Prediction of NO_X Vehicular Emissions using On-Board Measurement and Chassis Dynamometer Testing

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Abstract -

Motor vehicles' rate models for predicting emissions of oxides of nitrogen (NO_X) are insensitive to their modes of operation such as cruise, acceleration, deceleration and idle, because these models are usually based on the average trip speed. This study demonstrates the feasibility of using other variables such as vehicle speed, acceleration, load, power and ambient temperature to predict NO_X emissions. The NO_X emissions need to be accurately estimated to ensure that air quality plans are designed and implemented appropriately. For this, we propose to use the non-parametric multivariate adaptive regression splines (MARS) to model NO_X emission of vehicle in accordance with on-board measurements and also the chassis dynamometer testing. The MARS methodology is then applied to estimate the NO_X emissions. The model approach provides more reliable results of the estimation and offers better predictions of NO_X emissions. The results therefore suggest that the MARS methodology is a useful and fairly accurate tool for predicting NO_X emission that may be adopted by regulatory agencies in understanding the effect of vehicle operation and NO_X emissions.

Keywords -

Nitrogen Oxide; On-Board Emission Measurement System; Chassis Dyanmometer Testing System; Emission

1 Introduction

Vehicular emissions can bring serious impacts on the air quality, and have thus received increasing research concerns [1]. Outdoor air pollution is estimated to cause 1.3 million annual deaths worldwide [2]. Road transport often appears as the single most important source of urban pollutant emissions in source apportionment studies [3]. In the coming decades, road transport is likely to remain a large contributor to air pollution, especially in urban areas. For this reason, major efforts are being made for the reduction of polluting emissions from road transport. These include new powertrains and vehicle technology improvements, fuel refinements, optimization of urban traffic management and the implementation of tighter emission standards [4]. In recent decades, many emission models have been developed. Afotel *et al.* [5] proposed regression models to estimate light-duty gasoline vehicle emissions of CO_2 based on vehicle velocity, acceleration, deceleration, power demand and time of the day. However, the model did not include NO_X emissions. Oduro *et al.* [6] proposed multiple regression models with instantaneous speed and acceleration as a predictor variables to estimate vehicular emissions of CO_2 but not NO_X. Tóth-Nagy *et al.* [7] proposed an artificial neural network-based model for predicting emissions of CO and NO_X from heavy-duty diesel conventional and hybrid vehicles. The methodology sounds promising, but applied to heavy-duty vehicles only, and the fit function contains many details which make the model difficult to understand. Emission model based on instantaneous vehicle power, which is computed on total resistance force, vehicle mass, acceleration, velocity, and drive-line efficiency, was developed by Rakha *et al.* [8]. However, the model applies for fuel consumption and CO_2 emission factor and does not include the NO_X emission.

A key gap in our understanding of these emissions is the effect of changes in vehicle speed, power and load on average emission rates for the on-road vehicle fleet. Vehicle power, load and vehicle speed are closely linked to fuel consumption and pollutant emission rates [9]. Improved understanding of the link between operating conditions and emissions could develop accurate models for prediction of vehicle emissions. The quality of the application of any road vehicle emission model largely depends on the representativeness of the emission factor such as carbon dioxide (CO_2), carbon monoxide (CO), nitrogen oxides (NO_X), volatile organic compounds (VOCs) and particulate matter (PM). This refers to the accuracy with which the emission factor can describe the actual emission level of a particular vehicle type and driving conditions applied to it.

This work focuses on using the MARS methodology to improve the prediction accuracy of chassis dynamometer and on-board measurement systems. The dynamometer testing is one of the three typical vehicle tailpipe emission measurments methods, where emissions from vehicles are measured under laboratory conditions during a driving cycle to simulate vehicle road operations [10]. The real world on-board emissions measurement is widely recognized as a desirable approach for quantifying emissions from vehicles since data are collected under real-world conditions at any location travelled by the vehicle [11]. Variability in vehicle emissions as a result of changes in facility (roadway) characteristics, vehicle location, vehicle operation, driver, or other factors can be represented and analysed more reliably than with the other methods [12]. This is because measurements are obtained during real world driving, eliminating the concern about non representativeness that is often an issue with dynamometer testing, and at any location, eliminating the setting restrictions inherent in remote sensing. Though this measuring technique seems to be more promising, the need to improve the prediction accuracy of emission factor especially with NO_X emissions by using effective statistical techniques is important in any emission inventory.

