Artificial neural network (ANN) assisted prediction of transient NO\textsubscript{x} emissions from a high-speed direct injection (HSDI) diesel engine

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Abstract
The understanding and prediction of NO\textsubscript{x} emissions formation mechanisms during engine transients are critical to the monitoring of real driving emissions. While many studies focus on the engine out NO\textsubscript{x} formation and treatment, few studies consider cyclic transient NO\textsubscript{x} emissions due to the low time resolution of conventional emission analysers. Increased computational power and substantial quantities of accessible engine testing data have made ANN a suitable tool for the prediction of transient NO\textsubscript{x} emissions. In this study, the transient predictive ability of artificial neural networks where a large number of engine testing data are available has been studied extensively. Significantly, the proposed transient model is trained from steady-state engine testing data. The trained data with 14 input features are provided with transient signals which are available from most engine testing facilities. With the help of a state-of-art high-speed NO\textsubscript{x} analyser, the predicted transient NO\textsubscript{x} emissions are compared with crank-angle resolved NO\textsubscript{x} measurements taken from a high-speed light duty diesel engine at test conditions both with and without EGR. The results show that the ANN model is capable of predicting transient NO\textsubscript{x} emissions without training from crank-angle resolved data. Significant differences are captured between the predicted transient and the slow-response NO\textsubscript{x} emissions (which are consistent with the cycle-resolved transient emissions measurements). A particular strength is found for increasing load steps where the instantaneous NO\textsubscript{x} emissions predicted by the ANN model are well matched to the fast-NO\textsubscript{x} analyser measurements. The results of this work indicate that ANN modelling could strongly contribute to the understanding of real driving emissions.

Keywords
Deep learning, artificial neural networks, internal combustion engines, diesel, NO\textsubscript{x}, transient, Crank-angle resolved NO\textsubscript{x}

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Introduction
NO\textsubscript{x} emissions remain a key research area for the internal combustion engine community.\textsuperscript{1} Earlier studies focused on tailpipe emission control techniques such as exhaust gas recirculation (EGR) while running engines at steady-state.\textsuperscript{2} More recent studies have explored after-treatment techniques such as lean NO\textsubscript{x} traps (LNT) and selective catalytic reduction (SCR) for closer control of transient engine emissions.\textsuperscript{3} While after-treatment systems have improved gradually over the years, the significance of transient engine emissions on the conversion rate of these systems has also been highlighted.\textsuperscript{4} Studies have suggested, for example, an SCR catalyst requires a 1:1 ratio of NO/NO\textsubscript{2} for maximum conversion rate because the ratio influences both the oxygen and ammonia needed to reduce NO\textsubscript{x} and the speed of the reduction reaction.\textsuperscript{5,6} Although the importance of transient NO\textsubscript{x} emissions on after-treatment control techniques is well known, limited studies are found in the literature. The challenge arises as the time scale of instantaneous NO\textsubscript{x} formation is much shorter than the response time of conventional NO\textsubscript{x} analysers, which makes it difficult to measure and analyse engine emission under real (transient) driving conditions.

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Therefore, fast measurement methods and novel analysis techniques are required to extend the knowledge on transient NOx emissions.

Recently, Leach et al. measured cycle-to-cycle NO and NOx emissions from a high-speed light-duty diesel engine undergoing transient load steps using a commercial high-speed NOx analyser (Cambustion CLD500). The study revealed a strong correlation between the NOx emitted per cycle and the peak cylinder pressure of that cycle. This is consistent with previous studies of SI engines suggesting a close correlation between the maximum pressure and peak in-cylinder temperatures which can promote NO formation based on Zeldovich mechanisms. Further study, including the use of a newly developed fast LIF device for the direct measurement of NOx, also uncovered that changes in NO and NOx emissions, and hence NOx/NO ratio, are instantaneous upon a step change in engine load which further highlighted the importance of instantaneous NOx measurements for real-driving conditions emissions control. However, while an experimental instrument in a laboratory can now recover some emissions insights under real driving conditions, the accuracy and economics of having portable emission measurement systems for transient NOx emissions are still in question. With increasing computational power and a vast amount of testing data, numerical modelling becomes an alternative way for the predictions of transient NOx emissions.

