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Development of a neural network model for selective catalytic reduction (SCR) catalytic converter and ammonia dosing optimization using multi objective genetic algorithm

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ABSTRACT

In this paper, a mathematical model of the SCR catalytic converter is replaced with the neural network model to accelerate the optimization process. The Euro steady state calibration test data set is used to simulate the inlet properties of the SCR catalytic converter. For each chosen condition, a separate neural network is developed. In order to generate sufficient data to form a neural network for each condition, the original mathematical model was run several times at the temperature and inlet NO_x concentration of each condition with a range of different ammonia concentrations. Subsequently, using MATLAB® software, the neural network model is trained and tested for each condition. Ammonia dosing optimization is performed using multi objective genetic algorithm module of MATLAB®. The optimization objectives are NO_x reduction percentage and the outlet ammonia concentration of the SCR catalytic converter. It is convenient that the NO_x is reduced as much as possible while ammonia concentration does not exceed 25 ppm.

1. Introduction

As diesel engines are becoming more popular for applications in transportation (heavy-duty and passenger cars), emission topic is also becoming a more challenging issue. Consequently, the global emission standards have become much more stringent in the past few years [1] and because of the lean environment in diesel engine, their focus is mainly on NO_x (NO and NO_2) and exhaust gas PM (particulate matters). One of the major chemicals in the diesel exhaust gas is nitrogen oxide (NO) which is proved to be harmful for human health. It contains almost 90% of the diesel engine overall NO_x emission. Comparing the EU regulation of the standards for pollutant emissions for heavy-duty diesel commercial vehicles in 2008 (Euro 5 standards) and forthcoming 2013 regulations (Euro 6 standards), NO_x emission must be reduced up to 80% [2]. One way to decrease the engine exhaust NO_x is to circulate a portion of the exhaust gas back to the cylinders. This method is known as Exhaust Gas Recirculation (EGR). Applying this method results in some of the oxygen in pre-combustion mixture to be replaced by the exhaust gas. Consequently, NO_x will be reduced because the formation of NO_x strongly depends on nitrogen and oxygen mixing in high temperature. However, the result of this method is not satisfactory for the current and future requirements of the emission regulations [3]. Therefore, the application of an efficient after-treatment technology seems inevitable.

An efficient NO_x reduction method in diesel exhaust is the selective catalytic reduction (SCR) with ammonia [4]. This technology was first used in stationary applications and has also become very popular for both light-duty and heavy-duty vehicles over the last decade [5–7]. Urea SCR is undoubtedly one of the most effective methods of reducing NO_x because of its high selectivity and reactivity with NO_x in the presence of excess oxygen and is also very economical.

Among numerous models of SCR catalytic converter, a mathematical model was developed to study the behavior of SCR catalytic converter.

The objectives of this paper are (1) develop a neural network model of the SCR catalytic converter to replace the developed mathematical model and (2) optimize the performance of the SCR catalytic converter by determining the necessary amount of ammonia at each inlet NO_x concentration.

2. Mathematical model of the SCR catalyst

2.1. SCR reactions

SCR process using ammonia consists of 3 major stages:

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Nomenclature

C	concentration (mol/m^3)
C_p	specific heat capacity (J/kg K)
$C_{p,c}$	specific heat capacity of the monolith material
h	heat transfer coefficient between gas and solid phase (W/m^2 K)
h_o	heat transfer coefficient to the environment (W/m^2 K)
k_m	mass transfer coefficient (m/s)
L	catalyst length (m)
R	reaction rate (mol/m^2 s)
S_a	catalytic surface area per unit washcoat volume (m^{-1})
S_v	monolith internal surface area per unit monolith volume (m^{-1})
$S_{v,o}$	monolith external surface area per unit monolith volume (m^{-1})
T_g	exhaust gas temperature (K)
T_s	catalyst surface temperature (K)
T_{amb}	ambient temperature (K)
u	exhaust gas velocity (m/s)
ΔH	reaction enthalpy (J/mol)

Greek letters

Ω_{NH_3}	catalyst ammonia adsorption capacity (mol/m^3)
ε	void fraction of the monolith reactor
θ_{NH_3}	ammonia surface coverage
λ_s	thermal conductivity of catalyst
ρ_g	exhaust gas density (kg/m^3)
ρ_c	monolith density (kg/m^3)

Subscripts

ads	adsorption
des	desorption
g	gas phase
i	species index
j	reaction number
ox	oxidation
s	solid phase

1. Ammonia which is produced by the hydrolysis of urea is adsorbed on the catalyst.
2. NO_x reduction takes place using the adsorbed ammonia.
3. The remaining ammonia is desorbed from the catalyst to the gas flow.

There are also some side-reactions including the oxidation of ammonia at high temperatures.

The following reactions are considered in the mathematical model:

$$NH_3 \rightarrow NH_3^* \quad (1)$$

$$4NH_3^* + 4NO + O_2 \rightarrow 4N_2 + 6H_2O \quad (2)$$

$$4NH_3^* + 2NO + 2NO_2 \rightarrow 4N_2 + 6H_2O \quad (3)$$

$$4NH_3^* + 3NO_2 \rightarrow 3.5N_2 + 6H_2O \quad (4)$$

$$4NH_3 + 3O_2 \rightarrow 2N_2 + 6H_2O \quad (5)$$

$$4NH_3 + 5O_2 \rightarrow 4NO + 6H_2O \quad (6)$$

$$NH_3^* \rightarrow NH_3 \quad (7)$$

Reaction (1) is the adsorption of ammonia. Reactions (2)–(4) are NO_x reduction reactions. The oxidation of ammonia is described by reactions (5) and (6). Finally, reaction (7) is referred to as desorption of ammonia from the surface of the catalyst.