A number of the models discussed above either do not estimate NO_X emissions, or are so sophisticated as to require excessive data inputs. There needs to be a balance between the accuracy and detail of a model for its ease of application. Therefore, to enhance the prediction performance for the NO_X emissions, the MARS modelling approach is proposed in this paper. This, we aim to estimate, with high accuracy, the NO_X emissions. The effectiveness of the model is then determined by dividing the data into two parts, one for building the model (learning) and the other for validating the model (testing). The results are verified by comparing the real data and the MARS predicted values.

2 Methodology

2.1 Chassis Dynamometer Data Collection

This study uses secondary data corrected by the New South Wales (NSW) Road and Maritime Service (RMS), Department of Vehicle Emission, Compliance Technology Operation. The data were collected on the second by second basis and four vehicles were used for the test. The test vehicles include Toyota, Ford, Holden and Nissan from 2007 and 2008 model year with an engine displacement ranging from 1.8L to 2.0L. A chassis dynamometer set-up in the laboratory simulates the resistive power imposed on the wheels of a vehicle, as shown in Figure 1. It consists of a dynamometer that is coupled to drive lines that are directly connected to the wheel hubs of the vehicle, or to a set of rollers upon which the vehicle is placed, and which can be adjusted to simulate driving resistance. During testing, the vehicle is tied down so that it remains stationary as a driver operates it according to a predetermined time-speed profile and gear change pattern shown on a monitor. A driver operates the vehicle to match the speed required at the different stages of the driving cycle [13]. Experienced drivers are able to closely match the established speed profile.

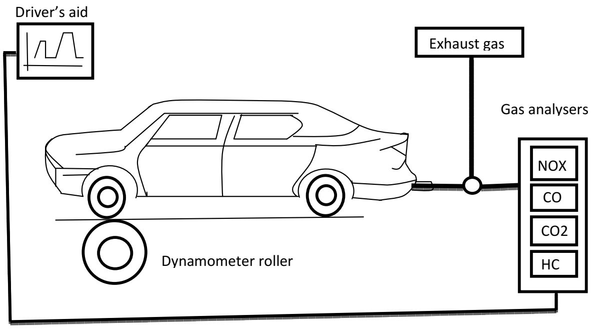

Figure 1. Schematic representation of a chassis dynamometer testing.

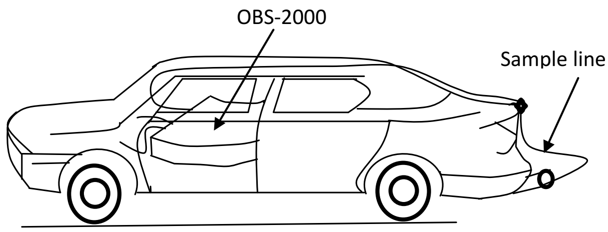

Figure 2. Schematic representation of on-board measurement.

2.2 On-Board Data Collection

Data from on-board instruments, can facilitate development of micro-scale emission models [10]. Compared with conventional dynamometer testing under carefully controlled conditions, on-road data reflects real driving situations. Accordingly, second-by-second emissions data were collected using a Horiba On-Board Measurement System (OBS-2000), as shown in Figure 2, with the same testing vehicles as with the dynamometer test cycle. The equipment is composed of two on-board gas analysers, a laptop computer equipped with data logger software, a power supply unit, a tailpipe attachment and other accessories. The OBS-2000 collects second-by-second measurements of nitrogen oxides NO_X, hydrocarbons (HC), carbon monoxide (CO), carbon dioxide (CO_2), exhaust temperature, exhaust pressure, and vehicle position (via a global positioning system, or GPS). Although the instrument measured other pollutants, the focus of this work was to build a model for NO_X emissions. For the measurement scale used, accuracy for the NO_X emission measurements, reported in percentage, was $\pm 0.3\%$. A two second lag in NO_X emission measurement was accounted for in the data spreadsheets. NO_X sensor calibration was carried out throughout the data collection period. To ensure consistently smooth and good data collection without frequent interruptions due to any possible unit malfunction, inability of batteries to stay charged and calibration issues throughout the period, proper maintenance and diagnostic procedures were strictly followed.

