were completely based on empirical results in the past, the development in technology has incorporated new model-based techniques [4-6].

Among different models that are developed for diesel engine combustion up to now, phenomenological models have sufficient accuracy to predict engine emissions and performance. In this paper a two-zone combustion model of a diesel engine, which yields the quantities of engine emissions (NOx and soot) and performance (IMEP) in a closed cycle, is applied. The target is to perform a simultaneous optimization of NOx and soot in a way that a reasonable engine performance is achieved. Classical methods for optimization, based on numerical techniques, have been applied to the optimization of diesel engines in different publications. In [8-9], a simple gradient method is used, where only one parameter is changed during iterations. In [10-12], a steepest descent method is followed.

However, Numerical methods for optimization suffer from some limitations such as the difficulty to escape from local minima and the dependence of the solution on the initial value chosen. But, genetic algorithm (GA) methods suggest an easy and trustable way to solve optimization problems. Although the computational time may be larger than that of numerical methods, where the search domain is rather large, GA is much more applicable due to its ability to search through the work space. Moreover, artificial neural networks (ANNs) are an emerging tool of artificial intelligence, which have been shown to be effective in solving a wide range of problems, including many applications to engine modeling [7]. The structure of ANNs enables them to model complex nonlinear multiple problems, which makes them a well-suited method for emission modeling. In addition, ANN can produce fast prediction responses, which represent an important advantage in comparison with alternative modeling techniques, such as physical and chemical models.

A single objective genetic algorithm, together with a neural network model of the engine based on experimental data, is implemented in [13]. Anyway, when we are engaged with a problem that has more than one objective, a single GA does not seem to be appropriate and a multi-objective algorithm should be applied. Hiroyasu has treated the problem of engine emission optimization by applying a multi-objective genetic algorithm coupled with a diesel engine combustion model in [14].

In this work, an ANN model based on a two-zone engine model is presented and optimized by NSGA-II as one of the powerful evolutionary algorithms of multi-objective optimization. For the optimization problem parameters of fuel injection, start of injection (SOI), injection duration and AFR (air to fuel ratio) are selected as design variables. The influence of these design variables on the engine operation is assessed by varying each parameter in a specific range and sampling the model outputs; thereby, a data sheet can be obtained. The data sheet will be used to generate an artificial neural network model of the engine as an alternative to the combustion model. Once the neural network model of the engine has been developed, results of trained neural network will be used for optimization. At first, the two-zone combustion model is briefly explained. Afterwards, neural network model and optimization algorithm are introduced. Finally, results of multi-agent optimization are presented.

COMBUSTION MODEL

In a two-zone combustion model, the combustion chamber is divided into two zones. The first zone is the unburned zone, which includes the unburned mixture of fuel, air and residual gas and the second zone is the burning zone. The current two-zone model includes
processes occurring during the closed cycle (compression and expansion strokes). Main in-cylinder processes which are air motion, fuel spray development and mixing, spray impingement on the wall, turbulent heat transfer and chemistry of combustion are modeled here. The fuel considered here is n-dodecane (C$_{12}$H$_{26}$), representing a common fuel for commercial diesel engines.

**Conservation and state equations**

In order to determine the temperature and pressure during compression stroke, the first law of thermodynamic for a closed system, and equation of state are used. Applying these two equations, temperature and pressure change per crank angle (an engine crank rotates 720 degrees per a complete cycle, and at the Top Dead Center the crank angle is assumed to be zero) can be stated as follows:

$$\frac{dT}{d\phi} = T\left(\frac{1}{P}\frac{dP}{d\phi} + \frac{1}{V}\frac{dV}{d\phi}\right)$$  \hspace{1cm} (1)

$$\frac{dP}{d\phi} = \frac{1}{V}\left[1 + \frac{R_{mol}}{C_V} \left(\frac{dV}{d\phi}\right) \right] + \frac{R_{mol}}{C_V} \frac{dQ}{d\phi}$$  \hspace{1cm} (2)

Equations (1) and (2) are solved simultaneously by the 4th-order Runge-Kutta’s method. The instantaneous volume of the cylinder is given by:

$$V = V_{cl} \left[1 + \frac{1}{2} (R_e - 1) \left(R + 1 - \cos \phi - (R^2 - \sin^2 \phi)^{\frac{1}{2}} \right)^2 \right]$$  \hspace{1cm} (3)

During combustion and expansion, the first law of thermodynamics for an open system is applied for each zone. Surrounding air just loses mass into the burning zone; therefore, the first law for this zone would be:

$$dQ = dE + PdV + h_d dm_a$$  \hspace{1cm} (4)

The burning zone not only receives mass from the air zone, but also there is an enthalpy flow from the fuel which is ready to be burned in the time step. So, the first law will be:

$$dQ = dE + PdV - h_d dm_a - h_t dm_f$$  \hspace{1cm} (5)

