Modeling the emissions of a gasoline engine during high-transient operation using machine learning approaches

Mohammad Hossein Moradi, Alexander Heinz, Uwe Wagner and Thomas Koch

Abstract

To perform a suitable optimization method in terms of emission and efficiency for an internal combustion engine, first highly accurate and possible real-time capable modeling for the transient operations should be provided. In this work, the modeling of NO_x and HC raw emission (before exhaust aftertreatment systems) in a six-cylinder gasoline engine under highly transient operation was performed using machine learning approaches. Three different machine learning methods, namely Artificial Neural Network, Long Short-Term Memory, and Random Forest were used and the results of these models were compared with each other. In general, the results show a significant improvement in accuracy compared to other studies that have modeled transient operations. Furthermore, the shortcoming of Artificial Neural Network for the prediction of the HC emission by the transient operation is observed. The coefficient of determination (R^2) for the best model for NO_x prediction is 0.98 and 0.97 for the training data and test data, respectively. This value is 0.9 and 0.89 for the best HC prediction model.

Keywords

Machine learning, artificial neural network, long short-term memory, Random Forest, internal combustion engines

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Introduction

One of the major challenges of the current decades is to reduce greenhouse gas and pollutant emissions from transportation and industry. Carbon dioxide (CO_2) is a greenhouse gas that causes global warming[1] and leads to enormous damage to numerous ecosystems.[2] Internal combustion engines are important to meet the future and medium-term CO_2 fleet limits, but they also emit pollution.[3] Therefore, the optimization of combustion engines in terms of efficiency and emissions is becoming increasingly important.[4] To perform optimization, the combustion engines are to be modeled first. Among different modeling approaches, Machine Learning is a real-time and powerful approach.[5] Using Machine Learning in internal combustion engine modeling is not an unknown concept and has been studied in previous studies for gasoline and diesel engines. Thompson et al.[6] developed an ANN, based on test bench data, which modeled the behavior of power and exhaust gas composition from a heavy-duty diesel engine along an FTP cycle with an error of less than 5%. The developed models by Hashemi and Clark[7] were also able to predict CO_2 and NO_x emissions of specific driving cycles with high accuracy. However, predictions of acyclic operation were associated with larger deviations. Sayin et al.[8] have developed the model for the steady-state operation to predict not only the fuel consumption and efficiency for a gasoline engine, but also carbon monoxide (CO) and hydrocarbon (HC) emissions. To assess the potential of ANNs, Tosun et al.[9] in compared a multilayer feed-forward (MLF) network trained with the Levenberg-Marquardt (LM) algorithm with linear regression models and observed a significant reduction in the mean absolute percentage error when using the ANN. Jaliliantabar et al.[10] tested the sensitivity of load, speed, and fuel composition on the performance and emissions of a diesel engine in steady-state operation for different

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biodiesel fuel and were able to find the relationship between the input parameters and engine performance and emissions using an ANN. The study of Fang et al.[11] indicated that an excess of input parameters for an MLF can lead to increased errors at low NO_x emission operating points of a diesel engine. To narrow down the number of inputs, both the significance value (p-value) and Pearson correlation coefficient were used. Here, the p-value turned out to be partially misleading and while looking at the Pearson coefficient allowed a reduction from 87 to 14 parameters. Particularly important for NO_x prediction were the degree of delivery, exhaust gas recirculation, inlet air temperature, and cylinder pressure. These studies have demonstrated that MLs can successfully model the steady-state and quasi-steady-state operation of an engine on a test bench. However, this cannot be easily transferred to the changing environmental parameters in everyday free driving. Based on real driving data, three different ML methods were applied in Altug and Kucuk[12] to predict the tailpipe NO_x emissions (measured by PEMS). Here, a coefficient of determination of $R^2 \leqslant 0.725$ was achieved with a long short-term memory (LSTM) network and $R^2 \leqslant 0.92$ with the XGBoost algorithm. The discrepancy was attributed to insufficient data. Fechert et al.[13] used ML methods as a virtual NO_x sensor to embed it in the AdBlue injection control system. The used LSTM network achieved a coefficient of determination of $R^2 = 0.81$. Ma et al.[2] applied an ANN in combination with particle swarm optimization to a diesel engine and were able to reduce NO_x, HC, and CO by 20.5%, 30.3%, and 43.1%, respectively, while reducing fuel consumption by 2.1%. These studies indicate that the research and application of MLs to internal combustion engines are of great interest and benefit.