2.2. Modeling

A one-dimensional model was used in this paper. As discussed in previous literature [8,9], the basic governing equations including Navier–Stokes equations and conservation of energy and species were used to simulate the behavior of SCR. The following assumptions were taken into account in modeling:

- A single SCR honeycomb channel can represent the overall behavior of the SCR catalyst.
- Laminar flow (considering each channel's width and gas velocity).
- One-dimensional flow (axial).
- No pressure drop.
- Ideal gas conditions.
- Surface reactions with first order kinetics.
- No species diffusion between gas phase and solid phase (catalyst surface).
- Axial heat conductivity in the solid phase.

Using the definitions of the terms specified in the nomenclature section, energy balances for gas phase and solid phases are

$$\varepsilon\rho_g C_{p,g}\frac{\partial}{\partial t}T_g = -\varepsilon\rho_g C_{p,g}u\frac{\partial}{\partial x}T_g - hS_v(T_g - T_s) \quad (8)$$

$$(1-\varepsilon)\rho_c C_{p,c}\frac{\partial}{\partial t}T_s = (1-\varepsilon)\lambda_s\frac{\partial^2}{\partial x^2}T_s + hS_v(T_g - T_s) - h_o S_{v,o}(T_s - T_{amb}) + \sum_j \Delta H_j R_j S_a \quad (9)$$

Mass balances for gas phase and solid phase are:

$$\varepsilon\frac{\partial}{\partial t}C_{g,i} = -\varepsilon u\frac{\partial}{\partial x}C_{g,i} - k_{m,i}\cdot S_v\cdot(C_{g,i} - C_{s,i}) \quad (10)$$

$$(1-\varepsilon)\frac{\partial}{\partial t}C_{s,i} = k_{m,i}\cdot S_v\cdot(C_{g,i} - C_{s,i}) \pm \sum_j R_{i,j}S_a \quad (11)$$

where ε denotes the volume fraction of the catalyst which is not filled with exhaust gas, h is the heat transfer coefficient between gas and solid phase, h_o is the heat transfer coefficient between monolith wall and the environment, ΔH_j is the enthalpy of the jth reaction inside the catalytic converter, R_j expresses the rate of the jth reaction inside the catalytic converter, C is species concentration, $k_{m,i}$ is the mass transfer coefficient of the ith species and finally, $R_{i,j}$ represents the rate of the jth reaction inside the catalytic converter affecting the ith species. The reaction rates are those employed by Chi and DaCosta [13].

All the terms used in Eqs. (8)–(11) are defined to clarify what phenomena they represent:

Energy balance:

$$\text{Gas phase}: \begin{cases} \varepsilon\rho_g C_{p,g}\dfrac{\partial}{\partial t}T_g \rightarrow \text{accumulation} \\ \varepsilon\rho_g C_{p,g}u\dfrac{\partial}{\partial x}T_g \rightarrow \text{convection} \\ hS_v(T_g - T_s) \rightarrow \text{gas–solid heat transfer} \end{cases}$$

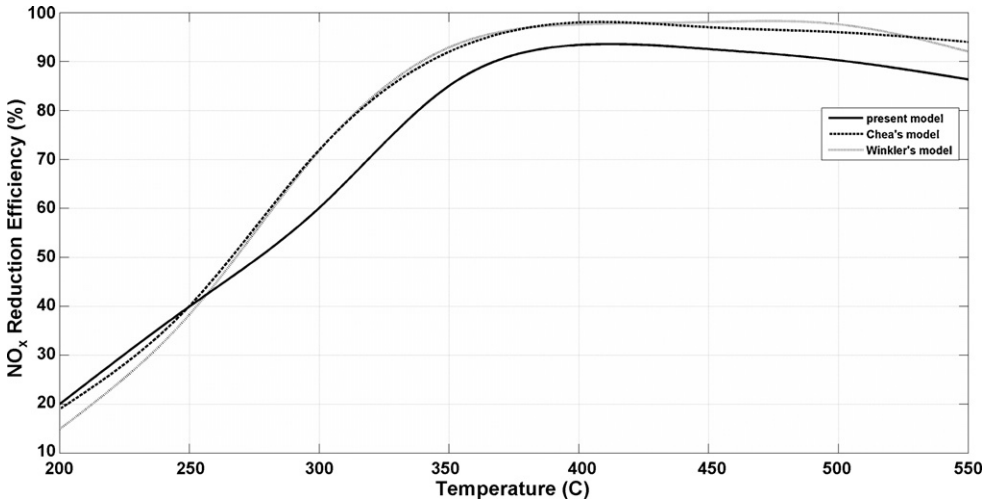

Fig. 1. A comparison between NO_x conversion efficiency calculated by the developed mathematical model and those of Winkler's and Chae's models.

