

Modeling of NO_x Emmissions in Internal Combustion Engine

Naim DONMEZ¹, and Orkun OZENER²

¹Automotive Division, Mechanical Engineering Faculty

Yıldız Technical University
34349 Istanbul
Turkey

ABSTRACT

In order to reduce fossil fuel emissions, which are among the biggest threats of human health in the global world, regulations are getting harder every day. Many technologies continue to be developed to reduce/eliminate emissions during combustion (at the source) or after combustion. Instead of physical sensors used for the measurement of emissions, virtual sensors (VS) are developed and used by physical, gray box and black box modeling methods. In the current study, the NO_x emissions generated at the engine output are modeled with steady state data by semi-physical modeling technique. The studies were carried out with data from 13 l, 6 cylinder and 353 kW diesel engine. The physical value used for the model is the maximum temperature calculated via a temperature sub-model based on the in-cylinder pressure measurement. The input data of the model are; calculated engine power at the electronic control unit (ECU), the estimated exhaust gas recirculation (EGR) ratio from ECU, the fuel rail pressure, the amount of injected fuel per stroke and the amount of trapped in cylinder air mass. The NO_x model created by these parameters are converted into empiric formula by statistical methods. The engine NO_x sensor data used as the target output data for validating and training the model parameters. Then validation results showed that the prediction accuracy of the developed NO_x model is between 1% and 10% range that can be acceptable for internal combustion applications.

Key Words: NO_x, NO_x modeling, Semi-physical modeling, Diesel engine, Exhaust emissions.

1. INTRODUCTION

It is very difficult to predict the amount of engine out emissions from internal combustion engines. This is due to the time-dependent variation of the combustion mechanism, fuel mixture ratio, cycle temperatures and pressure within the combustion chamber. The variables here are dynamic [1]. Estimation methods of emission generation process is based on the methods of thermodynamic assumptions, invariant constants or approximation theories. At present, emission models are efficiently used by engine developers both in dynamometer tests and via embedded models on the ECU [2]. In the case of internal combustion engines, data is sent to the ECU with instant sensor measurements. Depending on the driving variables (i.e. engine speed, accelerator pedal position, road conditions), a strategy (i.e. fuel injection angle, spray fuel-urea quantity) is followed for obtaining optimum fuel consumption-emission outputs regarding to targets. Considering to the todays automotive industry cost efficiency targets, engine manufacturers and researchers have developed real-time VS and related prediction algorithms to predict the target physical values [3]. In this context, VS are used to reduce component costs by replacing physical nitrogen oxide sensors and develop on-board diagnostic. Along with increasing solid emission limits, measurement is required activity to learn and optimize the formation of nitrogen oxides in diesel engines for VS. Data calculated via VS is also transmitted to the ECU, and is used for following the proposed strategies or error prevention. For example, today the data from the VS controls the efficiency of the NO_x conversion and SCR dosing control. There are some applications that use predictive algorithms to replace the physical NO_x sensor [1].

The first is the algorithm to diagnose the presence of the NO_x sensor physically with this algorithm coded on the ECU, it is checked whether the NO_x in the exhaust emissions are measured or not and the NO_x sensor is working properly [4]. The second application is the complete removal of the physical NO_x sensor. Development of the engine out NO_x predictive VS instead of the physical sensor, presents the advantages in terms of material supply, integration and ECU cabling [1].

On the other hand, the VS presents some disadvantages in case of accuracy problems. Incorrect measurement data from VS that is not accurate may cause incorrect NO_x conversion on the SCR system and as a reason NO_x emission exceeds the exhaust emission limits.

There are three types of models for NO_x estimation. These are,

- Physical models: Complex thermodynamic and combustion processes and high calculation process [5]
- Gray box (semi physical) models: Medium calculation process obtained by simplification of physical models
- Black box models: Including very few physical formulas and artificial neural networks, low calculation process [6]

The necessary steps for the creation of gray box and black box the models are:

- Input identification and model design,
- Model training,
- Validation [7]

The advantage of black box models are that they offer a minimum calculation time. However, assuming that the data based estimation is insufficient, it cannot be assumed that the model will work correctly under all circumstances. Many experimental studies that the engine parameters are varied is required for black box modeling calibration. Physically based and gray box based models are cost-disadvantageous due to the fact that they need computation time and sensor sets. However, a physically based or gray box based models created in research centers will require less data for NO_x estimation [6]. These model types uses engine-mapping data for training the models. In a gray box model to be created, the use of parameters based on physically based models will provide comprehensive and high quality estimation results. It was decided to use the non-integral estimation of the gray box model because the engine, test devices and sensor sets to be used for the estimation of nitrogen oxide emissions were sufficient [8].