Various studies have focused on the modelling of NOx emissions. Cho et al. implemented a real-time zero-dimensional model for predicting engine-out emissions of nitrogen oxides using in-cylinder pressure measurements. The proposed model uses a simplified Zeldovich NOx mechanism combining combustion-related parameters derived from simplified thermodynamic and combustion sub-models. Although the model was able to achieve ±10% accuracy at mid-to-high engine conditions, at low-load conditions the error was much higher making it more challenging for the application of real driving NOx predictions. Finesso et al. validated a real-time combustion model at steady-state conditions and in transient operation over several load steps. Although good predictions are given under steady-state, the transient predictions are less good, especially when EGR is adopted, giving higher uncertainties. Asprion et al. suggested a model that combines phenomenological and empirical approaches by extracting the most relevant physical phenomena and extending them by physically motivated empirical elements. Quantitative accuracy was proven for both steady and transient operations, however, due to the simplifications and assumptions necessary to allow for a sufficiently simple structure, the model is not able to predict the influence of multiple injections or even more fundamental changes of the combustion characteristics which is expected for modern engines. Park et al. proposed a real-time nitric oxide (NO) prediction model based on the in-cylinder pressure and on data available from the ECU. The NO formation model was developed based on both the analysis of computational fluid dynamics simulations as well as a physical model. The results showed that the model can predict engine-out NO emissions, making it suitable to be applied to engines and after-treatment systems without the use of a sensor. All these studies have proposed models driven by physical processes with various assumptions; however, the complex physical phenomena of NOx emissions are still yet to be recovered suggesting that additional terms may be needed for different conditions especially when the engines are running at low load. The coupling between interacting processes during the formation of NOx makes it even more challenging to isolate/identify the leading parameter or the combined effects of various parameters for a physical NOx model.

Modern engine development involves regular experimental testing, typically in engine test cells and on chassis dynamometers. The abundance of emissions data recorded under a wide range of operating conditions makes empirical or data-driven approaches attractive. In recent years, engine research studies have favoured Artificial Neural Networks (ANNs) as the predictive modelling tool for emissions and engine control predictions. Compared to other predictive empirical or data-driven models, the main advantage of ANN lies in its ability to identify cryptic, nonlinear, highly complex correlations, between the measured input and output data. The modelling process can have little to no governing equations for the parameters to be predicted, therefore substantially reducing the time and cost associated with engine development and model building. Being a machine learning tool, ANN also has the ability to re-learn when new data is available, which can further increase the model’s accuracy. A number of studies have also been conducted to predict the emission and performance of internal combustion engines (ICEs) by using the ANN approach. Deng et al. decoupled the effect of cetane number on emissions from other compositions and properties of diesel fuel using a neural network. The optimally designed back-propagating neural network was able to determine the functional relationships between total cetane number, base cetane number and cetane improver as well as total cetane number and nitrogen content and HC, CO, PM and NOx. Parlik et al. presented the ability of an ANN model in predicting specific fuel consumption and exhaust temperature of a diesel engine for various injection timings. The proposed new model was able to provide fast and consistent results with a low absolute relative error compared to the experiment. Mauro et al. used a large number of experiment datasets to construct a neural network capable of predicting the indicated mean effective pressure (IMEP) and its coefficient of variation (CoV of IMEP) in a spark-ignited internal combustion engine. A strong correlation between the modelled CoV and the experiments was captured by the model. However, a systematic...
overprediction of CoV was observed for low CoVs while higher CoVs were underpredicted by the ANN model suggesting missing physical parameters for the ANN input features. More recently Fang et al. studied different strategies for ANN input feature selection suggesting a Pearson correlation can be used to highlight significant parameters while providing a ranking of their relative importance. The ANN model predictions show good agreement to the experimental data with improved performance in the low-Nox region using input features given by Pearson correlation. Existing literature suggests ANN being a powerful tool capable of identifying the complex correlation between engine operating parameters and NOx emissions within the range of steady-state experimental test conditions. However, as crank angle resolved NOx emissions experimental data is still a challenge to obtain; very few numerical models, either physical or empirical, can be validated in the literature for transient cyclic NOx emissions. So the question arises: can one use an ANN model built from steady-state experimental data, which is largely available in engine testing facilities, to predict transient engine NOx emissions, therefore assisting after-treatment development and control?