$$\text{Solid phase}: \begin{cases} (1-\varepsilon)\rho_c C_{p,c}\dfrac{\partial}{\partial t}T_s \rightarrow \text{accumulation} \\ (1-\varepsilon)\lambda_s \dfrac{\partial^2}{\partial x^2}T_s \rightarrow \text{axial heat conduction} \\ hS_v(T_g - T_s) - h_o S_{v,o}(T_s - T_{\text{amb}}) \rightarrow \text{gas–solid heat transfer} \\ \displaystyle\sum_j \Delta H_j R_j S_a \rightarrow \text{released heat from chemical reactions} \end{cases}$$

Mass balance:

$$\text{Gas phase}: \begin{cases} \varepsilon\dfrac{\partial}{\partial t}C_{g,i} \rightarrow \text{accumulation} \\ \varepsilon u\dfrac{\partial}{\partial x}C_{g,i} \rightarrow \text{convection} \\ k_{m,i}\cdot S_v\cdot(C_{g,i} - C_{s,i}) \rightarrow \text{external mass transfer} \end{cases}$$

$$\text{Solid phase}: \begin{cases} (1-\varepsilon)\dfrac{\partial}{\partial t}C_{s,i} \rightarrow \text{accumulation} \\ k_{m,i}\cdot S_v\cdot(C_{g,i} - C_{s,i}) \rightarrow \text{external mass transfer} \\ \displaystyle\sum_j R_{i,j}S_a \rightarrow \text{catalytic reactions} \end{cases}$$

where convection indicates the change in temperature (in energy balance) and concentration (in mass balance) due to the flow through the channel.

Finally, ammonia surface coverage ($0 \le \theta_{NH_3} \le 1$) is obtained from the following equation:

$$\Omega_{NH_3}\cdot\frac{\partial}{\partial t}\theta_{NH_3} = R_{\text{ads}} - R_{\text{des}} - S_a(R_{\text{SCR}} + R_{\text{ox}}) \tag{12}$$

R_{ads}, R_{des}, R_{SCR} and R_{ox} correspond to the rate of ammonia adsorption on the catalyst surface, desorption of ammonia from the catalyst surface, reduction of NO_x and oxidation of ammonia respectively.

Initial and boundary conditions for the partial differential equations are as follows:

$$t = 0: \begin{cases} T_g(x) = T_s(x) = T_{\text{exhaust}} \\ C_{g,i}(x) = C_{s,i}(x) = C_{j,0} \\ \theta(x) = \theta_0 \end{cases}$$

$$x = 0(\text{inlet}): \begin{cases} T_g\,| = T_{\text{exhaust}} \\ \dfrac{\partial}{\partial x}T_s = 0 \rightarrow T_s\,| = T_s\,| \\ C_{g,i}\,| = C_{j,0} \end{cases}$$

$$x = L(\text{outlet}): \frac{\partial}{\partial x}T_s = 0 \rightarrow T_s\,| = T_s\,|$$

where m is the index of the grid points along the catalyst axis. In other words, n points (including inlet and outlet) are considered along the catalyst axis which divides it to $n-1$ equal parts. Therefore, $m = 1$ and $m = n$ are corresponding to $x = 0$ (inlet) and $x = L$ (outlet), respectively.

A computer code was developed in MATLAB® software environment to solve the system of 9 coupled partial differential equations; two equations for gas and catalyst temperatures, six equations for species concentrations in gas and solid phases (the species are NO, NO_2 and NH_3) and one equation for ammonia surface coverage using method of lines [10,11].

To confirm the validity of the developed model, the results of this model is compared to two other valid models presented by Winkler et al. [9] and Chae et al. [12] with the same inlet conditions in Fig. 1.

The comparison in Fig. 1 indicates that simulation results are almost in good agreement with two other valid models. Therefore, the model can be used to simulate the behavior of SCR catalytic converter.

3. Neural network model

Although the discussed mathematical model was developed to be as simple as possible, the run-time of the model is still a great concern. For example, it takes a 2.8 MHz CORE™ i7 cpu computer almost 4 min to solve the 400 by 100 grid system of governing partial differential equations in a single run. Therefore, the need to develop a neural network seems to be justified which leads to saving a great amount of time to obtain the necessary data at different initial conditions.

Table 1 shows the engine operating conditions used as the initial conditions to run the mathematical model [13]. The inputs and results (targets) are then used to develop the neural networks:

In Table 1, load refers to the injected fuel mass in an operating condition of the diesel engine per maximum injected fuel mass. Another parameter in this table is the space velocity which is one

Table 1
Engine operating conditions.

Mode	Engine speed (rpm)	Load (%)	Temperature (°C)	Space velocity (1/h)	Inlet NO_x conc. (ppm)
1	600	0	120	2081	150
2	1058	25	303	4444	749
3	1058	50	425	5907	1146
4	1058	75	493	7609	1294
5	1058	100	515	9532	1250
6	1321	25	290	6292	596
7	1321	50	368	8462	1045
8	1321	75	416	10880	1176
9	1321	100	470	13048	1215
10	1584	25	270	7871	497
11	1584	50	334	10493	778
12	1584	75	376	13166	1003
13	1584	100	439	14800	1133

of the inputs of the mathematical model. It stands for the volume of gas feed per hour per volume of the catalyst.

To develop a neural network, the following steps were taken:

- Assembling the training data (inputs and targets) derived from the mathematical model

The test modes in Table 1 provide the inputs for the neural network. As indicated in the table, each inlet NO_x concentration corresponds to a unique exhaust gas temperature. Therefore, the only parameter that can be used as a variable to control the system is the initial concentration of ammonia. Keeping the SCR inlet temperature and NO_x concentration constant, various amounts of ammonia were considered for each mode of the table. For each amount of ammonia the mathematical model was run and the obtained results were stored to be used to develop a neural network for each mode.