3 Multivariate Adaptive Regression Splines (MARS) Model

MARS was introduced for fitting the relationship between a set of predictors and dependent variables [14]. MARS is a multivariate, piecewise regression technique that can be used to model complex relationship. The space of predictors is divided into multiple knots in order to fit a spline function between these knots ([14], [15]). The basic problem in vehicular emission modelling is how best to determine the fundamental relationship between dependent variables, and vector of predictors, such as speed, acceleration, load, power, ambient temperature including other factors.

The MARS algorithm searches over all possible univariate hinge locations and across interactions among all variables. It does so through the use of combinations of variable called basis functions. The approach is analogous to the use of splines. This study aims at exploring the potential of applying the MARS methodology to model NO_X emissions using the following set of input parameters: speed, acceleration, load, power and ambient temperature of chassis dynamometer and on-board emission measurements. The problem can be stated as a multivariate regression problem. Suppose that N pairs of input-output parameters are available: $\{y_i, x_{1i}, \cdots x_{mi}\}_1^N$, where the depend variable y_i, $i = 1, 2 \cdots, N$, is the ith measure of NO_X and the predictor x_{li}, $i = 1, 2 \cdots, N$, $l = 1, 2, \cdots, m$, is the ith measure of the lth parameter. We assume that the data $\{y_i, x_{1i}, \cdots x_m\}_1^N$ are related through the following equation

$$y = f(x_1, \cdots, x_m), \ \ (x_1, \cdots, x_m) \in D \subset R^m, \quad (1)$$

where $f(\cdot)$ is an unknown multivariate deterministic function and D is the domain of inputs. Since the true mapping in (1) is not known, it is desired to have a function $\hat{f}(x_1, \cdots, x_m)$ that provides a "good" fit approximation of the output data. The good fit between $\hat{f}(x_1, \cdots, x_m)$ and the output data is using the integrated mean square error (MSE) estimated.

$$MSE = \frac{1}{N}\sum_{i=1}^{N}\left[y_i - \hat{f}(x_{1i}, \cdots x_{mi})\right]^2. \quad (2)$$

To regularize the problem, that is, make it well-posed, a restriction is imposed for the solution $\hat{f}(x_1, \cdots, x_m)$ as functions residing in the linear space:

$$F = f : f(\cdot) = \beta_o + \sum_{m=1}^{M}\beta_m h_m(\cdot), \quad (3)$$

where $\{h_m(\cdot)\}_{m=1}^M$ is a set of basis functions and $\{\beta_m\}_{m=0}^M$ are coefficients of representation. In this paper, $h_m(\cdot)$ is the splines basis function defined as:

$$h_m(\cdot) = \prod_{k=1}^{K_m}\left[s_{k,m}\cdot(x_{v(k,m)} - t_{k,m})\right]_+, \quad (4)$$

where $s_{k,m}$ are variables that take values ± 1, $v(k, m)$ labels the predictor variables and $t_{k,m}$ represents estimated values on the corresponding variables. The quantity K_m is the number of "splits" that give rise to each basis function β_m. Here the subscript "+" indicates a value of zero for negative values of the argument. The basis functions involved in (1) are known as "hockey sticks" basis function. MARS searches over the space of all inputs and predictors values (knots) as well as interactions between variables. Now, given the estimated coefficients $\{\beta_m^*\}_0^M$, basis functions $\{h_m^*(\cdot)\}_0^M$ and operation parameters describing a new measurement, the emission of the new measurement can be predicted by taking the following steps:

1. Segregate operation parameters including speed, acceleration, power, load and ambient temperature from the raw data.
2. Predict the emission NO_X by using the approximate function $\hat{f}(\cdot)$ with $\{\beta_m^*\}_0^M$ and $\{h_m^*(\cdot)\}_0^M$, that is $\hat{f}(x_{1i} \cdots x_{mi}) = \beta_0^* + \sum_{m=1}^{M}\beta_m^* h_m^*(x_{1i} \cdots x_{mi})$, $i = 1 \cdots N$, where $\{x_{1i} \cdots x_{mi}\}_1^N$ are from new measurements. The basis functions, together with the model parameters, are combined to produce the predictions given the inputs. The general MARS model equation is given as:

$$\hat{f}(X) = \beta_0 + \sum_{m=1}^{M}\beta_m h_m(X), \quad (5)$$

where $\{\beta\}_0^m$ are the coefficients of the model that are estimated to yield the best fit to the data, M is the number of sub-regions or the number of basis functions in the model, and $h_m(X)$ is the spline basis function given in (4). This model searches over the space of all inputs and predictor values (referred to as "knots") as well as the interactions between variables. During this search, an increasingly larger number of basis functions are added to the model to minimize a lack-of-fit criterion. As a result of these operations, MARS automatically determines the most important independent variables as well as the most significant interactions among them. From Put *et al.* [15], it is noted that the search for the best predictor and knot location is performed in an iterative process. The predictor as well as the knot location, having the most contribution to the model, are selected first. Also, at the end of each iteration, the introduction of an interaction is checked for possible model improvements.

3.1 Model selection and pruning

In general, non-parametric models are adaptive and can exhibit a high degree of flexibility that may ultimately result in over fitting, if no measures are taken to counteract it. The second step is the pruning step, where a "one-at-a-time" backward deletion procedure is applied in which the basis functions with the least contribution to the model are eliminated. This pruning is based on a generalized cross-validation (GCV) criterion. The GCV criterion is used to find the overall best model from a sequence of fitted models, where a larger GCV value tends to produce a smaller model, and vice versa. The GCV criterion is estimated using (7) as the lack-of-fit criterion [17]:

$$\mathrm{GCV} = \frac{1}{N}\frac{\sum_{i=1}^{N}\left(y_i - \hat{f}(X_i)\right)^2}{\left[1-\frac{\tilde{C}(M)}{N}\right]^2}, \qquad (6)$$

where $\left[1-\frac{\tilde{C}(M)}{N}\right]^2$ is a complexity function, and $\tilde{C}(M)$ is defined as $\tilde{C}(M) = C(M) + d.M$, of which $C(M)$ is the number of parameters being fit and d represents a cost for each basis function optimization and is a smoothing parameter of the procedure. The higher the cost d is, the more basis functions will be eliminated [16].

4 Results and Discussions

Five vehicular emission predictor variables, namely, speed (m/s), acceleration (m/s^2), power (W), temperature ($^\circ C$) and load (Nm) were used with the response variable of NO_X (g/s) in an attempt to identify the relationships that vehicular emission models developers wish to understand. To explore factors affecting vehicular emission models, the present study provides results and some interpretations from the MARS model. Table 1 and 2 summarize the variable selection results using MARS, whose beta factor coefficients β_m are denoted BF_m . In a MARS model, basis functions are used to predict the effects of independent variables on NO_X emission factor. The interpretation of MARS results is similar to but not as straight forward as that of classical linear regression models. A positive sign for the estimated beta factors for the basis function indicates increased NO_X emission, while a negative sign indicates the opposite. The value of beta factor implies the magnitude of effect of the basis function (i.e., variable effect) on the NO_X emission.

Table 1. List of basis functions of the MARS and their coefficients for on-board measurements.