**Spray modeling**

Spray characters have a great effect on diesel combustion. Among them, break-up time, break-up length, spray penetration and air entrainment are more important. Here, correlation of Hiroyasu et al., which is based on turbulent gas jet theory, is used for spray tip location as a function of time [15]. Correlations used for spray penetration and breakup time are as follows:

$$x = 0.39 \frac{2 \Delta p}{\rho_f} \cdot t \hspace{1cm} 0 < t \leq t_{br} \hspace{1cm} (6)$$

$$x = 2.95 \left(\frac{\Delta p}{\rho_a}\right)^{0.25} \sqrt{D_N \cdot t} \hspace{1cm} t \geq t_{br} \hspace{1cm} (7)$$

$$t_{br} = \frac{28.61 \rho_1 \cdot D_N}{\sqrt{\rho_a \Delta p}} \hspace{1cm} (8)$$

$\Delta p$ represents the pressure drop across the nozzle, which is calculated as follows:

$$\Delta p = P_{in} - P_{cyl} \hspace{1cm} (9)$$

**Combustion and emission modeling**

The main calculation procedure is based on the integration of the first law of thermodynamics and the perfect gas state equation combined with the various sub-models, for each zone separately. The semi-empirical model of Whitehouse and Way is used for calculating the rate of combustion. The injected fuel in the burning zone mixes up with the air entrained from the air zone via a mixing and diffusion process, while the burning rate of the fuel is expressed by an Arrhenious-type expression. The generally accepted kinetics formation scheme proposed by Lavoie et al. is used for calculation of nitride oxide [16]. The net soot formation rate is calculated by using the model proposed by Hiroyasu et al. [15], as modified by Lipkea and Dejoode [17]. Detailed explanation of the model can be found in [18-21].

**Modeling results**

Fig. 1 illustrates the predicted and measured quantities of pressure in the case of 80 % load and 2500 rpm. As can be seen there is a good agreement between measured and predicted data. In Figs. 2 and 3 simulated quantities of NOx and soot is illustrated for the case of 80 % load and 2500 rpm.

**NEURAL NETWORK**

Artificial Neural Network (ANN) is a powerful tool used in modeling of time series processing and
Fig. 1: Calculated and experimental pressure diagram, at 80% of full load, 2500 rpm and a static injection timing of 340° crank angle [21-22].

Fig. 2: Results of modeling for NOx, at 80% of full load, 2500 rpm and a static injection timing of 2° CA BTDC [21-22].

Fig. 3: Results of modeling for soot, at 80% of full load, 2500 rpm and a static injection timing of 2° CA BTDC [21-22].

Table 1: Ranges of the designed parameters used for data generation.

<table>
<thead>
<tr>
<th>Design Parameter</th>
<th>Range of Variation</th>
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<tbody>
<tr>
<td>SOI</td>
<td>330-350 crank angle</td>
</tr>
<tr>
<td>AFR</td>
<td>24-66</td>
</tr>
<tr>
<td>Injection Duration</td>
<td>16-41 crank angle</td>
</tr>
<tr>
<td>Engine Load</td>
<td>40%-100%</td>
</tr>
<tr>
<td>Engine RPM</td>
<td>1500-4000</td>
</tr>
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</table>

pattern recognition, and also has its root in engineering, neuro-science and mathematics. ANN consists of simple and adaptive processing units which is often called neurons.

A simple neuron is an information-processing unit that is fundamental to operation of neural network. Neurons are interconnected and form a large network. In neural modeling, the inputs are known or they can be measured and the behavior of outputs is investigated when input varies. The schematic of Fig. 4 shows the model of a neuron, which forms the basis of designing neural networks.

Three basic elements of the neuronal model are as follows [22]:

1- A set of synapses or connecting links, each of which is characterized by a weight or strength of its own as $W_{k}$.
2- A summation block for adding input signals, weighted by the respective synapses of the neuron.
3- An activation function $\varphi(\cdot)$ for limiting the amplitude of the output of a neuron.