- Creating the network object

Considering exhaust gas temperature and inlet concentrations of NO and ammonia as the inputs and NO_x reduction efficiency and NH_3 slip as the output, a feed-forward neural network was created. Fig. 2 shows a schematic of this network.

As shown in Fig. 2, the network consists of an input layer, one or – if necessary – more hidden layers with various number of sigmoid neurons followed by an output layer of linear neurons. Applying multiple layers of neurons with nonlinear transfer functions makes the network capable of learning nonlinear and linear relationships between input and output vectors. In Fig. 3, a schematic of a two-layer network is shown:

In Fig. 3, **W** and **b** correspond to the weight and bias of the neuron. The transfer function for hidden layer is "tansig" and the one for output layer is "purelin" [14]. The same transfer functions were used in present paper's neural networks. Fig. 4 shows these transfer functions.

- Training the network

After creating the network, the training process begins. To train a network, a set of network inputs and target outputs is needed. A key parameter of the created feed-forward network is the performance function which must be minimized during training by adjusting the weights and biases of the network iteratively. The performance function we deal with in this paper is Mean Square Error (MSE) which is the average squared error between the network outputs and the target outputs.

$$\mathrm{MSE} = \frac{1}{N}\sum_{p=1}^{P}\sum_{i=1}^{N}(Yp,i\mathrm{real} - Yp,i\mathrm{predicted})^2 \quad (13)$$

where i is the index in the output layer, p is the number of inputs, $Y_{\mathrm{predicted}}$ is the network outputs and Y_{real} is the mathematical model outputs (target outputs).

The numerical optimization technique used for training the neural network is Levenberg–Marquardt backpropagation which is referred to as "trainlm" in MATLAB® neural network environment [14]. This training algorithm updates the weights and biases of the network in the negative gradient direction which leads to a fast decrease in performance function:

$$x_{k+1} = x_k - \alpha_k g_k \quad (14)$$

Eq. (14) shows a single iteration of this algorithm, x_k is the vector of current weights and biases, g_k is the current gradient and α_k is the learning rate.

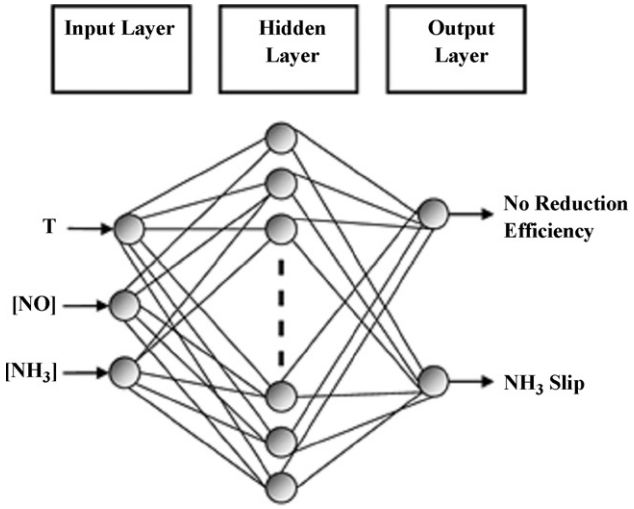

Fig. 2. A schematic of the neural network structure.

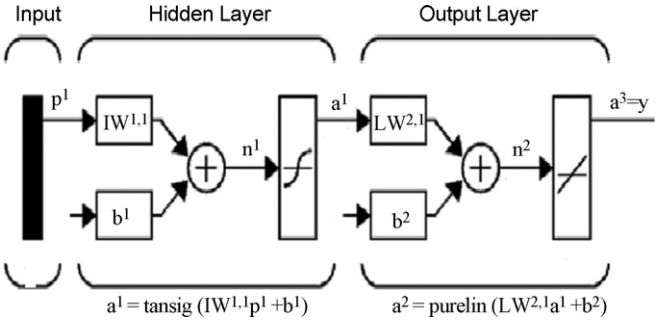

Fig. 3. A two-layer neural network [14].

