Remote NO\textsubscript{x} emission prediction model based on LSTM neural network

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**Keywords:** neural network, model, remote monitoring, NO\textsubscript{x} emission prediction.

**Abstract.** Test results from many researchers show that NO\textsubscript{x} emission from many on-broad heavy-duty diesel vehicles is higher than which been registered. Therefore, CN\textsubscript{VI} emission regulations clearly proposes that the heavy-duty diesel vehicles should be supervised by a T-BOX which can transmit CAN message from vehicle OBD interface to the remote monitoring platform. Based on the formation mechanism of NO\textsubscript{x} emission and the variety of OBD data flow, the LSTM (Long Short-Term Memory) neural network model inputs such as engine speed, torque, atmospheric pressure, coolant temperature, fuel consumption rate and intake air mass flow are selected by using partial least square method (PLS). 19877 groups of data from engine test results were used for model training and verification, the root mean square error of training and test are $R_{\text{TR}} = 29.7 \times 10^{-6}$ and $R_{\text{TE}} = 19.9 \times 10^{-6}$, with a high prediction accuracy which can fully meet the requirements of the SCR system DeNO\textsubscript{x} performance diagnosis module in the OBD remote monitoring system.

1 Introduction

With the rapid development of the national economy, the main contribution factors of urban pollution sources have begun to shift from fixed source emissions to mobile source emissions. Emissions of mobile sources in Beijing, Shanghai, Hangzhou, Jinan, Guangzhou and Shenzhen are the primary sources, accounting for 45.0%, 29.2%, 28.0%, 32.6%, 21.7% and 52.1% respectively \cite{1}. By the end of 2018, there were 18.18 million diesel trucks in China, accounting for 7.9% of the vehicle ownership, which were mainly commercial vehicles with high intensity of use, harsh operating environment and relatively high pollution emissions, and emissions of nitrogen oxides (NO\textsubscript{x}) and particulate matter (PM) accounted for 60.0% and 84.6% of the national vehicle emissions respectively.

Since the implementation of the CN\textsubscript{IV} and CN\textsubscript{V} emissions regulations, a number of research and testing institutions found that the real-road emissions of diesel vehicles,
especially commercial heavy-duty diesel vehicles, exceeded the standard limit seriously, and the cheating behaviors of on-board fault diagnosis (OBD) system and selective catalytic reduction (SCR) system in the on-road vehicle have not been effectively regulated\[2\]. Against this background, the country proposed the "Win the Blue Sky Guard Station Plan" at the end of 2017, and in the GB17691-2018 "Emission Limits and Measurement Methods for Pollutant Emissions of Heavy-Duty Diesel Vehicles (6th Phase of China) " released on June 22, 2018, the demand for remote monitoring of heavy-duty diesel vehicles were proposed for the first time \[3\]. In the same year, "Action Plan for the Control of Diesel Trucks" jointly issued by 11 departments such as the Ministry of Ecological Environment, which put forward the installation requirements of OBD remote online monitoring system for diesel trucks.

OBD remote online monitoring system needs to judge the operation and emission status of the target vehicles through various on-line models. At present, the domestic diesel vehicle in use are basically the vehicles below the national V, with a single downstream NO\textsubscript{x} sensor. Therefore, the diagnosis of the DeNO\textsubscript{x} performance of the SCR system cannot be directly realized, and a method that can predict the NO\textsubscript{x} emissions of the diesel engine through the OBD data flow is urgently needed to facilitate the realization of the above diagnosis function.