In this study, the NO_x emissions are modelled with non-integral semi physical modelling technique. Engine test results taken from dynamometers are used to train NO_x model. At the second step the model validated with new set of test points and the accuracy is tested. The results showed that the developed model is presenting good accuracy results and it can be used as a VS model in the ECU units for NO_x estimation.

2. MATERIAL AND METHODS

2.1 Experimental setup

In this study, a 13 l, 6 cylinder, turbocharged, diesel engine, which can produce a maximum power of 353 kW at Euro 6 emission standard, was used for experimental works. Engine properties are given at Table 1. The load to the engine was provided by an AVL APA INDY S50-4/3001 500kW AC Dynamometer with motoring and absorbing capability for both steady and transient conditions. The engine is instrumented with integrated with speed sensors, pressure transducers, thermocouples, fuel flow meters and in-line torque meter. The fuel consumption was measured by AVL735 Coriolis fuel measuring which was controlled and monitored by PUMA software. The cylinder pressure was measured using AVLGH22C model pressure sensor which was mounted on the cylinder head. The cylinder pressure signal was passed through AVL Indismart charge amplifier. The crankshaft position was obtained using a crank angle sensor to determine the cylinder pressure as a function of the crank angle. [9] The INCA program [10] is used to check the engine parameters and PUMA is the program where the sensor measurement data is read. The data was converted to model on MATLAB program.

Table 1. Properties of test engine

Engine type	Diesel
Emission type	Euro 6
Displacement (L)	13
Number of cylinders	6
Stroke (mm)	144
Rod(mm)	230
Diameter of piston (mm)	115
Compression ratio	17

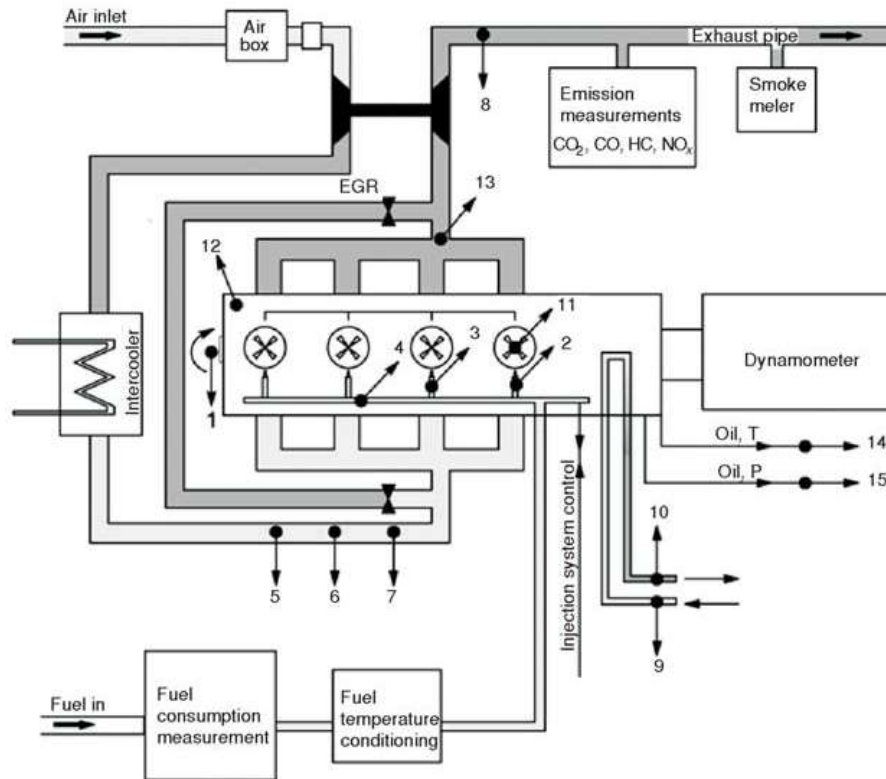


Figure 1: Experimental set-up [11]