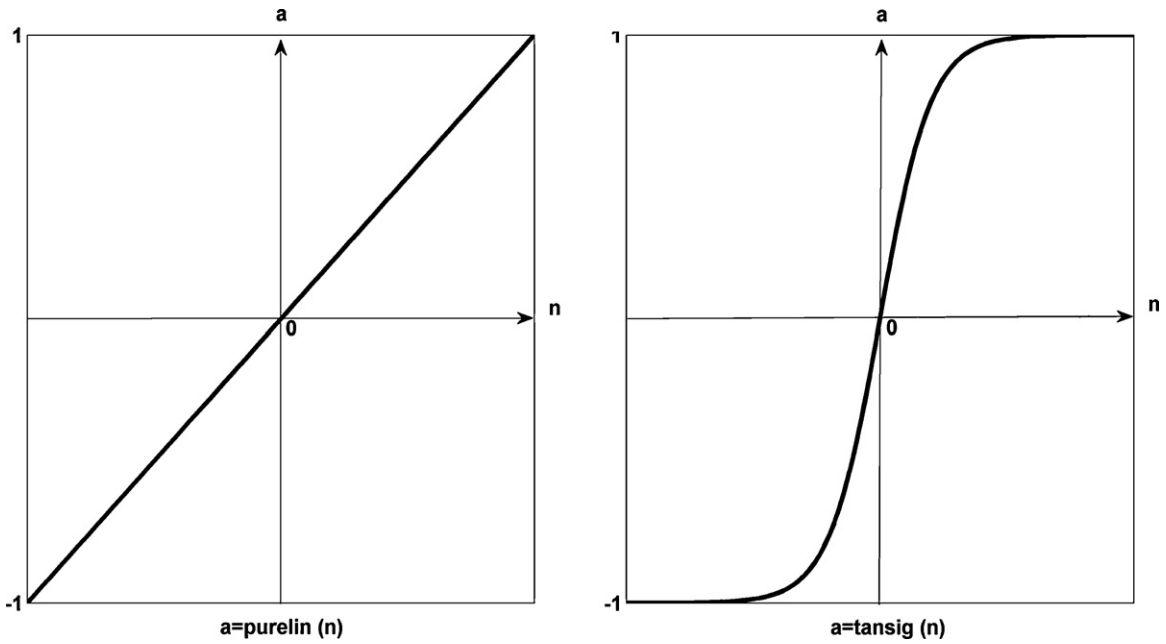

Fig. 4. Transfer functions used in the neural network.

4. Optimization

The purpose of optimizing a function is to maximize or minimize some of its variables through finding a set of design parameters that the mentioned variables are dependent on. There are various optimization techniques whose task is to find a set of optimal design parameters which minimize or maximize certain variables of a function.

In this paper, the objective of optimization is to find the optimal inlet ammonia concentration (as the design parameter) to maximize the NO_x conversion efficiency of SCR catalyst and minimize the ammonia slip simultaneously. Therefore, the multi objective genetic algorithm was applied due to its simplicity of use and robustness.

4.1. Multi-objective optimization problems (MOPs)

MOPs can be defined as below [15,16]:

$$\begin{cases} \min \vec{f}(\vec{x}) = \left\{ f_1(\vec{x}),\ f_2(\vec{x}), \ldots,\ f_k(\vec{x}) \right\}^T \\ x \in X = \left\{ \vec{x} \in R^n \,\middle|\, g_j(\vec{x}) \le 0\,(j = 1, \ldots, m) \right\} \end{cases}$$

where $\vec{x}$ is the vector of design variables that maximize or minimize k objective functions within m constrains. The objective of MOP is to find $\vec{x}$.

$\vec{f}$ and $\vec{g}$ are the functions of objectives and constrains:

$$\begin{cases} f_i(\vec{x}) = f_i(x_1, x_2, \ldots, x_n), i = 1, \ldots, k \\ g_j(\vec{x}) = g_j(x_1, x_2, \ldots, x_n), j = 1, \ldots, m \end{cases}$$

In many MOPs, the considered objectives are in conflict with each other. Therefore, it is impossible to achieve a solution that optimizes each objective function concurrently. The answer to such problems is a set of solutions, called *Pareto optimal*. But, before defining this term, the concept of *dominant* must be introduced. Assume that $\vec{x}_1$ and $\vec{x}_2$ are vectors in n-dimensional space ($\vec{x}_1, \vec{x}_2 \in R^n$) and f is a function. $\vec{x}_1$ dominates $\vec{x}_2$ if the following conditions satisfy:

$$\begin{cases} f_i(\vec{x}_1) \le f_i(\vec{x}_2)\,(\forall i = 1, \ldots, k) \\ \text{and} \\ f_i(\vec{x}_1) \prec f_i(\vec{x}_2)\,(\exists i = 1, \ldots, k) \end{cases}$$

A solution which is not dominated by any other solution in the solution space is known as *Pareto optimal*. The main characteristic of the Pareto optimal solution is that it cannot be improved with respect to an objective unless deteriorating at least one other objective. A set of all these non-dominated solutions is called *Pareto optimal set* and the corresponding objective function values in the objective space are the *Pareto front*. Finding the Pareto front, which consists of Pareto optimum solutions, is the major goal in MOPs [15–17].

4.2. Genetic algorithm (GA)

The genetic algorithm is based on natural selection which is the concept of biological evolution. In nature, weak species become extinct in their environment due to natural selection. The reason is that strong species are more likely to pass their genes to future generations through reproduction. Consequently, the species with the correct combination in their gens become dominant in their population after a number of generations [17]. This algorithm is suited to solve multi-objective problems because:

- The ability to search various regions of the solution space enables it to find diverse solutions even in non-convex, discontinuous and multi-modal solution spaces.
- The user does not have to prioritize, scale or weight objectives.

There are several GAs for MOPs and they usually have the same working pattern including the following steps [15,17]:

- *Step 1* (Initialization): The individuals (search points) are initialized.
- *Step 2* (Evaluation): The fitness value of each individual is evaluated by Pareto ranking. For each solution, Pareto ranking is the

Table 2
Genetic algorithm optimization parameters.

Parameter	Definition	Value/type
Number of generations	Maximum number of iterations	400
Population size	The number of individuals in the optimization process	60
Crossover fraction	The fraction of the next generation that crossover produces	0.8
Mutation function	The assigned function randomly generates directions with respect to the last successful or unsuccessful generation	Adaptive feasible
Stopping criteria	Function tolerance: the algorithm stops if the cumulative change in fitness function value is less than this value.	0.0001

number of solutions dominant to the focused solution +1. The fitness value is reciprocal number of the Pareto ranking.