Beta factor	Basis function	Value
BF0		0.249827
BF1	Max(0, SPEED-8.1127)	–0.000142123
BF2	Max(0, SPEED-11.667)	0.000342034
BF3	Max(0, SPEED-12.5242)	0.000442178
BF4	Max(0, SPEED-16.3889)	0.0032363
BF5	Max(0, SPEED-23.8889)	0.011587
BF6	Max(0, SPEED-24.1667)	0.0439038
BF7	Max(0.95-ACCEL, 0)	–0.0013075
BF8	Max(0, ACCEL-1.25)	0.0073075
BF9	Max(0, ACCEL-5.85)	0.0113075
BF10	Max(0, ACCEL-7.21)	0.0311017
BF11	Max(0, AMBT -22.12)	0.00023075
BF12	Max(0, AMBT -23.47)	0.00313022
BF13	Max(0, AMBT -24.76)	0.02113075
BF14	Max(0, LOAD -10.53)	0.01561811
BF15	Max(0, LOAD -52.34)	0.0179656
BF16	Max(0, LOAD -60.16)	0.023224571
BF17	Max(0, Power -8.98)	0.0148769
BF18	Max(0, Power -21.32)	0.01567893

For the effect of each basis function, max $(0, x-t)$ is equal to $(x-t)$ when x is greater than t; otherwise the basis function is equal to zero. As shown in Table 1 and 2, the MARS model contains 19 and 15 basis functions for on-board and dynamometer testing respectively. The on-board measurements and dynamometer testing have similar interpretations. It can be observed that all the five predictor variables play crucial roles in determining NO_X vehicle emission. From Table 1, beta factors BF1, BF2, BF3, BF4, BF5 and BF6 account for the nonlinear effect of vehicle speed in the emission model. The effect of speed on NO_X emissions can be explained as follows. By using the onboard measurements method, if the speed of the vehicle is less than 8.1127 m/s or 29.2 km/h, it has negligible effect on the NO_X emission (indicated by

BF0), but from 11.667 m/s or 42 km/h this effect is increased with an increase in speed (indicated by BF2-BF5). The emission rate can reach 0.0439 g/s when the speed is about 24.1667 m/s or 82 km/h (indicated by BF6).

Table 2. List of basis functions of the MARS and their coefficients for dynamometer testing.

Beta factor	Basis function	Value
BF0		0.313578
BF1	Max(0, SPEED-6.428)	–0.00017255
BF2	Max(0, SPEED-9.356)	0.000625
BF3	Max(0, SPEED-18.368)	0.00575
BF4	Max(0, SPEED-25.136)	0.0635
BF5	Max(0, ACCEL-1.119)	0.00943
BF6	Max(0, ACCEL-4.235)	0.0567
BF7	Max(0, ACCEL-6.243)	0.0663
BF8	Max(0, AMBT -21.54)	0.000321
BF9	Max(0, AMBT -23.15)	0.00443
BF10	Max(0, AMBT -24.62)	0.0372
BF11	Max(0, LOAD -15.67)	0.0132
BF12	Max(0, LOAD -45.67)	0.053
BF13	Max(0, Power -13.76)	0.0168
BF14	Max(0, Power -20.64)	0.0212

This expected finding is consistent with previous findings in literature. From Carslaw *et al.* [18], it is noted that NO_X emissions rise and fall in a reverse pattern to hydrocarbon emissions (HC). As the speed of the vehicle increase the mixture becomes leaner with more HC's at high temperatures in the combustion chamber, there appear excess oxygen molecules which combine with the nitrogen to form NO_X. From Table 1, as the speed increases (indicated by BF2-BF6) the total NO_X emission emitted from the tail pipe also increases.