Regarding the estimation of NO\textsubscript{x} emissions, domestic and foreign scholars have done a lot of research and put forward a variety of methods to build a prediction model, such as Taskinen\[4\] using combustion simulation software KIVA-2 to establish the NO\textsubscript{x} emission prediction model of medium-speed diesel engines. This method has a strong explanation for NO\textsubscript{x} generation, but the modeling method is complicated, the input parameters are more, the requirements for computing resources and data are higher, and it is not suitable for remote monitoring needs. d’Ambrosio, Asprion and Finesso etc. \[5-7\] used a semi-experienced approach to build a NO\textsubscript{x} emission prediction model of diesel engines based on Zeldovich theory. This model has a simple structure and can explain the generation of NO\textsubscript{x} to a certain extent, but it is difficult to use for remote diagnostic due to the need for accurate cylinder pressure signals as input. For diesel engines without in-cylinder pressure sensors, Banerjee, Anand, and Li Nan, etc. \[8-10\] used neural networks (NN) to establish a NO\textsubscript{x} emission prediction model for diesel engines. The neural network method has good nonlinear fitting and is simple to use, but it requires many training samples and has a large prediction error for the untrained area. The diesel engine NO\textsubscript{x} emission prediction model Chang Yingjie etc. \[11\] built using the partial least square (PLS) requires less training data and good robustness, but its nonlinear fitting ability is low. Since the method of PLS modeling can only solve nonlinear problems in a very small extent, for many nonlinear practical problems, the PLS method is not very effective \[12\]. Hu Jie etc. \[11\] use the neural network partial least square (NNPLS) to establish a NO\textsubscript{x} emission prediction model of diesel engines, which also has the characteristics of both PLS ( requires few training sample point and can fully extract useful information from independent variables ) and NN ( high degree of nonlinear fitting ) and it can obtain higher prediction accuracy under the training of a small number of sample points. However, for remote online monitoring systems, the amount of data is often abundant, so this paper selects a recurrent neural network \[14-15\] that is more suitable for prediction of sequence and large amounts of data to build a NO\textsubscript{x} emission prediction model, which can accurately predict NO\textsubscript{x} emissions of the target engine and then realize the diagnosis of DeNO\textsubscript{x} performance of SCR system and NO\textsubscript{x} sensor signal.
2. OBD remote monitoring system

2.1 Introduction of systems and functions

OBD remote monitoring system is mainly composed of OBD remote monitoring terminal (also known as vehicle terminal/T-BOX) and remote monitoring platform. As shown in Figure 1, OBD remote monitoring terminal is usually installed in the vehicle OBD diagnostic interface, which can collect the main operating parameters of the vehicle during operation through the CAN bus (e.g. engine speed, intake mass flow, fuel consumption rate, engine net output torque, SCR inlet temperature/SCR outlet temperature, urea injection volume, urea level sensor signal, downstream NOx sensor measurement etc.). Through the wireless communication module of the terminal, the data will be sent to the remote monitoring platform in the format specified by the platform using the 2G/4G network. The platform can accept the data uploaded by the terminals installed on different vehicles, and carry out a series of data pre-processing, storage and calculation operations to achieve the normalized tracking of continuous, real-time and online status monitoring of vehicle operating condition information, I/M status information and pollutant emissions.

After processing a large number of long-term running data from on-line vehicles, many common cheating behavior of vehicles are identified based on temperature sensor signal diagnosis module, NOx sensor signal diagnosis module, urea injection system working status diagnosis module etc. Based on the feedback results of the real state of the actual vehicle, train the neural network self-learning model that determines the diagnosis result, determine the threshold of core criteria and the weight factor of diagnosis result of sub-model. The learned model can accurately identify the abnormal using behavior of vehicles such as complete or partial pull-out of the temperature sensor, partial dilution of the NOx sensor, pull-out of the NOx sensor, failure of the NOx sensor, the using of temperature/ NOx sensor signal generator, reflux of the injected urea, the using of poor quality urea and poor performance of SCR catalysts.

This paper focuses on the NOx emission prediction method used for the diagnosis of DeNOx performance of the vehicle SCR system to ensure that the accuracy of prediction output by the model meets the needs of remote diagnostics.
2.2 Method of SCR system DeNOx performance diagnosis

After the platform accepts the OBD data uploaded by the vehicle, the filtered data is used as the input to the DeNOx performance diagnostics module. Due to the technology configuration of a single downstream NOx sensor used in diesel vehicles, it is necessary to diagnose the DeNOx performance of the SCR system through the following methods:

1) Predict upstream NOx emission level through the NOx emission prediction model of the platform, as shown in figure 2.