- *Step 3* (Selection): According to the fitness values, some of the individuals are selected.
- *Step 4* (Reproduction): If the terminal condition is not satisfied, new search points must be generated. The operators that GA uses to generate new solutions are *crossover* and *mutation*. Crossover results in the convergence of the population by making the individuals alike. On the other hand, mutation applies random changes to the individuals to avoid the search from local optima. Usually, a combination of these operators is applied.
- *Step 5*: The process repeats from step 2.

As the described process goes on and the number of generations increases, the population evolves and the optimal solution is obtained.

In multi objective genetic algorithm optimization, the concept discussed above is used to minimize the objective vectors. Since one of the objectives in the SCR catalytic converter (NO_x conversion efficiency) is to be maximized, all the members of this objective vector were inversed in order to be used in the algorithm.

In this paper, fast non-dominated sorting genetic algorithm (NSGA-II) [18] was used. To use this algorithm in MATLAB®, some parameters must be introduced to the software including the number of variables, the objective function and also suitable constrains. The created neural network was used as the objective function which returns separate objective vectors for NO_x conversion efficiency and ammonia slip. Ammonia inlet concentration was considered to be the only variable of the system. The system variable constrains were defined in the form of lower and upper bounds.

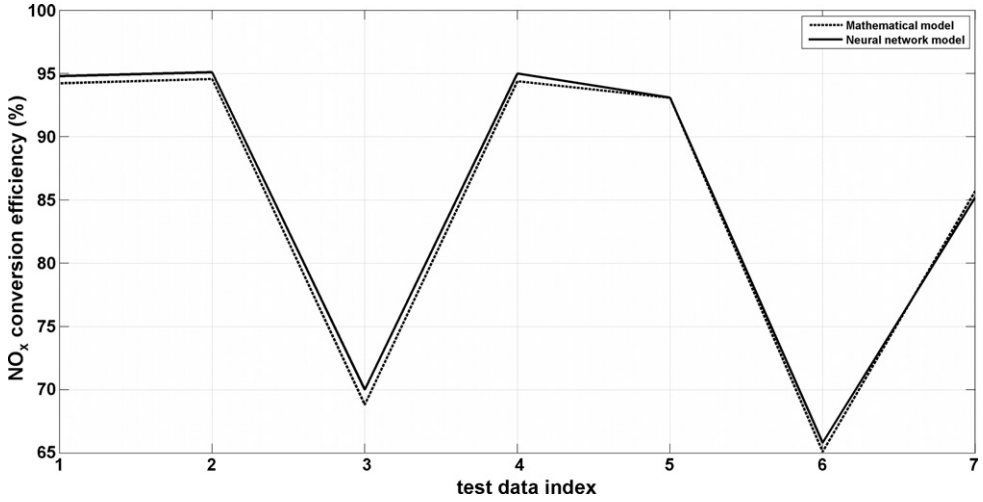

Fig. 5. Verification of the neural network response (NO_x conversion efficiency) to random test data.

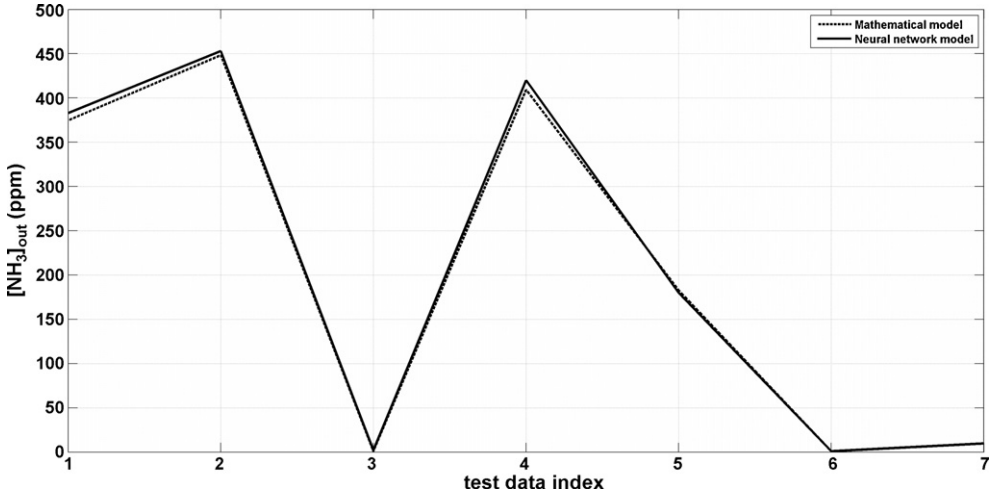

Fig. 6. Verification of the neural network response (NH_3 concentration) to random data.