In this study, we explore the applicability of the ANN method for the prediction of NOx emissions of a high-speed direct injection diesel engine undergoing transient load steps. The model is built from a substantial experimental dataset, which includes 7 months of engine testing (1108 individual experiments) from the University of Oxford single-cylinder diesel research engine running under various steady-state conditions. The engine and the test cell have been designed to give the highest quality data, and much of this dataset has already been published. The previously constructed ANN model based on this steady-state state dataset is given transient input features including crank angle resolved cylinder peak pressure to predict the transient NOx emissions. The predicted transient NOx emissions are then quantitatively compared both with results from a conventional test-bed emissions analyser and a fast-NOx emissions analyser which have been published previously. The differences between predictions and measurements from each analyser are highlighted.

### Experimental setup and data uncertainty

#### Engine and instrumentation

The engine used was a single-cylinder direct injection diesel engine. Exhaust Gas Recirculation (EGR) was achieved via a high-pressure EGR system, with the exhaust gases passing through an EGR cooler, entering a dedicated volume where mixing with the fresh intake charge took place prior to entering the inlet manifold. In-cylinder pressure data were measured using a Kistler 6046Asp-3-2 cylinder pressure transducer in the same cylinder from which the NO and NOx measurements were taken. Emissions measurements were obtained from two different instruments. Referred to as the ‘fast’ analyser, a two-channel Combustion CLD500 probe is fitted approximately 70 mm downstream of an exhaust port to sample the NO and NOx emissions. The instrument uses chemiluminescence method coupled with a constant pressure heated sampling system to give a fast sample response time and to isolate the measurements from temperature and pressure variations in engine exhaust. The resultant NOx channel has a $T_{10-90\%}$ response time of 10 ms. Cylinder pressure and fast-NOx measurements are logged with a high-speed data acquisition unit at a resolution of 0.1 CAD.

Low frequency channels were logged at 1 Hz using a CADET engine control system by Sierra-CP Engineering. Engine-out emissions, including NO and NOx, were measured by a Horiba MEXA-ONE, referred to as the ‘slow’ analyser. The MEXA-ONE samples the exhaust through a 12 m sample line sampling approximately 3 m downstream of the engine exhaust valves, after the high pressure EGR is taken off, and a 25 L smoothing tank. This gives the slow analyser a response time of around 15 s. More information in terms of both emissions instruments can be found in Leach et al.

#### Test conditions and training set

The ANN training and verification data sets comprise a series of experiments conducted over includes 7 months period of engine testing within a larger research program. All of these tests included the slow analyser and were focusing on steady-state engine performances at different load conditions with different EGR compositions. Each test point logged by the low-speed data acquisition system was repeated several times over different days.

On the other hand, tests using the fast analyser focusing on transient engine conditions (which are used solely as the validation data set for the ANN) were conducted on a single day of testing for which the analyser was available. For these data, the low-speed engine
data including the slow analyser were logged for 180 s while the high-speed data – cylinder pressure and fast-NOx were logged for 300 cycles. In addition to the raw 0.1 CAD resolved logs, the high-speed data are also logged as an average of 300 cycles through the CADET system (the low-speed data acquisition system) with their values updated every 300 cycles. This allowed for a test file that integrated both low and high-speed data, which are the test points of interest in this study, but with a substantial time-offset.

For testing conditions that have high-speed data, the engine load steps were run in such a way that the step in engine load was initiated a short while after logging had begun (less than 100 cycles). So if an engine load step up was being measured, there will be more cycles logged at the higher load (more than 200) than the low load side (less than 100), and if a step down, vice-versa.

As mentioned before, the purpose of this study is to check whether a steady-state trained ANN model is capable of predicting transient fast-NOx responses. The test set involving steady-state data is, therefore, exclusively used as the training data. Whereas the testing dataset with fast-NOx analyser is only used for the validation of model NOx predictions. For steady-state data, a wide range of speed/load conditions is performed together with five-point EGR sweeps with the exception under full-load conditions. Table 2 presents the different steady-state test points considered for the training, validation and verification of an ANN model. With each test point logging 180 s of data, the total number of test points used in training this model is \( \approx 128,000 \) points after data pre-processing.