2.2 Input Identification and Model Design

2.2.1 Input identification

When installing the gray box model, five selected ECU data is used as input for the system. In-cylinder maximum temperature data is calculated using via the in-cylinder pressure sensor from the test engine [5], [12]. Fuel consumption and rail pressure data that can be read from the ECU [13]. Total air quantity is the sum of the mass of air measured by the physical MAF sensor on the engine and the mass of EGR in the ECU. EGR / air ratio is the ratio of the EGR mass information in the ECU with the total air quantity in the ECU [8], [14]. Power is an information that has a map in the ECU (from speed and torque information) [5]. The maximum temperature in the cylinder is the white box part of the gray box model consisting of sensor information and theoretical physical formulas. The model inputs and outputs are identified at Figure 2.

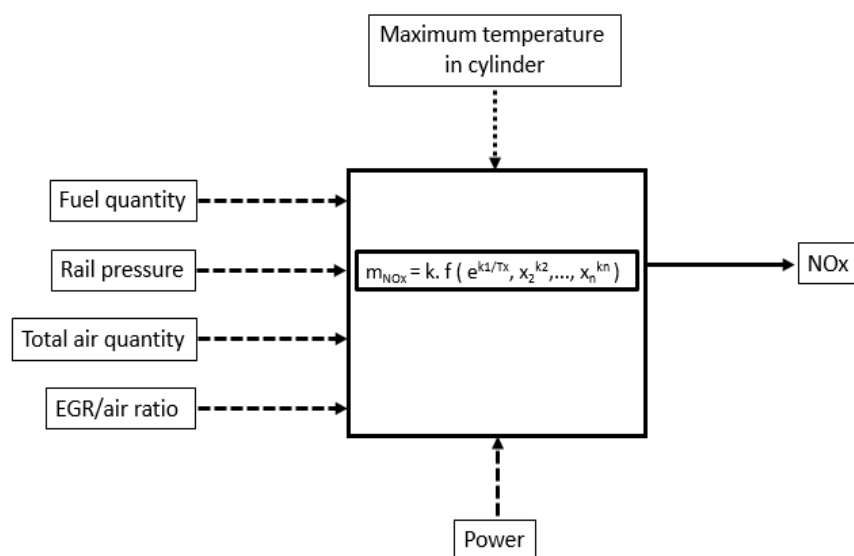


Figure 2: Gray box model inputs

2.2.2 Cylinder temperature model

The maximum temperature of gases, T_{max} is calculated as function of in cylinder pressure. The calculation starts from the pressure at the intake valve opening position and ends at the pressure at the exhaust valve closing position.