2) Estimate the maximum conversion capacity of the catalyst through inlet and outlet temperature of the SCR system, estimate the theoretical maximum reaction capacity of the SCR system under the actual injection condition by the reactant real-time injection volume, and obtain the DeNOx quantity, as shown in Figure 3.

3) Predict downstream NOx emission mass through upstream NOx primary emission cumulative mass and the theoretical DeNOx mass. Finally, compare the downstream NOx emission mass and the actual NOx emission mass calculated by NOx sensor (as shown in Figure 4) to evaluate the real-time conversion capability (performance) of the SCR system.

The evaluation method of the real-time conversion capacity of the SCR system is as follows. Since the conversion efficiency of normal vanadium based SCR catalyst can generally reach more than 60% under the conditions above the starting temperature,
Condition 1 gives the basic judgment of the catalyst conversion efficiency, Condition 2 is to diagnoses the DeNO\textsubscript{x} efficiency of SCR system by checking the logic correspondence among the accumulated mass of the upstream NO\textsubscript{x} emission, the accumulated mass of urea injection and the accumulated mass of the downstream NO\textsubscript{x} emission. When Condition 2 fulfilled, the conversion performance of SCR system is considered normal.

\begin{equation}
\text{cond. 1: } \frac{\sum_{i=1}^{5}(A_i-C_i)}{\sum_{i=1}^{5} A_i} > 50\% \tag{1}
\end{equation}

\begin{equation}
\text{cond. 2: } 0.6 \sum_{i=1}^{5} C_i < \sum_{i=1}^{5} (A_i - B_i) < 1.5 \sum_{i=1}^{5} C_i \tag{2}
\end{equation}

In the formulas:
- \( A \) is the accumulated mass of the engine out NO\textsubscript{x} emission during a certain time;
- \( B \) is the theoretical accumulated DeNO\textsubscript{x} mass corresponding to the consumed urea during a certain time;
- \( C \) is the accumulated mass of tailpipe NO\textsubscript{x} emissions during a certain time.

When the downstream NO\textsubscript{x} sensor works normally and the signal is reliable, the accuracy of this diagnosis method mainly depends on the accuracy of the upstream NO\textsubscript{x} emission prediction model.

This paper uses the LSTM neural network method to predict the engine out NO\textsubscript{x} emission of the target vehicles because OBD remote monitoring platform can easily get a lag quantity of real-time data that can be quickly classified in to different models and brands.

### 3 Remote NO\textsubscript{x} emission estimation model

#### 3.1 Influence factors of diesel NO\textsubscript{x} generation and preliminary confirmation of input parameters

Three conditions are required for the formation of diesel exhaust NO\textsubscript{x}: excess oxygen in the combustion chamber, high temperature of the combustion process, and duration of high temperature \cite{17}.

As the advance angle of fuel injection is delayed, the amount of fuel involved in the mix combustion decreases, and the initial heat release and peak of the heat release are reduced. Thus, the maximum combustion temperature is reduced. Meanwhile, the duration of high temperature in combustion chamber get shorted and the NO\textsubscript{x} emission is significantly reduced.

The diesel engine speed can affect both the high temperature and the duration of the combustion process. When the injection angle is fixed, the higher the speed, the shorter the actual injection time. At the same time, the charge coefficient decreases with increasing speed, resulting in a reduction in NO\textsubscript{x} emission concentration.

The load represents the maximum combustion temperature and the duration of the high temperature. Torque, cycle fuel injection quantity (mg/stk), excess air coefficient etc. represent the load factor. And the torque can be obtained by product of the rated torque in the vehicle static information and the percentage of net output torque in the OBD data flow; cycle fuel injection quantity can be calculated by the proportional relationship between the number of engine cylinders in the vehicle static information and the speed and the fuel consumption rate in the OBD data flow; excess air coefficient can be calculated by the intake quantity and the fuel consumption rate in the OBD data flow.

For diesel engines with EGR, the EGR rate is also an important factor that affects the original NO\textsubscript{x} emission. However, most of heavy-duty vehicles that meet the implementation of the CN_IV and CN_V Emissions Regulations adopt the SCR-only DeNO\textsubscript{x} technology.
route, the proportion of vehicles using EGR is small, so the EGR rate is not considered in this paper.