In order to remove any outliers in the dataset, pre-processing is performed where data points with variations more than the acceptable limit for the target IMEP (±0.2 bar) and speed (±20 RPM) are excluded. The operator errors are, therefore, minimized during this process. In addition, for the low speed/low load conditions, under maximum EGR rates, the engine was found to enter a low-temperature combustion regime, indicative of very low NOx (≈10 ppm), which is very susceptible to combustion instability. Consequently, EGR values above 60% were removed from the training set as they showed very high variance in IMEP and NOx. This is expected to increase the model’s accuracy even under low NOx values. Test points 6 and 7 are set aside for verification purpose during ANN model construction therefore excluded from training. For reasons of commercial confidentiality, all emissions results have been rescaled by an arbitrary value (and hence are presented in arbitrary units).

For transient data with the fast analyser, two test points are shown in Table 3 representing different levels of NOx emissions. Test point 1 represents low speed low load, with alternating load steps. Test point 2 refers to the high speed high load. No EGR is considered for both fast-NOx tests due to a lack of data availability. A full engine map carried out for both slow and fast-NOx analyser is shown in Figure 1. The fast-NOx conditions are clearly marked well outside the range of all training data. Figure 2 shows a sample window for test point 2, where both fast-NOx and slow-NOx are recorded at the same time with fast-NOx focusing on the transient load steps (the fast-NOx emissions data is not plotted on the same graph for clarity). It is worth noting the testing is not performed in one continuous run, and the discontinuity in time is highlighted by the zigzag line. Additional time alignment between the slow and fast analyser is needed to compare the results from two analysers. The pre-processing applied to the fast analyser data is detailed later in this work.

### Data uncertainty

The accuracy of any empirical model will heavily depend on the accuracy of the experimental data. The source of errors in measurements can be traced back to either unexpected sources of error which are random in

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**Table 2.** Range of test conditions for the training and verification dataset used.

| Test point | 1 | 2 | 3 | 4 | 5 | Verification test |
|------------|---|---|---|---|---|-------------------|
| Speed (RPM) | 1500 | 1500 | 2000 | 2500 | 4000 | 1750 | 2000 |
| nIMEP (bar) | 3.8 | 6.9 | 25.8 | 17.6 | 21.6 | 13.9 | 12.3 |
| Rail pressure (MPa) | 47–69 | 46–235 | 131–178 | 78–228 | 217–222 | 84–132 | 77–227 |
| Boost pressure (barG) | 0.05–0.07 | 0.24–0.56 | 1.84–2.22 | 1.5–1.86 | 1.54–1.61 | 1.07–1.40 | 1.10–1.50 |
| Back-pressure (barG) | 0.29–0.38 | 0.34–1.30 | 2.20–3.10 | 2.10–3.10 | 2.40–2.50 | 1.80–3.00 | 1.80–3.10 |
| Inlet temperature (°C) | 55–70 | 20–60 | 35–60 | 30–75 | 50–55 | 30–70 | 35–75 |
| EGR (%) | 0–59 | 0–57 | 0–23 | 0–30 | 0 | 0–43 | 0–43 |

**Table 3.** Fast-NOx test conditions and load steps.

| | TP\textsubscript{fast}^1 | TP\textsubscript{fast}^2 |
|----------------|--------------------|--------------------|
| Engine speed (RPM) | 1500 | 2000 |
| Lower nIMEP (bar) | 1.9 | 19.4 |
| Higher nIMEP (bar) | 3.8 | 25.8 |
| Back-pressure (barG) | 0.31 | 2.9 |
| Inlet temperature (°C) | 55 | 40 |
| EGR (%) | 0 | 0 |
nature or inaccuracies associated with the measurement equipment. As careful calibration has been performed for each instrument minimizing equipment errors (notably the slow-NOx analyser was calibrated at least twice daily over the months that this data was taken, and the fast-NOx analyser was calibrated roughly every hour, and the results drift-corrected), this section focuses on uncertainties with random nature. As already mentioned, each test point under steady-state conditions was logged for 180 s by the low-speed data acquisition system and repeated several times over different days, therefore removing any environmental bias error. The associated uncertainty for each test point in the training set was given by the 95% confidence level.