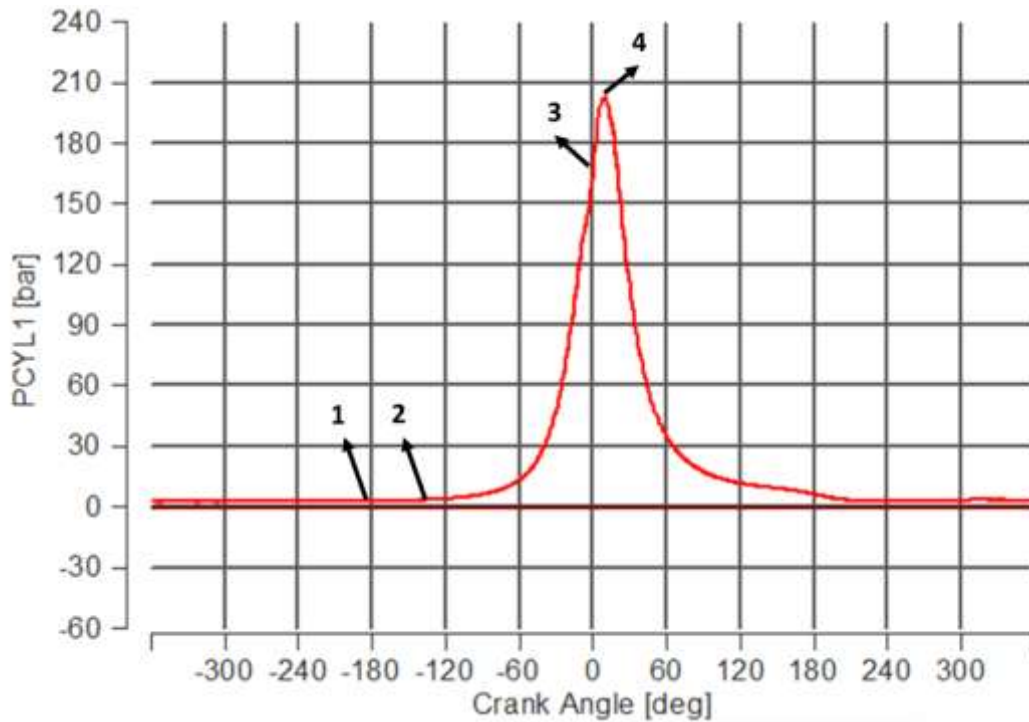


Figure 3: Indicating measurement

The combustion equation according to the first law of thermodynamics:

$$\eta_y H_u = U_4 - U_2 + L_{2,4} \tag{1}$$

In this equation, the total work generated by the difference in the internal energy change of the gas between 2 and 4 is equal to the total heat energy of the air-fuel burning in the cylinder. The internal energy change at point 2 can be written as follows:

$$U_2 = U'_2 + U''_2 \tag{2}$$

The total work between points 2 and 4 is expressed by the following equation:

$$L_{2,4} = P_4 V_4 - \rho P_2 V_2 \tag{3}$$

$$P_4 V_4 = (n_{yu} + n_r) \bar{R} T_4 \tag{4}$$

$$P_2 V_2 = (n_e + n_r) \bar{R} T_2 \tag{5}$$

If 4th and 5th equations are written into the 3rd equation:

$$L_{2,4} = (n_{yu} + n_r) \bar{R} T_4 - \rho (n_e + n_r) \bar{R} T_2 \tag{6} \quad \text{the equation was found.}$$

The theoretical coefficient of variation μ is calculated as follows:

$$\mu = \frac{(n_{yu} + n_r)}{(n_e + n_r)} \tag{7}$$

The residual gas coefficient γ_r is calculated as follows:

$$\gamma_r = \frac{n_r}{n_e} \tag{8}$$

If all these equations are written into equation 1, the following equation is found:

$$\frac{(\eta_y H_u)}{n_e(1+\gamma_r)} + \frac{u_2'+\gamma_r u_2''}{1+\gamma_r} + \bar{R}\rho T_2 = \mu(u_4'' + \bar{R}T_4) \quad (9)$$

According to equation 9, the $T_4 = T_{max}$ temperature is the maximum burnt gas temperature in the cylinder. The mathematical model created in MATLAB program was fed with the data taken from the test engine and the temperature was calculated for each test point. [12]

2.2.3 Model design

The reference model to be fed with the data from the test engine is formed as follows to generate estimates in steady state points:

$$m_{NOx} = K \cdot P^{k_1} \cdot q_{tot}^{k_2} \cdot e^{\frac{k_3}{T_{max}}} \cdot P_{rail}^{k_4} \cdot \left(\frac{m_{egr}}{m_{air}}\right)^{k_5} \cdot m_{air}^{k_6} \quad (10)$$

In which, m_{NOx} is the mass of NO_x emissions, P is the power, q_{tot} is the quantity of fuel, T_{max} is the maximum temperature in cylinder, P_{rail} is the pressure of rail, m_{egr} is the mass of EGR gases, m_{air} is the total mass of gases taken into the cylinder and K, k_1 , k_2 , k_3 , k_4 , k_5 , k_6 are the coefficient parameters.

3. RESULTS AND DISCUSSIONS

3.1 Model Training

The engine mapping test consisting of 186 data was performed to train the reference model. The speed-torque points of the test are shown in Figure 4.