Beta factors (BF7-BF10) on Table 1 show the nonlinear effect of vehicle acceleration on the NO_X which can be described as fellows. If the vehicle acceleration is less than 0.95 m/s^2, NO_X emission will reduce by 0.0013075 g/s (indicated by BF7), but if the acceleration is increased from 1.25 m/s^2, to 5.85 m/s^2, the NO_X emission will increase by 0.0113075 g/s (indicated by BF8 and BF9). The NO_X emission can reach more than 0.0311017 g/s when the acceleration exceeds 7.21 m/s^2. This result is similar to that of the speed because of depressing the accelerator pedal increase acceleration as well as speed simultaneously. The ambient temperature is also found to influence the NO_X emission as indicated by BF11, BF12 and BF13 of Table 1, the effects of ambient temperature on NO_X emission occurrence include: (1) if the ambient temperature is less than 22.12°C then it has no effect on vehicle NO_X emission (indicated by BF11); (2) if the ambient temperature is greater than 22.12°C but less 23.47°C, NO_X emission will increase by 0.00023075 g/s for 1°C increase of ambient temperature (indicated by BF11 and BF12); (3) if the ambient temperature is greater than 23.47°C but less than 24.76°C, the vehicle NO_X emission will increase by 0.00313022 g/s for 1°C increase in ambient temperature (indicated by BF12 and BF13) and (4) if the ambient temperature is greater than 24.76°C the NO_X emission will increase by 0.02113075 g/s for 1°C increase in ambient temperature (indicated by BF13). The higher ambient temperature resulting in

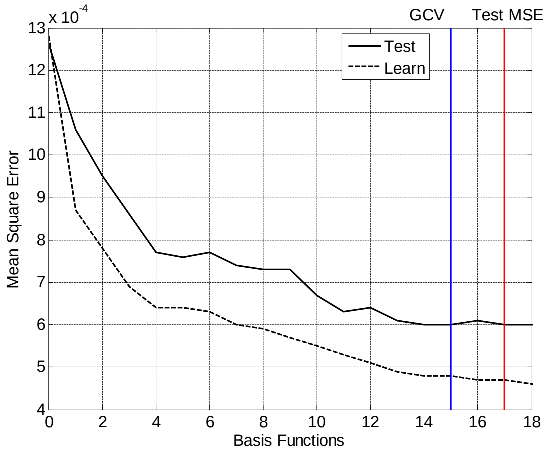

Figure 3. MARS model for On-Board System.

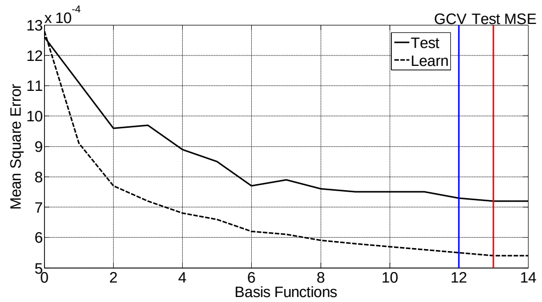

Figure 4. MARS model for Chassis Dynamometer System.

more vehicle NO_X emission is expected, because NO_X is formed in a larger quantity in the cylinder as the combustion temperature exceeds the required limit. This finding is also consistent with previous explanation. In addition, temperatures greater than 24.76°C (B13) will significantly produce NO_X emissions. As indicated by BF14, BF15 and BF16, the MARS results show the effect of load: (1) if the load is less than 10.53 Nm, then it has no effect on NO_X emission (indicated by BF14); (2) if the load is greater than 10.53 Nm but less 52.34 Nm, the NO_X emission will increase by 0.01561811 g/s for 1 Nm increase of load (indicated by BF14 and BF15); (3) if the load is greater than 52.34 Nm but less than 60.15 Nm, the vehicle NO_X emission will increase by 0.0179656 g/s for 1 Nm increase in load (indicated by BF15 and BF16) and (4) if the load is greater than 60.15 Nm the NO_X emission will increase by 0.02324571 g/s for 1 Nm increase in load (indicated by BF16). As far as the effect of power on NO_X emission, BF17 and BF18 indicate that the occurrence can be described as: (1) if the power is less than 8.98 W, then it has no effect on vehicle NO_X emission (indicated by BF17); (2) if the power is greater than 8.98 W but less 21.32 W, NO_X emission will increase by 0.01567893 g/s for 1 W increase of power (indicated by BF17 and BF18); (3) if the power is greater than 21.23 W, the vehicle NO_X emission will increase by 0.01567893 g/s for 1 W increase in power (indicated by BF18). The NO_X emission as a result of the increasing load and power is expected, following the remark by Pierson *et al.* [19] that driving a vehicle against a higher resistance will increase the engine load and power which will result in increases of the carbon dioxide (CO_2) and NO_X emissions.