Intake resistance, exhaust resistance, temperature after intercooling etc. also have a great impact on emissions, but these parameters mainly depend on load factors, which has been reflected in the fuel consumption rate factors and will not be considered.

The environmental factors such as the atmospheric pressure, ambient temperature, ambient humidity of the engine-post-processing system also have an impact on the generation of NO$_x$, and the atmospheric pressure can be obtained through the on-board sensor signal, the ambient temperature and ambient humidity etc. can be confirmed through the input in the platform atmospheric environment module with the GPS signal later. Then correct NO$_x$ emissions.

According to the requirement of GB17691 for remote monitoring of OBD data flow, the types of data that are shown in Table 1 must be read from OBD interface.

| Number | Data items                                        |
|--------|--------------------------------------------------|
| 1      | Vehicle speed                                   |
| 2      | Atmospheric pressure (direct measurement or estimation) |
| 3      | Maximum benchmark torque of the engine          |
| 4      | Engine net output torque                        |
| 5      | Friction torque                                 |
| 6      | Engine speed                                    |
| 7      | Engine fuel flow                                |
| 8      | NO$_x$ sensor output                            |
| 9      | SCR inlet temperature (if applicable)           |
| 10     | SCR outlet temperature (if applicable)          |
| 11     | DPF differential pressure                       |
| 12     | Intake air mass flow read by the air quality flow sensor |
| 13     | Urea tank level                                 |
| 14     | Fuel tank level                                 |
| 15     | Engine coolant temperature                      |
| 16     | Latitude and Longitude                          |

Based on the standard output parameters of OBD interface in Table 1, combined with the parameters related to the formation of NO$_x$ emissions, preliminarily select seven parameters, such as engine speed, engine net output torque, atmospheric pressure, cooling water temperature, fuel consumption, SCR inlet temperature, and intake mass flow, as the initial input of the model. Then filter and confirm relatively independent characteristic parameters as the final input of the neural network by the PLS method.

3.1 PLS method

The PLS method uses the idea of main component analysis and reduce the multiple correlation of the independent variables by extracting the component. However, it is different from principal component analysis. Partial least square method extracts components in groups of independent and dependent variables at the same time. The extracted components satisfy the following two conditions [18]:

1) The extracted component group should contain the variation information in the independent variable and the dependent variable as much as possible;

2) The correlation between the independent and dependent variable components in the same group is as large as possible, that is, their correlation coefficients are as large as possible.

If $t$ represents the component extracted from the independent variable $X$ and $r$ represents the component extracted from the dependent variable $Y$, the above two conditions mean
choosing the largest variance \( \text{Var}(t) \) and \( \text{Var}(r) \) and the largest correlation coefficient \( \text{Corr}(t, r) \).

Assuming that there are \( w \) and \( v \) that make formula \( t = X_w \) and \( r = Y_v \) true, the above condition can be expressed the extremum problem in formula (3):

\[
\max \sqrt{\text{Var}(t) \text{Var}(r)} \text{Corr}(t, r) = \max \text{Cov}(Xw, Yv) = \max (w^T X^T Y v)
\] (3)

Solve \( w \) and \( v \) using singular value decomposition. A set of eigenvectors \( t=X_w \) and \( r=Y_v \) can be obtained through decomposition of the equation \( X^T Y = \sum e_i f_i g_i^T \), where \( w=f_1 \) and \( v=g_1 \). It has been proved in literature \([19]\) that the covariance \( \text{Cov}(t, r) \) at this time is the largest.