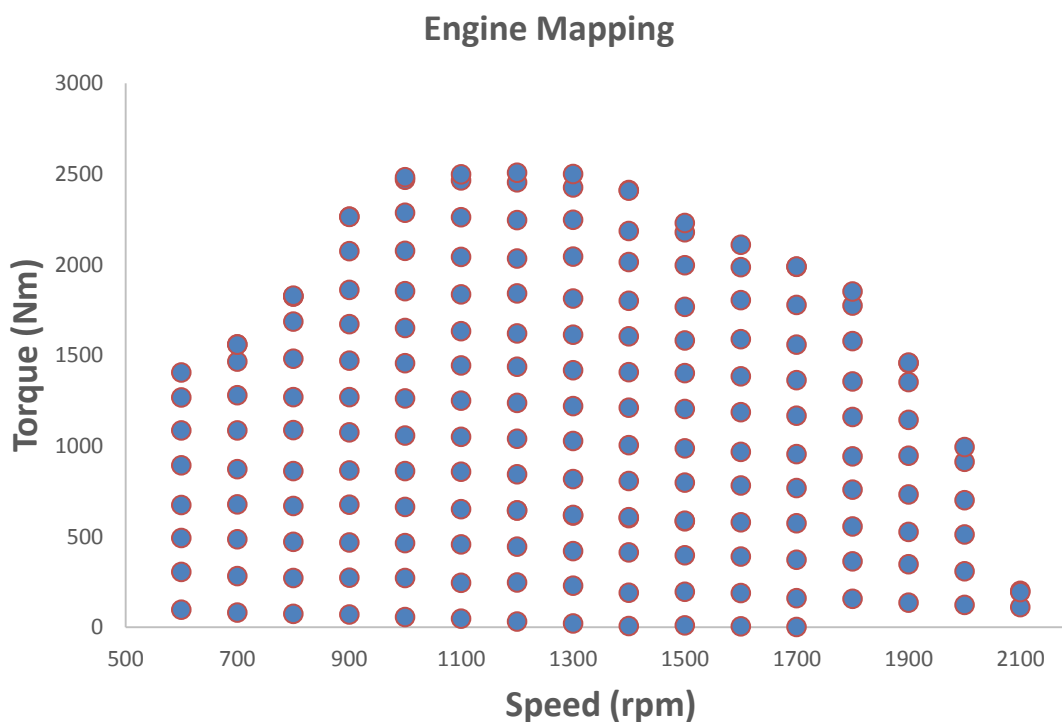


Figure 4: Engine mapping test speed - torque points

Log-log regression method [15] was used for coefficient estimation in the model equation. In this way, coefficients are estimated in MATLAB program. According to the results, the new model formula is as follows:

$$m_{NOx} = 2,385 \cdot P^{0,083} \cdot q_{tot}^{0,831} \cdot e^{\frac{3930,62}{T_{max}}} \cdot P_{rail}^{1,343} \cdot \left(\frac{m_{egr}}{m_{air}}\right)^{-0,14} \cdot m_{air}^{-1,683} \quad (10)$$

The results of regression statistics for training data are shown in Figure 5.

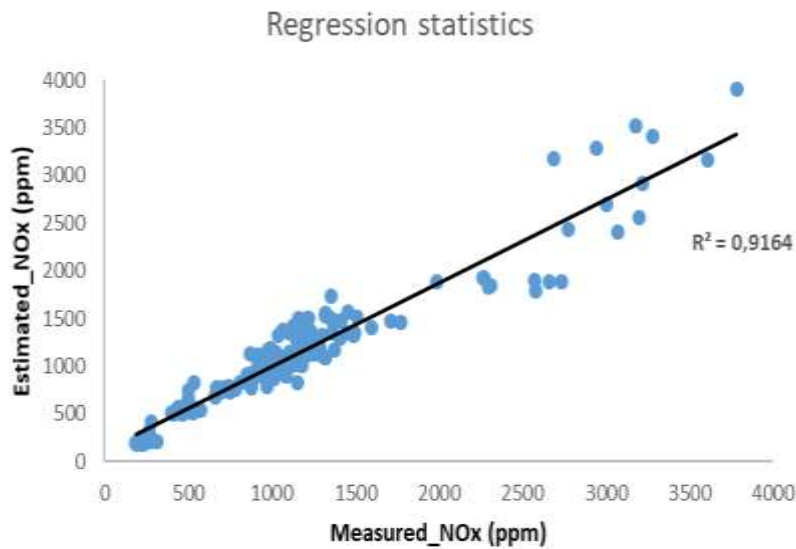


Figure 5: Regression statistics

The NO_x estimation of training data is as given at Figure 6.