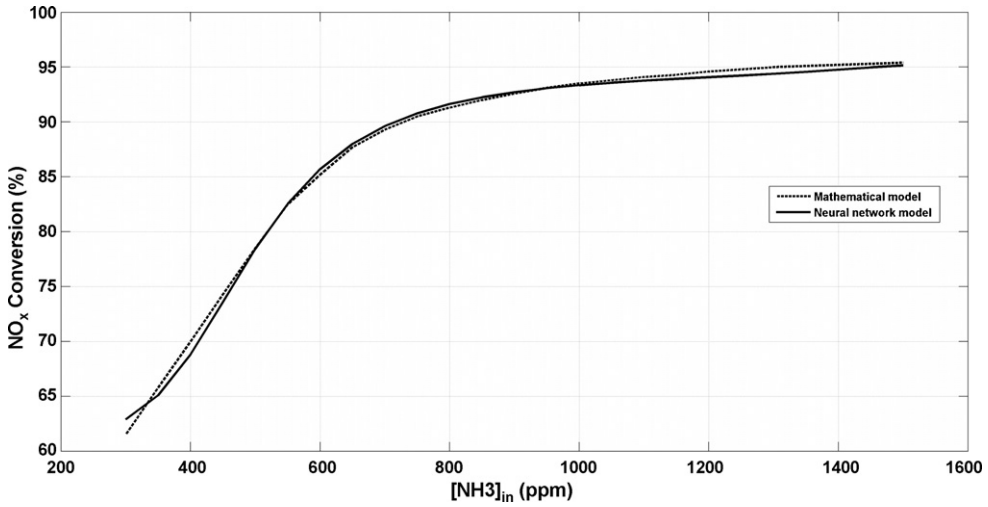

Fig. 7. Comparison of the mathematical model results and the neural network results (NO_x conversion efficiency).

The parameters used in the genetic algorithm optimization are presented in Table 2:

5. Results and discussion

5.1. Neural network simulation results

To observe how the whole process functions, we shall consider mode 3 in Table 1 as an example. Twenty-five runs were performed on the mathematical model of the SCR, each one with a different inlet ammonia concentration. A set of 18 input/output data was used to train a neural network and the remaining data was used to test it. A computer code was developed to extract totally random test data in order to verify how well the network has been trained.

Figs. 5 and 6 show the neural network test results for NO_x conversion efficiency and output concentration of ammonia as the targets of the network, respectively.

According to Figs. 5 and 6, the created network was trained properly and it is able to give reasonable answers when it is fed with the inputs that it has never seen before. Therefore, the mathematical model can be replaced with the neural network in this particular mode.

In Figs. 7 and 8, the responses of the mathematical model to Euro test set mode 3 conditions were compared to those of the neural network.

5.2. Optimizations results

The optimization was run and terminated after 212 iterations for test mode 3. Fig. 9 shows the Pareto front plot of the objectives.

As shown in Fig. 9, the optimal result is highlighted and has the coordinates of (88, 24). This point corresponds to inlet ammonia concentration of 674 ppm. In other words, for mode 3, with the inlet NO_x concentration of 1146 ppm, the best amount of ammonia which results in the optimal performance of SCR catalytic converter (88% reduction of NO and 24 ppm ammonia slip) is 674 ppm.

Obviously, the demand to increase NO_x conversion efficiency results in ammonia slip exceeding the maximum allowed value of 25 ppm and acting as a pollutant – known as unregulated emission – itself. On the other hand, moving toward lower ammonia slip decreases the ability of the SCR catalyst to reduce NO_x. In other words, improving the solution with respect to one objective leads to worsening the other objective. As indicated before, this is the main concept of the Pareto optimal solution.

In Fig. 10, the optimization result of test mode 5 is shown.

In this mode, the optimal point has the coordinates of (57, 21) that occurs at inlet ammonia concentration of 876 ppm. As demonstrated in Fig. 10, the trend is similar to that of mode 3, but the NO_x conversion efficiency has decreased distinctly. This decrease is caused by the 90° initial temperature difference between mode

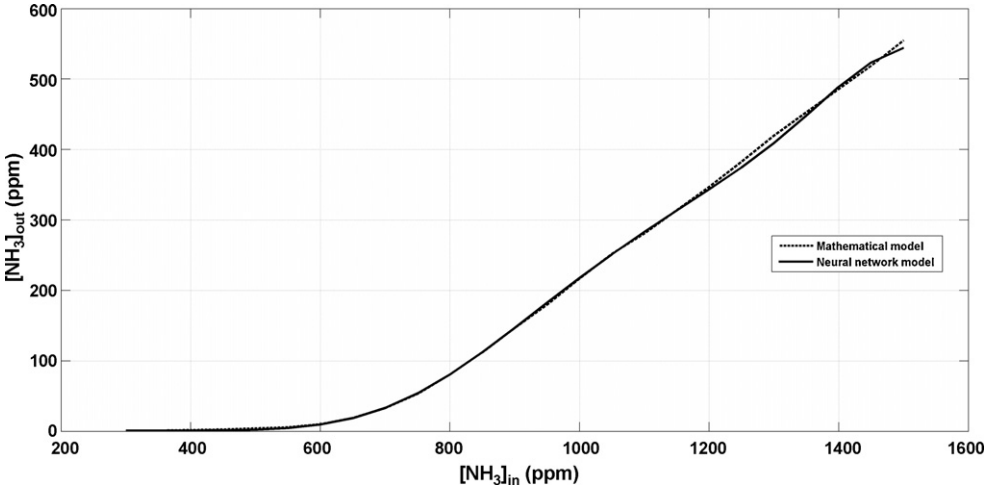

Fig. 8. Comparison of the mathematical model results and the neural network result (ammonia output concentration).