But as shown in the literature review, there are still few studies that have addressed the modeling of raw emissions (before exhaust aftertreatment systems) from the internal combustion engines in high transient operation. The accuracies of the developed models for transient operations are also in need of improvement. In this sense, in this study different ML methods, namely, Artificial Neural Network, Long short-term Memory, and Random Forest have been used to develop appropriate models for a six-cylinder gasoline engine. It involves an Engine-in-the-Loop (EiL) test bench located at the Institute of Internal Combustion Engines at IFKM, KIT. The test bench is equipped with all necessary modern measurement techniques. Furthermore, it uses CarMaker from IPG as the EiL simulation component to enable the highly transient operation of the engine with real-world relevance. The results of this study show a significant improvement in accuracy regarding the prediction of raw emission in highly transient operations.

Experimental setup and results

The experiments were performed on an engine test bench with an Engine-in-the-Loop vehicle simulation component. The test bench is equipped with an AMA4000 emission analysis system. The emissions were sampled behind the turbocharger but in front of the aftertreatment system of the engine. An overview of the experimental setup is shown in Figure 1. A six-cylinder inline turbocharged spark-ignition engine was used for this investigation. Some of the technical data is given in Table 1. For the experiments, the serial operating maps were used on the engine control unit (ECU) with slight alteration for the use on an engine test bench. With this experimental setup, the simulated test runs on virtual street courses were performed. The three courses were selected for conformity with Real Driving Emission (RDE) tests. Contrary to Commission Regulation (EU) 2017/1151, the following critical alterations were used:

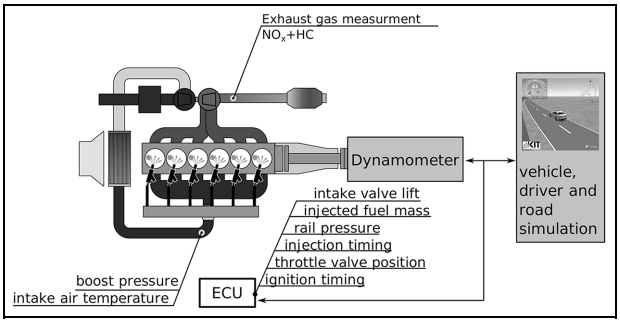

Figure 1. Experimental setup.

Table 1. Technical engine data.

Type	Gasoline direct injection
No. of cylinders	Six in line
Displacement	2979 cm^3
Compression ratio	10.2:1
Injector position	Central
Valve timing	Variable
Aspiration	Turbocharger
Rated power	225 kW at 5800 rpm
Rated torque	400 N · m at 1200–5000 rpm
Emission certification	Euro V
Fuel	Gasoline E5

- The engine coolant and oil temperature was conditioned externally to 85°C.
- The exhaust was sampled before the exhaust aftertreatment system.
- The dynamic boundaries for $va_{pos,95}$ were overstepped.
- All ECU and test bed data was recorded with or downsampled to 10 Hz instead of 1 Hz.

With this alteration, a higher degree of reproduction ability was achieved as well as a wider operating range of the engine. The experimental basis for the modeling consists of nine simulated RDE runs on three RDE courses using three different driver configurations. The

Table 2. Vehicle speed and dynamic range of the used RDE runs.

	Driver	Speed range		
	Dynamic	Urban	Rural	Motorway
v_{mean} [km/h]	Lower	35.9–38.4	74.7–75–5	115–119
	Medium	35.2–35.9	74.4–75.4	115–118
	Higher	32.7–34.3	74.0–76.3	116–119
$va_{pos,95}$ [m^2/s^3]	Lower	15.7–17.4	19.3–22.4	18.2–20.7
	Medium	18.1–19.9	23.3–31.6	24.6–33.9
	Higher	21.6–25.6	26.1–34.4	33.1–36.7