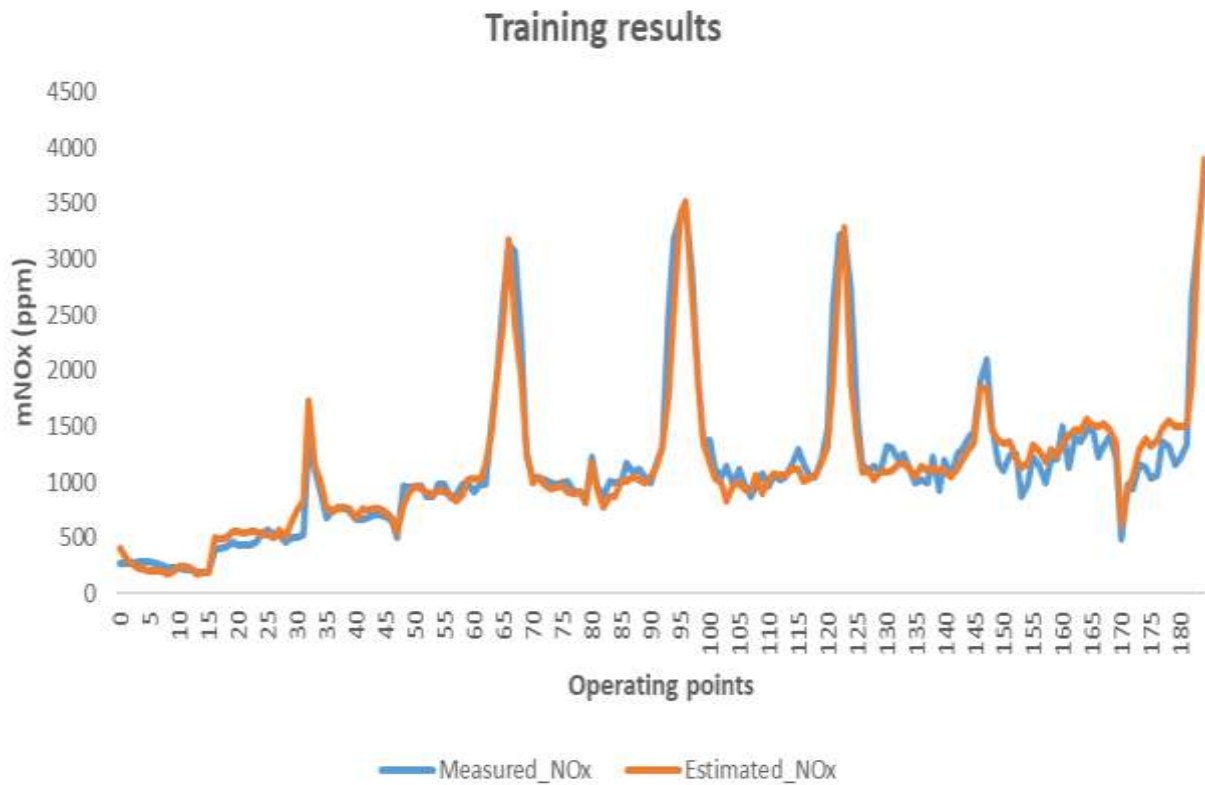


Figure 6: Training data results

3.2 Validation

The model formula obtained from the training data is validated with the data obtained from the test engine and the model accuracy is checked. The test points to be validated in the test engine were selected as given at Table 2.