The load vectors of feature vector are defined as \( m = X^T t / t^T t \), \( n = Y^T r / r^T r \); The regression factor of the regression model \( \hat{r} = c t \) is \( c = t^T t / r^T r \) and the components of the first group extracted are \( tm^T \) and \( ctn^T \). The independent variables and dependent variables were decomposed to: \( X = X_1 + tm^T \), \( Y = Y_1 + ctn^T \), and do the same thing for \( X_i \) and \( Y_i \). Assuming \( A \) times of decomposition, independent variables and dependent variables can be expressed as:

\[
X = t_1 m_1^T + \ldots + t_A m_A^T + X_A
\] (4)

\[
Y = c_1 t_1 q_1^T + \ldots + c_A t_A q_A^T + Y_A
\] (5)

The relationship between the variables \( X \) and \( Y \) can be expressed as the following:

\[
Y = X_1 b_1 + \ldots + X_B b_B + Y_E
\] (6)

Where \( B \) is the number of independent variables, \( B_i \) is the regression factor of the \( i \)th independent variable, \( X_i \) is the \( i \)th independent variable, and \( Y_E \) is the residual matrix.

### 3.1.1 Screening of independent variables

Although the partial least square method extracts the most relevant components from independent variables and dependent variables, the insignificant variables in the independent variables will still have an adverse effect on the model \([20]\), so the independent variables must be filtered. The independent variables are tested by the significance coefficient as follows:

The regression factor \( b_i \) is calculated using all samples for the \( i \)th independent variable and the regression factor \( b_{i(-j)} \) is calculated using the sample except the \( j \)th sample point, and the following parameters are defined:

\[
\sigma_{bi} = \sqrt{\frac{\sum_{i=1}^{n} (b_{i(-j)} - b_i)^2}{n-1}}
\] (7)

The significance of the independent variable is judged by whether the significance coefficient \( |b_{ij}| / t_{0.05, n-1} \sigma_{bi} \) is greater than 1. The greater the significance coefficient, the higher the significance of the independent variable. When the significance coefficient is less than 1, the independent variable is not significant.

However, simply filtering the independent variables by whether the significance coefficient \( |b_{ij}| / t_{0.05, n-1} \sigma_{bi} \) is greater than 1 does not result in the best results. Therefore, two parameters in the formula (7) and formula (9) are used to determine the accuracy of the model.
to assist in the selection of independent variables. The root mean square error can show the average prediction effect of the model.

In the modeling process, the sample is divided into two parts: the modeling sample and the testing sample. Training samples are used to build the model, and test samples are used to verify the prediction performance of the model.

The root mean square of the training sample prediction error:

\[ R_{tr} = \sqrt{\frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{n}} \]  \hspace{1cm} (8)

where \( y_i \) represents the actual value of the \( i \)th training sample in the dependent variable, \( \hat{y}_i \) represents the predicted value of the \( i \)th training sample and \( n \) is the number of training samples.

The root mean square of the test sample prediction error:

\[ R_{te} = \sqrt{\frac{\sum_{i=1}^{m} (y_j - \hat{y}_j)^2}{m}} \]  \hspace{1cm} (9)

where \( y_j \) represents the actual value of the \( j \)th test sample in the dependent variable, \( \hat{y}_j \) represents the predicted value of the \( j \)th test sample and \( m \) is the number of test samples.

After judging the significance coefficient is less than 1, adopt the method of screening one by one to remove the insignificant variables. First calculate the \( R_{tr} \) and \( R_{te} \) values of the model before removing an independent variable, and then calculate the \( R_{tr} \) and \( R_{te} \) values again after removing the independent variable. If both \( R_{tr} \) and \( R_{te} \) become smaller, it is reasonable to remove the independent variable, otherwise it should not remove the independent variable. If the final \( R_{tr} \) and \( R_{te} \) values are large, it means that the relevant information has been missed or the nonlinearity was serious, and the information should be re-extracted.

### 3.1.2 Removal of specific sample points

Because of experimental errors or other reasons, a small number of sample points deviate too much from other sample points, and when they are used to model or validate the model, there is a large deviation in the mode. Therefore, this part of the data needs to be eliminated. There are a statistical test method proposed in the literature [18].

The contribution rate of the \( j \)th sample to the \( h \)th component \( t_h \) is defined as:

\[ T_{hj}^2 = \frac{\hat{t}_{hj}^2}{(n-1)s_h^2} \] \hspace{1cm} (10)

where \( \hat{t}_{hj}^2 \) is the square of the \( h \)th component value calculated with the \( j \)th sample. \( s_h^2 \) is the variance of component \( t_h \).