Figures 3 and 4 show the uncertainty associated with the scaled fuel flow rate and the normalized slow analyser NOx emissions readings for the 1500 RPM/3.8 bar nIMEP test point. The chosen test point represents the worst case scenario in terms of experimental uncertainty as the signal to noise ratio is expected to be the highest. The results presented here are averaged over three runs, and as can be seen, the associated uncertainty is small, indicating a high fidelity experimental dataset. The associated uncertainty for both nIMEP and the rail pressure was measured to be less than 0.3% at the 95% confidence level for the results. A detailed uncertainty analysis on other datasets used in this work can also be found in a previous publication.19

As detailed in previous studies,23 the fast-NOx data was quench and drift-corrected before analysis. The signal from the fast-NOx analyser is only valid when the exhaust valves are open (i.e. when there is exhaust flow) and so the average emission from a single engine cycle must be taken during that period. By aligning the data with the EVO and EVC points (see Table 1) a mean value can then be estimated over the valve opening period which represents the cyclic NOx emissions for that cycle. This is shown in Figure 5. As noted above, there are very different response rates for the instrumentation (approximately 15 s for the slow analyser and 10 ms for the fast analyser), and these response rates vary with exhaust pressure amongst other
parameters. As a result, careful time alignment of the data was necessary, using the load step (which also corresponded to a substantial change in in-cylinder pressure as well as a ‘NOx step’) was used as a common feature between all of the datasets, and all were time-aligned to this common reference point. Nevertheless, as will be seen in the results section, not all of the transit delays in the slow analyser can be (or should be) compensated for.

**Neural network setup**

In this study, a commonly recognized and used ANN structure shown in Figure 6, multilayer perceptron, was constructed. For the model used in this study one input layer, one hidden layer and one output layer is used. The activation function is chosen to be the continuous differentiable log-sigmoid function with an error function based on the mean squared error (MSE). The backpropagation algorithm is given by a nonlinear numerical optimization technique, called Levenberg-Marquardt (LM). Details of number of neurons and the process of selection the above mentioned structure is detailed in previous studies. Here we will highlight the performance of the model from the perspective of both the correlation coefficient ($r$) and coefficient of determination ($R^2$). The definition of the coefficient of determination and Pearson correlation used in this study are:

\[
 r = \frac{\sum_{i=1}^{n} (x_i - \overline{x})(y_i - \overline{y})}{\sqrt{\sum_{i=1}^{n} (x_i - \overline{x})^2(y_i - \overline{y})^2}}
\]

where $n$ is the sample size of given paired data $(x_1, y_1), \ldots, (x_n, y_n)$. $\overline{x}$ and $\overline{y}$ are the sample mean for variable $x$ and $y$.

\[
 R^2 = 1 - \left( \frac{\sum_{i=1}^{n} (t_i - O_i)^2}{\sum_{i=1}^{n} (O_i)^2} \right)
\]

where $t_i$ is the experimental output and $O_i$ is the model output.

Figure 7 shows the performance of the ANN model predictions with the correlation coefficient indicating the relationship between two or more parameters. The ANN model shows a very high correlation coefficient with all data points clustered near the unity slope line. The results also demonstrate the ability of ANN in predicting experimental observations for a wide range of

![Figure 5. Crank angle based NO and NOx emission.](image1)

![Figure 6. Schematic diagram of a feedforward neural network.](image2)

![Figure 7. Regression plot for LM based ANN model predictions versus experimental results for all data types.](image3)
operating conditions, including those excluded from the training dataset (validation data).

The constructed ANN model also highlighted the important parameters for input features. Parameter selection was achieved via a filter algorithm which distinctively isolates the input variable selection process from the ANN training. All parameters considered were experimental data and not modelled parameters. Various auxiliary statistical analysis techniques were compared to measure the relevance of individual, or combinations of input variables. For the current ANN model, the Pearson correlation was chosen as the statistical analysis tool for the parameter selection process. To minimize cross correlation between variables, the importance of each parameters with NO\textsubscript{x} emissions was highlighted when the correlation coefficient was greater than 2/√n, where n is the number of parameters tested.\textsuperscript{25} The detailed process of feature selection is highlighted in our previous study.\textsuperscript{19} The results suggest 14 input features in the dataset are needed for the construction of an ANN NO\textsubscript{x} model. A brief discussion of each parameter chosen is included in this article.

Table 4 shows the parameters with the highest Pearson correlation coefficient, with respect to NO\textsubscript{x} emissions, that were used as input parameters in the ANN model. EGR has a negative correlation coefficient with NO\textsubscript{x}, an effect that is very well understood and widely covered in literature. Volumetric efficiency is also shown to be correlated to NO\textsubscript{x}.\textsuperscript{26} This is expected as an increase in volumetric efficiency results in more air being trapped in the cylinder and consequently more oxygen; the effects of oxygen availability in NO\textsubscript{x} formation and the positive correlation of oxygen and NO\textsubscript{x} are well understood.