To illustrate the NO_X emission during real-world driving conditions and the dynamometer testing drive cycle, Figures 3 and 4 show the MARS model that has the best performance basis on independent test samples. There were 557 data points used in the analysis, 65% of which for building the model (Learn) and 35% for validation (Test).

Table 3. Comparison of MARS and Multiple Linear Regression (MLR) model

Model	Summary Statistics	On-Board	Dynamometer
MARS	R^2	0.63	0.57
	Adjusted R^2	0.62	0.56
	MSE	3.35×10^{-6}	1.33×10^{-5}
MLR	R^2	0.51	0.50
	Adjusted R^2	0.50	0.49
	MSE	2.57×10^{-5}	3.12×10^{-5}

The on-board system model has nineteen basis functions with the best model with the least mean square error occurring at 17^{th} basis function, R^2 value of 63% while the chassis dynamometer has the R^2 of 57% with the best model occurring at BF12. Table 3 compares the MARS and Multiple Linear Regression (MLR) model and presents the model summary statistics. It is clear that the MARS model perfoms better than the MLR model as the latter gives R^2 of 51% and 50% for both the on-board and the dynamometer test. The 12% and 7% differences in contribution achieved by the MARS model confirms its ability in improving the prediction accuracy of the NO_X emission. Among all the predictor variables the speed appears to have the highest contribution to NO_X emissions. Figures 5 and 6 provide a detailed plot of the real data and prediction using MARS techniques. Note that the predicted emissions follow the real data with sufficiently good precision although there is a slight deviation in the dynamometer predictions. The MSE of the on-board system was 3.355×10^{-6} while that of dynamometer was 1.33×10^{-5}.

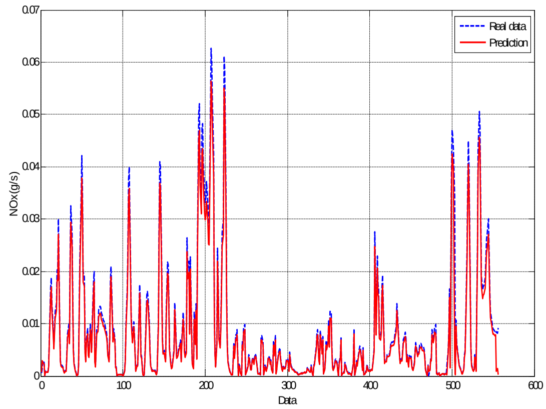

Figure 5. Predicted values of NO_X and the real data plotted for on-board measurements.

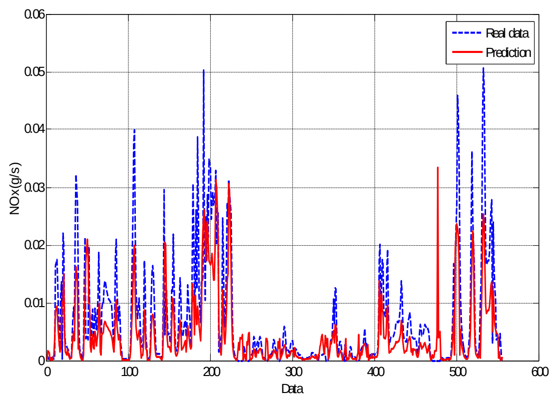

Figure 6. Predicted values of NO_X and the real data plotted for dynamometer testing.

5 Conclusion

This paper has presented a MARS modelling approach to effectively estimate vehicular NO_X emissions. The model approximates the nonlinear relationship between the NO_X emission which is a function of speed, acceleration, temperature, power and load as predictor variables. The MARS model is implemented with 19 and 15 effective piecewise-linear BFs. The model predicts the NO_X emission by forming a weighted sum of the predictor variables; thus, the predicted emission changes in a smooth and regular fashion with respect to the input virations, offering some performance improvements. The results obtained indicate a promising application of the proposed method in the estimation of NO_X emissions with a reasonable accuracy. The proposed method may usefully assist in a decision-making policy regarding urban air pollution.

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