The cumulative contribution rate of the \( j \)th sample is:

\[ T_j^2 = \sum_{h=1}^{m} \frac{t_{hj}^2}{(n-1)s_h^2} \] \hspace{1cm} (11)

where \( m \) is the number of extracted components.

When the cumulative contribution is too large, the probability that the component will deviate the result is high. The specific determination conditions are as follows:

\[ T_j^2 < F(m, n - m) \frac{m(n^2 - 1)}{n^2(n - m)} \] \hspace{1cm} (12)
The sample point is retained if the above conditions are met, otherwise it should be eliminated.

### 3.1.3 Determination of the structure of the PLS model

The number of extracted components will directly affect the effect of partial fitting of neural network. Determine the optimal number of components by increasing the number of components one by one. The method steps are as follows: the number of components increases one by one from 1. We can use the method in Figure 5 to determine the optimal structure of the neural network part with current number of components to obtain the PLS model with different components. As the number of components increases, the prediction error of the model first decreases. When the number of components of the model is 6, the test sample error is minimum. And then the number of components starts to increase, and the error of training sample changes little when the number of components is 4 to 6. Therefore, the optimal number of components of this model is 6.

![Fig. 5. The process of determining model structure.](image)

This paper finally confirms that the parameters used for the neural network model estimate are as follows: engine speed, torque, atmospheric pressure, cooling water temperature, fuel consumption and intake mass flow. The engine test bench data are used for model training and validation. We combined with the sensor signal of the T-BOX and all environmental factors are used as input of the environmental correction factor MAP when estimating emissions for the vehicle.

### 3.1.4 Possible error in the PLS model

Based on previous experience in establishing the NO\textsubscript{x} emission estimation model in the injection control strategy, it has been found that the deviation of the PLS model is mainly due to the following aspects \cite{14}:

(1) Error of the test data. There are some errors in the data obtained from the experiment, which will result in the error of the model prediction results. The errors are randomly distributed, and the influence of this error on the model decreases gradually as the training sample increases.

(2) The deviation caused by fitting. The PLS method is only applicable to linear fitting. Although the accuracy of the model is improved to a certain extent by adding some quadratic terms, the quadratic curve still has a large deviation from the actual curve;

(3) Error caused by the residual terms. During modeling with the PLS method, there is always a residual \(Y_c\) for the dependent variable that cannot be eliminated, and it also have an impact on the model;
(4) Others. The selected independent variables and training samples are not representative, so the model is poorly optimized.

In order to reduce the error of the PLS model, the PLS method of neural network is used. The composition extracted by the PLS method is fitted directly to the dependent variable, eliminating the influence of the residual terms. At the same time, the error caused by fitting can be greatly reduced by using of the neural network method.

3.2 Determination of neural network model

Although the BP (back propagation) neural network is popular and technologically sophisticated in the industry, recurrent neural network is more appropriate for sequence prediction and large amounts of data [15]. Moreover, the LSTM neural network overcomes the problem of gradient disappearance and gradient explosion caused by long-distance memory, and is a more suitable choice for training the network model [21].

2. 2.1.1 Selection of activation functions and learning algorithm

The main function of the activation function is to strengthen the ability of network learning and provide nonlinear modeling ability for the network [22]. Different activation functions have different characteristics and application situation. In the LSTM neural network, the Sigmoid function can be selected as the gate activation function. The Sigmoid function can produce values between 0 and 1. 1 means remember and 0 is forgot. In addition, activation functions such as Tanh, ReLU, Sigmoid can be selected as state activation functions. Compared with the ReLU function, Tanh function is more robust, and its convergence speed is faster than Sigmoid function, so we choose the Tanh function as the state and output function.

The common learning algorithm of LSTM neural networks is BPTT (back-propagation through time). The BPTT algorithm is a common method for training RNN, in fact, its essence is still the BP algorithm. It calculates the hidden state and output, error and partial derivative of weight of each layer, and then optimize the parameter of vertical propagation between levels and lateral propagation on time using gradient descent [23].