Similarly, the mass flow rate of the inlet is also correlated to NO\textsubscript{x} since an increase in the mass flow rate of air would result in a higher oxygen concentration in the cylinder as well as higher in-cylinder pressures (and hence temperatures). In addition, due to mass continuity, exhaust mass flow rate shows an equally high correlation.

The inlet and EGR cooler outlet temperatures are found to be negatively correlated to NO\textsubscript{x}, a result attributed to thermal throttling. Thermal throttling occurs when an increase in temperature leads to a reduction in charge density and consequently in a reduction of oxygen availability, thus reducing NO\textsubscript{x} emissions. However, an increase in inlet temperature can result in higher charge temperatures, thus increasing peak cylinder temperature and consequently NO\textsubscript{x}. It has been shown that the two competing events described above cancel out, leading to minor changes in NO\textsubscript{x}.\textsuperscript{26} However, due to the nature of the tests included in the dataset, the inlet and EGR cooler outlet gas temperatures are directly linked to EGR levels which explains their negative correlation with NO\textsubscript{x}.

Various parameters related to engine load were also highlighted by the Pearson correlation test. From those parameters, peak cylinder pressure (P\textsubscript{max}) showed the highest importance. Perhaps surprisingly peak cylinder temperature (here calculated by the bulk gas temperature) did not show a high correlation with NO\textsubscript{x} emissions, a well documented behaviour in literature.\textsuperscript{27} Leach et al.\textsuperscript{7} also showed that peak cylinder pressure correlates very closely to NO\textsubscript{x} in a diesel engine and over a range of combustion parameters only IMEP showed a comparable, albeit lower, correlation to NO\textsubscript{x}. This was attributed to the errors introduced in the calculation of other parameters such as IMEP and cylinder temperature from the pressure signal. This is discussed further in later sections as this is directly related to the current approach in predicting the transient NO\textsubscript{x}.

Finally, the temperature change across the engine for the cylinder head and the jacket also showed a high correlation to NO\textsubscript{x}. As already discussed, NO\textsubscript{x} formation is highly dependent on cylinder P\textsubscript{max}, which can lead to increased heat transfer to the cylinder walls due to higher bulk gas temperatures. This then explains the correlation of the coolant temperature difference across the cylinder head and cylinder jacket with NO\textsubscript{x} emissions, presented in Table 4.

### Transient inputs data for NO\textsubscript{x} prediction

In order to predict transient NO\textsubscript{x} emissions from the constructed steady-state ANN model, it is necessary to align slow response input feature signals with the fast-NO\textsubscript{x} analyser data. As mentioned before, while logging the fast analyser, all other data channels are also logged through CADET system (the low-speed data acquisition system) with their values updated every 300 cycles. Data logged with low-speed data acquisition systems are then advanced 300 cycles for each condition investigated. A recent study\textsuperscript{28} has suggested that transient NO\textsubscript{x} is closely related to the peak in cylinder temperature (T\textsubscript{max}), the maximum cylinder pressure (P\textsubscript{max}) and the indicated mean effective pressure (IMEP). Therefore, it is crucial to have such information included as the input for NO\textsubscript{x} predictions. However, a strong link between P\textsubscript{max} and T\textsubscript{max} suggests the formation of NO and NO\textsubscript{x} through the extended Zeldovich mechanisms can be directly associated to P\textsubscript{max} alone. Therefore, among the 14 parameters used in the model

| Parameters                  | Parameters                  |
|-----------------------------|-----------------------------|
| Brake power                 | Coolant jacket δT           |
| Cylinder head coolant δT    | Cylinder P\textsubscript{max} |
| EGR                         | EGR cooler outlet T          |
| Exhaust mass flow rate      | Fuel flow rate              |
| gIMEP                       | Inlet mass flow rate        |
| Inlet pressure              | Inlet temperature           |
| Net power                   | Volumetric efficiency       |