The activation function limits the amplitude range of the output signal to some finite value. There are various types of activation functions, such as threshold function, piecewise-linear function, and sigmoid function. Here, we have made use of a certain ANN architecture known as the multilayer feed-forward neural network or multilayer perception (MLP).
Network Implementation

The range of variation of the design parameters is shown in table 1. These data are used for training and testing the neural network. For every set of engine load and speed a network is trained with SOI, AFR and injection duration as inputs and NOx, soot and IMEP as outputs. 256 samples are applied for training in each set of data. The input layer uses 3 nodes, two hidden layers are constructed of 15 nodes in each layer and the output layer includes 3 nodes. The training procedure is based on “Quick Propagation” algorithm. 128 samples were used in testing procedure of each data set. A sample validation for NOx, soot and IMEP quantities at 80 % load and 1500 rpm is displayed in Figs. 5, 6 and 7. Surprisingly the results are so satisfactory, that one can not distinguish test and trained curve (solid and dashed curves) from each other. Network errors are calculated based on mean square error (MSE) formula given as below:

$$\text{MSE} = \frac{1}{P} \sum_{p=1}^{P} \sum_{i=1}^{N} \left( \frac{Y_{\text{real}}^{p,i} - Y_{\text{predicted}}^{p,i}}{N} \right)^2$$

Where i is number of nodes in output layer, p is the number of samples and $Y_{\text{predicted}}$ is network outputs and $Y_{\text{real}}$ is the correct data of well depths, which extracted before. MSE value is 0.0023 for the trained data. This value for test data is equal to 0.0065.

MULTI-OBJECTIVE OPTIMIZATION

In reality, most optimization problems deal with more than one objective. Usually, the target is to find design
variables like \( x \) that minimize or maximize \( k \) objective functions within \( m \) constraints. This type of optimization problems is called Multi-objective Optimization Problems (MOPs) and can be formulated as follows \[23, 28\]:

\[
\begin{align*}
\min_{\mathbf{x}} & \quad f(x) = \begin{bmatrix} f_1(x), f_2(x), \ldots, f_k(x) \end{bmatrix}^T, \\
\text{s.t.} & \quad x \in X = \left\{ x \in \mathbb{R}^n \mid u_j(x) \leq 0 (j=1,\ldots,m) \right\}
\end{align*}
\]  

(11)

If the objective functions are in the trade-off relationship, it is difficult to minimize or maximize all objective functions at the same time. In this case, the concept of dominance and Pareto optimum solution should be utilized.

**Dominant solution definition**

Suppose \( \bar{x}_1, \bar{x}_2 \in \mathbb{R}^n \) are two solutions, when

\[
\begin{align*}
f_i(\bar{x}_1) & \leq f_i(\bar{x}_2) \quad (\forall i = 1,\ldots,k) \quad \text{and} \\
f_i(\bar{x}_1) & < f_i(\bar{x}_2) \quad (\exists i = 1,\ldots,k).
\end{align*}
\]

Then \( \bar{x}_1 \) dominates \( \bar{x}_2 \) and is a better solution.

In Fig. 8, the concept of the Pareto optimum solutions is illustrated in the case of two objectives, which are supposed to be minimized. Solution A yields better results for both \( f_1 \) and \( f_2 \) than solution C. In this case, it is said that C is dominated by A. Therefore, A is better than C. On the other hand, the value of \( f_1 \) of A is better than that of B, but \( f_2 \) for B is better than that of A. Therefore, it is not possible to conclude which of the two solutions is better. In this case A and B are called non-dominant solutions. In practice, multi-objective optimization problems deal with non-dominant solutions. A set of these non-dominant solutions is called a Pareto optimum set. The line of the Pareto optimum solution is called a Pareto front.

**Genetic algorithms for MOPs**

The Genetic algorithms (GA) can be applied to the problems whose search space is discrete. Since GA’s are multipoint search methods, these algorithms are very suitable for finding a Pareto optimum set \[24\]. Several algorithms for multi-objective optimization problems have been reported up to now. SPEA-2 and NSGA-II are two examples of these algorithms \[25\]. In multi-objective GAs, the Pareto ranking is often used for determining the fitness value \[26\]. The Pareto ranking is determined according to the following procedure. For each solution, the number of the solutions that are dominant to the focused solution is counted. Pareto ranking is this number + 1. The concept of the Pareto ranking is shown in Fig. 9. In this example, there are four solutions: A, B, C, and D. A, B, and C are non-dominant solutions, and therefore, their Pareto rankings are 1. D is dominant to A and B and the Pareto ranking of D is \( 1 + 2 = 3 \).

**NSGA-II**

Among various multi-objective EAs, those who use an elite-preserving operator are of more interest. No matter how the elitism is introduced, it makes sure that a good solution found early in the run will never be lost unless a better solution is discovered. Moreover, the presence of elites enhances the probability of creating...
better offspring. Some EAs, like Rudolph’s elitist MOEA, use only an elite-preservation strategy, but NSGA-II also uses an explicit diversity-preserving mechanism. In Fig. 10 the procedure of NSGA-II is shown. Procedure of NSGA-II is outlined in appendix “A”.