3.2.2 Determination of the number of nodes in hidden layer

The number of nodes in the hidden layer has a great impact on the performance of the LSTM neural network. If the number of hidden layer nodes is too small, the information processing ability and generalization ability of the network will decrease. Conversely, if there are too many hidden layer nodes, the network will also be complicate, the model training speed will be affected, and the risk of "overfitting" will increase. However, based on the Kolmogorov theorem, it can be seen that this hidden layer has 2n -1 neurons, where n represents the number of neurons in the input layer. Because the number of input layer nodes of LSTM model created in this paper is 6, the number of hidden layer nodes is 13.

3.2.3 Adam optimization algorithm

The optimization algorithm is essentially a mathematical method. And common optimization algorithms include SGD (Stochastic gradient descent, SGD), Momentum, Nesterov Momentum, Adagrad (Adaptive sub-gradient, Adagrad), RMSprop, Adam etc. [21]. Adam is actually the result of an optimized combination of Momentum and RMSprop. Adam can not only store exponential decay averages of squares of past gradients like RMSprop, but also can store exponential decay averages of past gradients like momentum. In short, Adam can automatically adjust the learning rate of parameters, increase training speed, and improve
network stability. The main parameters of the recurrent neural network based on LSTM are listed in Table 2:

**Table 2. Main parameters of LSTM-based recurrent neural network model.**

| Training parameters                          | Modes and values |
|----------------------------------------------|------------------|
| Number of hidden layer nodes                 | 13               |
| State activation function                    | Tanh             |
| Gate activation function                     | Sigmoid          |
| Loss function                                | RMSE             |
| Optimize iterative algorithms                | Adam             |
| Training cycle                               | 400              |
| Gradient threshold                           | 1                |
| Learning rate                                | 0.01             |

### 4. Validation of the model

#### 4.1 Experimental acquisition of model data

We used the bench test results of a commercial heavy-duty vehicle diesel engine as the training and validation data for the model are from and the specific parameters of the engine are shown in Table 3:

**Table 3 Test engine specifications**

| Parameters                   | Content                                      |
|------------------------------|----------------------------------------------|
| Engine model                 | 7H                                           |
| Configuration                | 6-cylinder inline                            |
| Displacement                 | 6.8L                                         |
| Ignition sequence            | 1-5-3-6-2-4                                   |
| Number of intake valves      | 2                                            |
| Number of exhaust doors      | 2                                            |
| Compression ratio            | 17.7                                         |
| Type of supercharger         | Variable Geometry Turbocharger (VGT)         |
| Fuel injector                | Double solenoid valve electronic unit injector |
| Peak torque                  | 1000Nm@1200~1900rpm                          |
| Rated power                  | 209kW@2300rpm                                |

Measure parameters including engine data flow and gas emissions using instruments shown in Table 4, and figure 6 shows the bench test site.

**Table 4 Parameter measurement scheme**

| Test instruments                  | Test parameters                                                        |
|-----------------------------------|------------------------------------------------------------------------|
| AVL electric dynamometer test bench | engine speed, torque, coolant temperature, inlet temperature and pressure, exhaust pressure, atmospheric humidity, atmospheric temperature, atmospheric pressure |
| FTIR                              | Engine out NO_x emission concentration                                  |
| ES581                             | Fuel delivery per cycle, engine speed, engine net output torque, atmospheric pressure, coolant temperature, SCR inlet temperature, intake mass flow |
19877 groups of data are divided into the data set and training set by hierarchical sampling method, and 14877 groups are used as sample training data and 5000 groups are used as test data. Because the unit of each input data is different and the order of magnitude is different, it is necessary to normalize the data first.

![Image](image1.jpg)

**Fig. 6.** Engine & after-treatment system test bench.

### 4.2 Results analysis

LSTM neural network and PLS model were combined to the final neural network model. And the engine speed, torque, atmospheric pressure, cooling water temperature, fuel consumption, intake mass flow were taken as inputs of neural network. The predicted results of training and test sets of the model (the network model output value after denaturalization), the error of training set and the test set, as shown in figure 7 to figure 10 respectively.