Table 4. Engine parameters for the ANN model based on the Pearson correlation coefficient.
Fast response crank-angle resolved maximum cylinder and indicated mean effective pressures are included as the input to predict transient NOx behaviour. Previous studies also confirmed $P_{\text{max}}$ has indeed the highest correlation with cycle NOx emissions among parameters such as initial burn duration (CA0-10), burn duration (CA10-90), maximum in-cylinder temperature ($T_{\text{max}}$) and cycle IMEP, therefore, making the current model suitable for transient NOx predictions. The successful prediction of transient NOx relies heavily on the availability and accuracy of cyclic $P_{\text{max}}$ and IMEP data. Before including the cyclic pressure data as the input feature, the high fidelity experimental data is first checked in terms of their correlation with transient NOx emissions. A high correlation is indeed found between NOx emissions from the engine and the maximum cylinder pressure of that cycle. A sample Pearson correlation is shown in Figure 8 for the low load conditions (test point 1). For other aligned slow signal channels, the values are repopulated into the cyclic base making sure all 14 input features are available simultaneously in a cyclic form for the model.

**Results and discussion**

In this section, transient simulation results of a previously built steady-state neural network configuration will be discussed in detail for different engine speeds. The real road transient behaviour is highlighted through the load variations. Figures 9 and 10 showed the time averaged cyclic NOx emissions from the 'fast' and 'slow' analysers at two conditions where the predicted time averaged NOx emissions are also highlighted. First, there exists a clear difference for the start of rising NOx emissions, which is linked to the physical position of the slow analyser further downstream in the exhaust. The difference in peak NOx emissions is also likely caused by the location of the analyser. The agreement between the two analysers is discussed in detail in previous studies assuring the fidelity of both measurements. The simulation was able to predict the higher peak NOx emissions relying on transient data, especially at load step-up, which is closely matching measured fast-NOx. More interestingly here, for both conditions, a clear faster rise of NOx is captured by the simulation compared to the slow analyser. This is well aligned with the fast-NOx analyser. The simulation and the fast analyser reaches steady-state almost instantaneously whereas for, both

![Figure 8](image1.png)

**Figure 8.** Test point 1 cyclic $P_{\text{max}}$ versus NOx emissions via Pearson correlations.

![Figure 9](image2.png)

**Figure 9.** Test point 1 comparisons between the cycle averaged ANN NOx model predictions, the cycle averaged fast-NOx analyser readings and the slow-NOx analyser readings. Four separate test sets (identified by the zigzag line) are concatenated together for the same test conditions.
conditions, the slow analyser takes around 6–8 s to reach a steady-state value after the load step, suggesting that engine-out NOx emissions follow a slow transient path on a load step. Physically, a delay in the NOx formation caused by a NOx converter as shown by the slow-NOx channel would suggest that there is more NO measured than NOx, which is not an accurate representation of the NOx formation process. A close alignment of NOx and NO from the fast-NOx analyser has also confirmed the NO2/NOx ratio has a similarly instantaneous response. Both the simulation and the fast-NOx analyser suggest the engine-out emissions are, in fact, instantaneous. The simulation of such event is achieved through the instantaneous response of the engine in-cylinder peak pressure to the load demand with following similarly instantaneous response of engine thermal conditions. It can be seen that there is excellent repeatability between different engine test runs for the same condition. The delay in response and lower values here for slow analyser are likely caused by the combination of the slower response rate of the analyser itself and the longer path from the exhaust path to the slow analyser, and longer mixing time in the engine exhaust before the slow analyser acquiring a sample. With the inclusion of cyclic $P_{\text{max}}$ signal, the ANN model is indeed able to predict the transient NOx emissions during load steps. This is, to the best of the authors’ knowledge, the first confirmation of experiment and simulation in this fast transient NOx behaviour. The application of such a model can, therefore, help to estimate the real road NOx emissions without the use of a lab grade fast-NOx analyser.