Table 2. Validation point inputs

	Speed(rpm)	Power (PS)	q _{tot} (mg/str)	P _{rail} (bar)	m _{air} (kg/h)	m _{EGR} (kg/h)	T _{max} (K) (math. model)
1	1000	123.30	89.02	974.605	615.83	124.8	2185.67
2	1200	144.17	87.00	1100.131	758.04	129.0	2057.54
3	1400	160.98	88.06	1400.465	910.10	184.8	2101.12
4	1600	178.85	86.37	1760.436	1058.32	241.0	2177.36

5	1800	195.22	85.65	1999.448	1207.59	278.3	2087.30
6	2000	201.08	82.02	1950.057	1087.17	70.0	2194.84
7	1200	316.91	186.23	1360.037	1134.73	169.3	2294.28
8	1400	362.16	188.09	1644.361	1340.82	209.4	2300.81
9	1600	414.72	193.03	2080.540	1455.39	227.2	2480.90

When validation data is applied to the model, the estimated NO_x mass and the measured NO_x mass are as follows:

Table 3. Comparison of NO_x data between measured and estimated

	Measured NO _x (ppm)	Estimated NO _x (ppm)	Difference *
1	1030.4	1063.7	-3%
2	1044.2	1005.4	4%
3	1002.8	976.7	3%
4	1027.3	942.2	8%
5	902.1	966.4	-7%
6	1294.0	1178.1	10%
7	1157.0	1139.4	2%
8	1105.3	1119.1	-1%
9	1121.1	1220.5	-9%

* = ((Estimated – Measured)/Measured) x 100

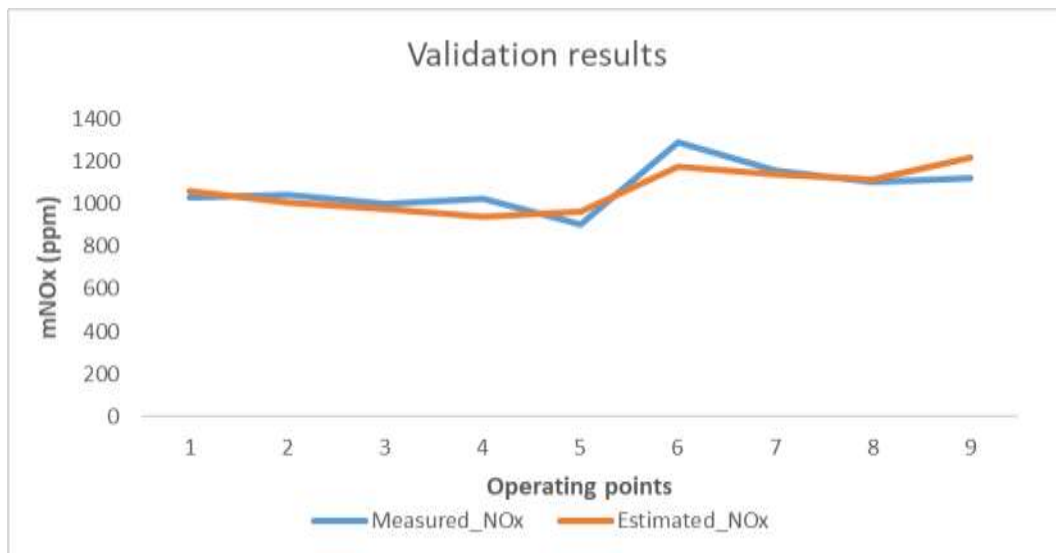


Figure 7: Validation results

The validation results showed that the minimum prediction error is 1% and the maximum prediction error is obtained as 10% range, which can be acceptable range.

4. CONCLUSION

In this study, a semi-physical (gray box) model was developed for NO_x estimation for use in steady state measurements of internal combustion diesel engines. The model estimates the NO_x emission with the data generated at the steady state points of the test engines tested at the dynamometer. The model forms the measurable inputs of the gray box model with internal and external (in cylinder pressure sensor) sensors on the engine. The model was trained with engine mapping test data and validated with randomly selected operating point data. The obtained model coefficient estimation results are within the targeted results for this study. When the data selected for validation were applied to the new model, the estimation error rate was 5.5%. The study can be used to confirm the accuracy of the NO_x emission measured during the dynamometer tests of the test engines at the development stage.

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