**Genetic Algorithm Implementation**

We have developed a NSGA-II code in Matlab software. There are two setting parameters to execute the optimization code. Firstly, the number of population should be set, which is chosen 200. It could be noted that the search domain will grow as the population number increases. Therefore, the chance for finding the global minima rises in a certain number of generations. Secondly, generation number - the number of iterations to achieve the global minima - is adjusted to 1000. The structure of Multi-objective Optimization using genetic algorithm, NSGA-II consists of three input parameters and three objectives. Inputs are selected from trained neural network outputs and outputs are optimized values of NOx, soot and IMEP. Optimized quantities of design variables for each set of engine load and speed are determined. In order to reduce the calculation cost and to strengthen the optimization process the results of the trained networks has been applied for optimization instead of the combustion code. According to the weights of the trained networks a fitness function has been introduced and optimized.

In Fig. 11 diagram of the derived Pareto solutions for the case of 2000 rpm and 60 % load is shown. All the plotted solutions are those that dominate other derived solutions during searching through the objective space. Every single point in this diagram introduces an optimized set of NOx, soot and IMEP that is in accordance with a specific set of design variables.

In order to determine a single set of optimized design variables for the engine operation, one should suggest a specific constraint. In other words, a logical constraint like the relation between objectives’ quantity should be considered and imposed on the achieved Pareto solutions. Hence, just the Pareto solution that satisfies the constraint would be the final answer.

The constraint which we consider in this paper is the value of NOx due to its strong and serious effects on human health parameters. Hence, the solutions that have lower value of NOx in comparison with others are selected. As a result of considering the NOx-value to be the criterion, IMEP value - the representative of generated power in engine - will decrease. Definitely, it can be completely different when we get engaged upon different situations. These situations include other aspects of engine application. For instance, there may be a demand on simultaneous minimizing of NOx and soot. This could be done by allocating a weight factor for the NOx and soot separately, showing the importance of each one, and by considering a new fitness function that is generated by the sum of weighted objectives. In general, the problem of multi-objective optimization has to reduce to a single objective problem, otherwise the achieved Pareto solutions can not be applied for a specific application.

Regarding to the aforementioned constraint, optimized quantities of engine outputs are calculated for some sets
Table 2: Results of optimization.

<table>
<thead>
<tr>
<th>Rpm</th>
<th>Load (%)</th>
<th>AFR</th>
<th>DUR (deg)</th>
<th>SOI (deg)</th>
<th>NOx (ppm)</th>
<th>Soot (mg/m^3)</th>
<th>IMEP (bar)</th>
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<tr>
<td>1500</td>
<td>40</td>
<td>36</td>
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of load and rpm. To obtain the corresponding design variables quantities, a new neural network has been trained. Inputs of this network are the optimized values of emissions and performance and outputs are the optimized values of design variables. In table 2, achieved data for every set of engine load and speed is shown. In Figs. 12, 13 and 14 optimized values of AFR, SOI and injection duration are plotted for different sets of load and engine speed. Using this optimization algorithm a pre map of engine for minimum emission and optimum performance can be obtained.

CONCLUSIONS

In this paper, the problem of optimization of diesel engine emissions and performance has been studied. As the objectives of the optimization (NOx-soot) are in a trade-off mode with each other, applying a multi-objective algorithm was inevitable. Derivation of the Pareto optimum solutions by GAs requires a large number of calculation iterations. Hence, a neural network model of the engine, which has proved to be an efficient tool for simulating diesel engine combustion, was developed. Finally, applying the constraint of minimum values of NOx, the multi-objective problem was reduced to a single objective one and the Pareto solutions that satisfied the constraint were highlighted as the final answer. As the main result of this work, is the pre calibration of the engine concerning emissions and performance, which plays an important role in test time and cost saving.

Nomenclatures

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
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<tr>
<td>R_c</td>
<td>Compression ratio</td>
</tr>
<tr>
<td>V_c</td>
<td>Clearance volume of cylinder (m^3)</td>
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Fig. 12: Optimized values of AFR for different rpm-load.

Fig. 13: Optimized values of SOI for different rpm-load.

Fig. 14: Optimized values of injection duration for different rpm-load.

R  Ratio of connecting rod length to crank radius
P_f  Fuel line pressure (Pa)
P_cyl  Cylinder pressure (Pa)
T  Temperature (K)
\( \phi \)  Crank angle (degree)
V  Instantaneous cylinder volume (m³)
R_{mol}  Universal gas constant, 8314.3 (J/kmol K)
C_v  Constant volume specific heat capacity (J/kmol K)
Q  Heat transfer to the cylinder wall (J)
t_{bc}  Break-up time (s)
\( \rho_l \)  Liquid fuel density (kg/m³)
\( \rho_a \)  Air density (kg/m³)
D_N  Nozzle hole diameter (m)
H  Specific enthalpy (J/kg)

Acronyms
DI  Direct injection
GA  Genetic algorithm
MOP  Multi-objective optimization

Received: 22nd July 2008; Accepted: 13th April 2009

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