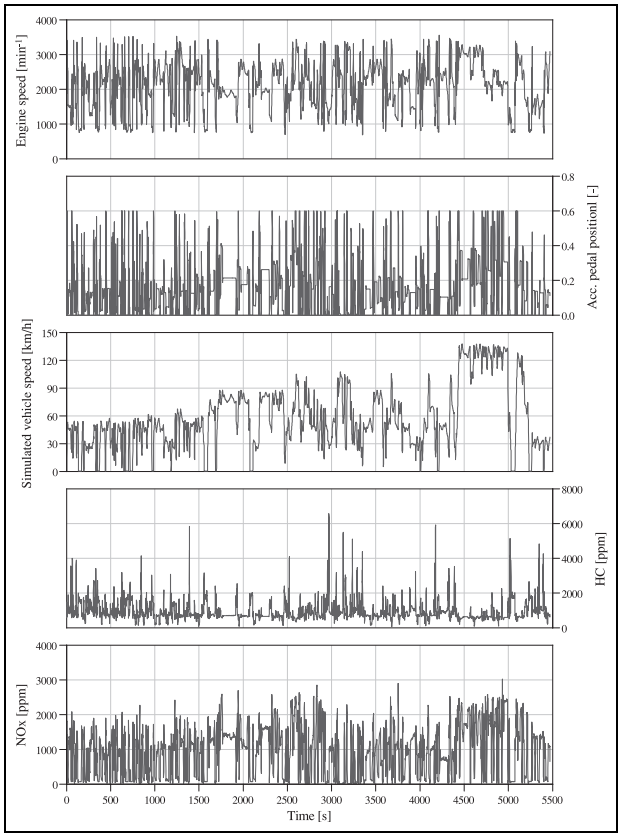

Figure 2. Exemplary experimental data of a simulated RDE run.

different drivers varied mainly concerning maximum acceleration target and gear changing behavior. The training data was obtained from the simulated RDE runs.

Figure 2 shows exemplary test data for one of the simulated road curses. Shifting behavior, and therefore engine speed limit is controlled by the driver parameterization as well as the accelerator pedal position limit. As can be seen from this example the driver input and the simulated road course lead to highly transient load demand and engine speeds. Since no traffic was simulated the resulting simulated vehicle speed is determined by the speed limit and the lateral acceleration limits for corner speeds. Peak HC emissions occur often with load changes from a higher to a lower load.

Table 2 shows an overview over vehicle speed and dynamic range of the used RDE runs. The definition and calculations of mean vehicle speed (v_{mean}) and the dynamic parameter ($va_{pos,95}$) are compliant with the EU regulation. The driver configurations result in dynamic parameters which are under the limit (lower), near the limit (medium), and over the limit (higher) defined by the regulation.

Methodology

The used machine learning approaches

In this study, three different Machine Learning (ML) methods, that is, Artificial Neural Network (ANN), Long Short-Term Memory (LSTM), and Random Forest (RF) were used to model gasoline engine emissions.

Artificial neural network (ANN). In the field of artificial neural networks, the cascade-forward neural network has been used. In Cascade-forward ANN, each layer is connected with all previous layers. In this sense, Cascade-Forward ANN differs from Feed-Forward ANN in that each layer is only connected with a previous layer (neighbor layer).[14,15] Furthermore, to enable learning of complex relationships, more than one hidden layer (deep cascade-forward neural network) was used to develop neural networks and process the input parameters.[14,16] The transform functions for the hidden layers were chosen between the Sigmoid, Tanh, or ReLu function, whereas linear transform functions were always applied for the input and output layers.

Long short-term memory (LSTM). LSTMs (A method from the family of RNNs) can learn long-term relationships in time series data. In particular, when the time delays between relevant information increase, LSTMs have an advantage over RNNs.[17] Inputs to the LSTM block are the cell state at time step $t\ \ 1$ ($c_{t\ \ 1}$), the hidden state at time step $t\ \ 1$ ($h_{t\ \ 1}$), and the features of input data at time step t (x_t). Each of the LSTM block gates (forget-, update-, and output-gate) has its own weights, recurrent weights, and bias. Based on these learnable weights, respective gate decides about the influence of $h_{t\ \ 1}$ and x_t on the cell state.[18] In order to control the influence of information from the past, cell state is initially computed by the forget gate. In the next step, the

update gate decides about adding new information to cell state. Therefore, relevant information, learned from previous time steps, are stored in the cell state.[19] Score is to minimize root mean squared error (RMSE).[17]