In order to further study the accuracy of the chosen model, Figure 11 shows the absolute error for the ANN model predictions for all test points. As seen from the graph, the majority of the points are clustered around zero error line in terms of absolute error, which shows the good predictability of the model across different engine speed and load. Bear in mind, the conditions investigated here are well outside training range even for steady-state range and no transient fast-NOx was incorporated in training. Previous studies both from the literature and the authors of this study have suggested an accuracy of 3% can be reached for operating conditions within the training range. This suggests using such a tool at facilities with large dataset can be beneficial given the retrain abilities also demonstrated by the current model. It is worth noting though, during load stepping there is a slight difference between the time-averaged ANN predicted NOx values and the measured fast-NOx emissions. This is likely due to the
fast analyser picking up the cycle-to-cycle variations which the model is not trained with. Figures 12 and 13 present the cyclic predictions of the ANN model using the repopulated signals compared with the experimental measurements. Indeed cycle-to-cycle NOx variations are present in fast-NOx analyser for both conditions. For test point 1 the predicted NOx is well within the range of cyclic NOx measurements for both load step-up and load step-down. For test point 2, predicted NOx also shows good agreement with measured cyclic NOx under load step-up. However, a deviation is observed under load step-down. This small deviation around 100 arbitrary NOx units at load stepping down is thought to be attributed to the lack of extensive training data at these high loads, compared to other operating conditions as can be seen in Figure 1. The deviation is also within the accuracy limits of the steady state NOx model as shown in the previous model development study. This also explains why at step up there is little deviation between the predictions and experiments as the model is well trained at these conditions. For the current study, safety concerns limited extensive experiments at high speed and high load conditions. With more data available at high loads and speed the slight deviation at stepping down could also be mitigated. This is supported by a correlation study between the experimental data and the NOx experiments.

Figures 14 to 17 shows the correlation between the simulation and fast-NOx emissions for each condition with a focus on load step-down. Here, the correlation coefficient is used to describe the relationship between two or more parameters. Globally both test points show a high correlation for all test points with better correlation found in test point 1. This is expected as lower cycle-to-cycle variations were observed. Test point 2 still has a very high global correlation of 0.88. A close look is given to load step down for both test

![Figure 12. Comparison of ANN cyclic NOx predictions with fast-NOx analyser at test point 1.](image12)

![Figure 13. Comparison of ANN cyclic NOx predictions with fast-NOx analyser at test point 2.](image13)

![Figure 14. Test point 1 load step down correlation between cycle averaged simulation and fast-NOx.](image14)

![Figure 15. Test point 1 overall correlation between cycle averaged simulation and fast-NOx.](image15)
A high correlation is again found even for test point 2 despite the lower prediction. This suggests the transient trend is well predicted where a deviation from the experimental values is likely caused by a global parameter for example: exhaust flow rate fluctuations. This highlights the delicacy of the ANN model as it is very sensitive to slight changes in signal. The transient behaviour, however, is well aligned with the fast-NO\textsubscript{X} predictions. More importantly the prediction is simultaneous and has comparable or better results compared to the slow-NO\textsubscript{X} analyser. The high correlation between the NO\textsubscript{X} predictions and the experiments is closely aligned with the high correlation given by the cylinder peak pressure and NO\textsubscript{X} emissions, highlighting the importance of cyclic peak cylinder pressure in the prediction of transient NO\textsubscript{X} emissions for ANN based models.

Conclusions

In this study, the transient predictive ability of artificial neural networks where a large number of engine testing data are available has been studied extensively. Significantly, the proposed model is trained from steady-state engine testing data. The trained data with 14 input features are provided with transient signals which are available from most engine testing facilities. Crank-angle resolved NO\textsubscript{X} measurements have been taken from a high-speed light duty diesel engine at a variety of engine test conditions from low load and speed to high load and speed which provides data with the highest quality for the validation of model predictions. The maximum cylinder pressure of each cycle is combined with other thermophysical signals given by a slow response analyser as the input for the ANN model.

The model is found to be able to predict transient NO\textsubscript{X} at conditions well outside the transient conditions covering different load steps with a high degree of accuracy. The response in NO\textsubscript{X} levels to step changes in engine load is predicted as instantaneous, which is consistent with fast-NO\textsubscript{X} analyser suggesting that the in-cylinder conditions change similarly instantaneously. No significant transient effects were observed by the model following the step change. The importance of in-cylinder peak pressure in transient NO\textsubscript{X} formation is further verified. This is only previously reported by the data used in this study. The study also aligned well with previous input feature selection study emphasizing the importance of in-cylinder peak pressure in NO\textsubscript{X} modelling. The predicted model is, therefore, likely to be capable of predicting transient RDE NO\textsubscript{X} on an engine-out basis. Moreover, since the model has previously been applied to steady-state predictions and different engine configurations, the capability of the current model is therefore further extended.

Although the model is found to be able to predict transient NO\textsubscript{X} emissions, the capability of cycle-to-cycle variations is still not yet developed as limited diesel engine experimental data is available. Therefore, the authors intend to further study the capability to incorporate physical models into the ANN model for future studies.

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