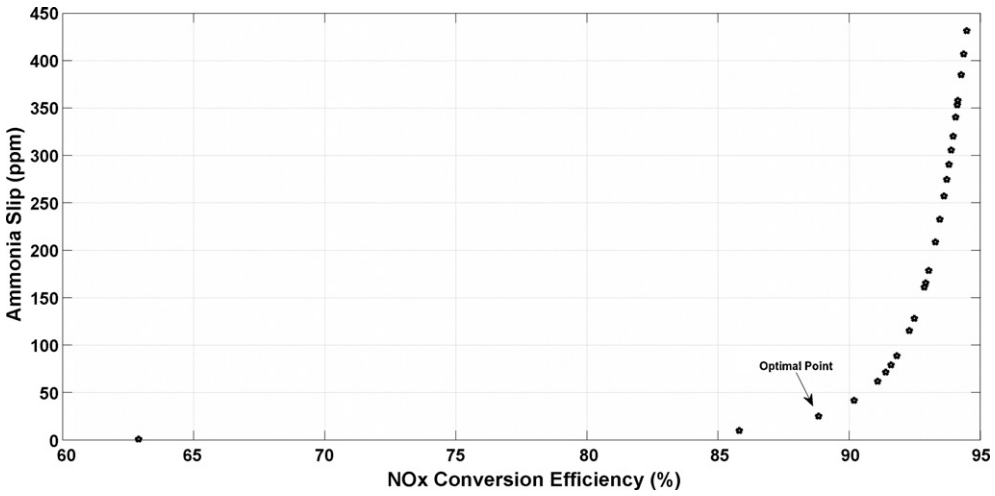

Fig. 9. Optimization result (Parteo front) for mode 3.

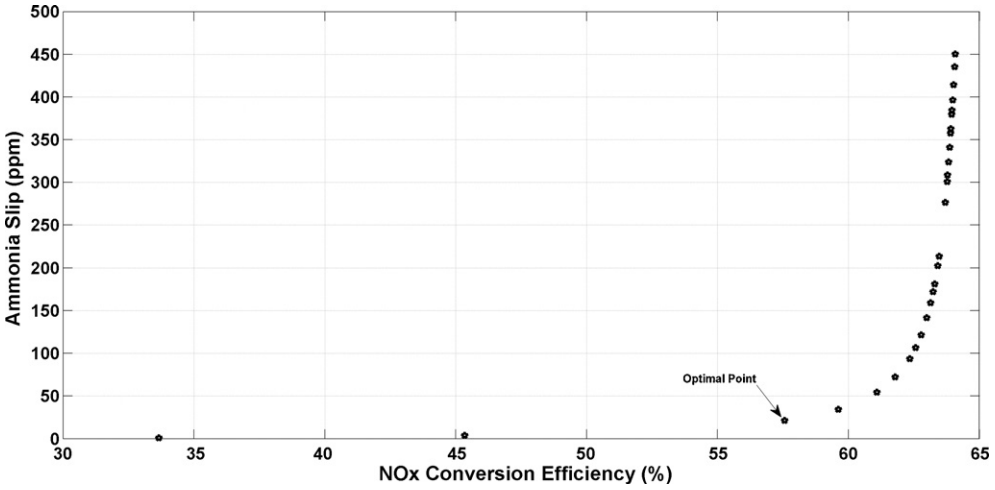

Fig. 10. Optimization result (Parteo front) for mode 5.

Table 3
Optimization results for the engine speed of 1058 rpm.

Mode	Temperature (°C)	Inlet NO_x conc. (ppm)	Optimal NH_3 (ppm)	NO_x conversion (%)	NH_3 slip (ppm)
2	303	749	586	86	6.3
3	425	1146	674	88	24
4	493	1294	901	70.6	24.6
5	515	1250	876	57	21

3 and mode 5. As the temperature inside the SCR catalyst exceeds a certain value (around 450 °C), ammonia oxidation takes place especially through reaction (5). The product of this reaction is NO. Therefore, increasing the temperature leads to a decrease in NO_x conversion efficiency and also ammonia slip.

Finally, the optimization results for modes 2–5 (engine speed = 1058 rpm) of Table 1 are summarized and presented in Table 3:

The applied genetic algorithm (NSGA-II) is one of the most efficient, fast convergent and well tested algorithms suitable for multi-objective problems. However, NSGA-II uses a crowding distance method to determine the population density around a solution in order to obtain a uniform spread of solutions along the best-known Pareto front [17]. The main drawback of this method is that crowding distance is capable of working in the objective space only. Therefore, NSGA-II might be surpassed by another method known as *Strength Pareto Evolutionary Algorithm* (SPEA-2) [19].

6. Conclusion

With the intention of saving time and computational efforts, the conventional mathematical model of SCR catalytic converter was replaced with a neural network model. Then, it was used as an objective function to optimize the performance of the SCR catalytic converter using multi objective genetic algorithm. The purpose of optimization was to find the best amount of inlet ammonia concentration for each inlet NO_x concentration in order to maximize the NO_x conversion efficiency and to keep the ammonia slip under a certain amount simultaneously.

As predicted, NO_x conversion efficiency increased with increasing inlet ammonia concentration and it resulted in high ammonia slip which is not favored at all. Thus, in order to accomplish both objectives, the optimal point which had the highest possible NO_x conversion efficiency while keeping the ammonia slip below 25 ppm was chosen at each mode.

The main achievements of this paper are

- By substituting the SCR catalytic converter model with neural network model, the run time was decreased from almost 4 min to almost real-time speed.
- Finding the optimized inlet ammonia concentration through multi objective genetic algorithm resulted in the highest possible NO_x efficiency and low ammonia slip.

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