As can be seen from figure 7 and figure 8, the predictive model has good learning ability and generalization ability, and with the increase of training times, the mean square error becomes smaller and smaller. The training sample error of the model \((R_{TR})\) is \(29.7 \times 10^{-6}\). And the RMSE of the model is 2.27% when the maximum NO\(_x\) emission of the training data is \(1310 \times 10^{-6}\). The test sample error of the model \((R_{TE})\) is \(19.9 \times 10^{-6}\). And the RMSE of the model is 2.64% when the maximum NO\(_x\) emission of the training data is \(753 \times 10^{-6}\). And the position with the largest error in the test set is in the 1001 data, with an error -267.2. The test set sample error percentage is shown in Figure 11. It can be seen from Figure 11 that the maximum error percentage of the test set is only 1.18%, which has reached a very high estimation accuracy. The data with the largest error mainly appears in the first few sets of data for in each layer of the training set, which is caused by the basic characteristics of the recurrent neural network and performs well in other cases.
19877 groups of data are divided into the data set and training set by hierarchical sampling method, and 14877 groups are used as sample training data and 5000 groups are used as test data. Because the unit of each input data is different and the order of magnitude is different, it is necessary to normalize the data first.

Fig. 6. Engine & after-treatment system test bench.

4.2 Results analysis

LSTM neural network and PLS model were combined to the final neural network model. And the engine speed, torque, atmospheric pressure, cooling water temperature, fuel consumption, intake mass flow were taken as inputs of neural network. The predicted results of training and test sets of the model (the network model output value after denaturalization), the error of training set and the test set, as shown in figure 7 to figure 10 respectively.

As can be seen from figure 7 and figure 8, the predictive model has good learning ability and generalization ability, and with the increase of training times, the mean square error becomes smaller and smaller. The training sample error of the model (RTR) is $29.7 \times 10^{-6}$. And the RMSE of the model is 2.27% when the maximum NO\textsubscript{x} emission of the training data is $1310 \times 10^{-6}$. The test sample error of the model (RTE) is $19.9 \times 10^{-6}$. And the RMSE of the model is 2.64% when the maximum NO\textsubscript{x} emission of the training data is $753 \times 10^{-6}$. And the position with the largest error in the test set is in the 1001 data, with an error -267.2. The test set sample error percentage is shown in Figure 11. It can be seen from Figure 11 that the maximum error percentage of the test set is only 1.18%, which has reached a very high estimation accuracy. The data with the largest error mainly appears in the first few sets of data for in each layer of the training set, which is caused by the basic characteristics of the recurrent neural network and performs well in other cases.

Fig. 7. Comparison of prediction results of training.

Fig. 8. Comparison of prediction results of test.

Fig. 9. Errors of training results.

Fig. 10. Errors of test results.
Fig. 11. Percentage errors of test results.

5. Conclusion

(1) The PLS model based on the LSTM neural network model. First of all, select the parameters according to their availability, NO\textsubscript{x} emission correlation, and their significance. And then determine the structure of model by incrementing one by one. Finally establish the diesel engine NO\textsubscript{x} emissions prediction model and confirm engine speed, torque, atmospheric pressure, cooling water temperature, fuel consumption, mass air flow as the input of the model.

(2) The training sample error of the model (R\textsubscript{TR}) is 29.7×10^{-6}. And the RMSE of the model is 2.27% when the maximum NO\textsubscript{x} emission of the training data is 1310×10^{-6}. The test sample error of the model (R\textsubscript{TE}) is 19.9×10^{-6}. And the RMSE of the model is 2.64% when the maximum NO\textsubscript{x} emission of the training data is 753×10^{-6}.

(3) For this diesel engine, the maximum error percentage of test set is only 1.18%, which can fully meet the requirements for remote diagnosis of DeNO\textsubscript{x} performance of SCR system and can be used for reasonable diagnosis of downstream NO\textsubscript{x} sensor signal.

Open Fund of the National Engineering Laboratory for Mobile Pollution Source Emission Control Technology (NELMS2017A08)

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