Random Forest (RF). Random Forest is a method that can be used for both classification and regression. In this method, each element (here decision trees) is trained with the randomly selected input data (bootstrap samples). The samples that are not used as bootstraps for a tree are counted as out-of-bag samples for that tree. The out-of-bag samples are used after training for the validation of the developed model. The final prediction of the Random Forest models is also the average of the prediction of different trees. The most important hyper-parameter for the Random Forest is the number of trees. A major advantage of Random forest compared to the other ML methods is that in this method there is no over-fitting risk. In other words, the more trees used, the more accurate the results will be. But above a certain amount of trees, no significant improvement in method accuracy will happen. Whereas with the increasing number of trees the calculation time will increase significantly.[20,21]

It should be noted that all the models were developed in MATLAB Software.

Input parameters

As indicated before, in the modeling of this study, the output parameters are the NO_x in the unit of ppm and HC in the unit of ppm. Ten parameters were initially selected to serve as input to develop models. Since the local conditions in the combustion chamber, which are predominantly important for emission formation, are unknown, several external parameters were chosen for the modeling approach. They are listed below together with their influence on in-cylinder conditions:

- *Injected fuel mass* (mg per stroke): fuel mixture, load, and maximum pressure.
- *Throttle valve position* (%), *intake valve lift* (mm): load, fuel mixture, and in-cylinder flow.
- *Engine speed* (rpm): in-cylinder flow.
- *Boost pressure* (mbar): maximum in-cylinder pressure.
- *Rail pressure* (MPa), *Injection timing* (degree of Crankshaft BTDC): Mixture formation and homogenization.
- *Intake air temperature* (°C): Knocking behavior.
- *Ignition timing* (degree of Crankshaft BTDC): Combustion characteristics including maximum pressure.
- *Volumetric efficiency* (-): additional and optional load parameter.

The summary of the applied input parameters is listed in Table 3. To confirm the dependence of output parameters on the selected input parameters, the Pearson and Spearman coefficients were calculated. The Pearson and Spearman coefficients indicate the linear and non-linear correlation, respectively. The calculated values are presented in Table 4.

Table 3. Summary of the applied input parameters.

Input parameter	Unit
Fuel flow	mg per stroke
Throttle	%
Intake valve lift	mm
Engine speed	rpm
Boost pressure	mbar
Rail pressure	MPa
Intake air temperature	°C
Injection timing	degree of Crankshaft BTDC
Ignition timing	degree of Crankshaft BTDC
Volumetric efficiency	–

Table 4. The Pearson and Spearman coefficients for HC and NO_x emissions.

Inputs parameters	HC		NO_x	
	Pearson	Spearman	Pearson	Spearman
Fuel flow	0.291	0.554	0.806	0.867
Throttle	0.278	0.707	0.625	0.798
Intake valve lift	0.312	0.728	0.724	0.815
Engine speed	0.405	0.628	0.256	0.289
Boost pressure	0.121	0.006	0.409	0.059
Rail pressure	0.276	0.540	0.706	0.630
Intake air temperature	0.163	0.260	0.221	0.265
Injection timing	0.119	0.020	0.285	0.147
Ignition timing	0.322	0.300	0.438	0.467
Volumetric efficiency	0.286	0.582	0.792	0.865

The results show a significant linear and non-linear correlation between input and output parameters. It confirms the fact that the selected input parameters play a crucial role in determining and predicting NO_x and HC emissions.

Data pre-processing

The data from different measurement systems were synchronized in the first step. After that, 20% of the data were randomly removed to be used for testing the developed models. With the remaining data, the models were trained. The value of 20% is suggested by the other studies.[5] These data samples should cover the entire ranges of change of the input parameters, to be able to perform holistic testing of models in all areas of ranges of change. In Figure 3(a) to (e), it can be seen that the test samples (marked in red) represent suitable coverage for the change ranges of input parameters. In this sense, if the computed errors of test data converge to the computed errors of training data, the

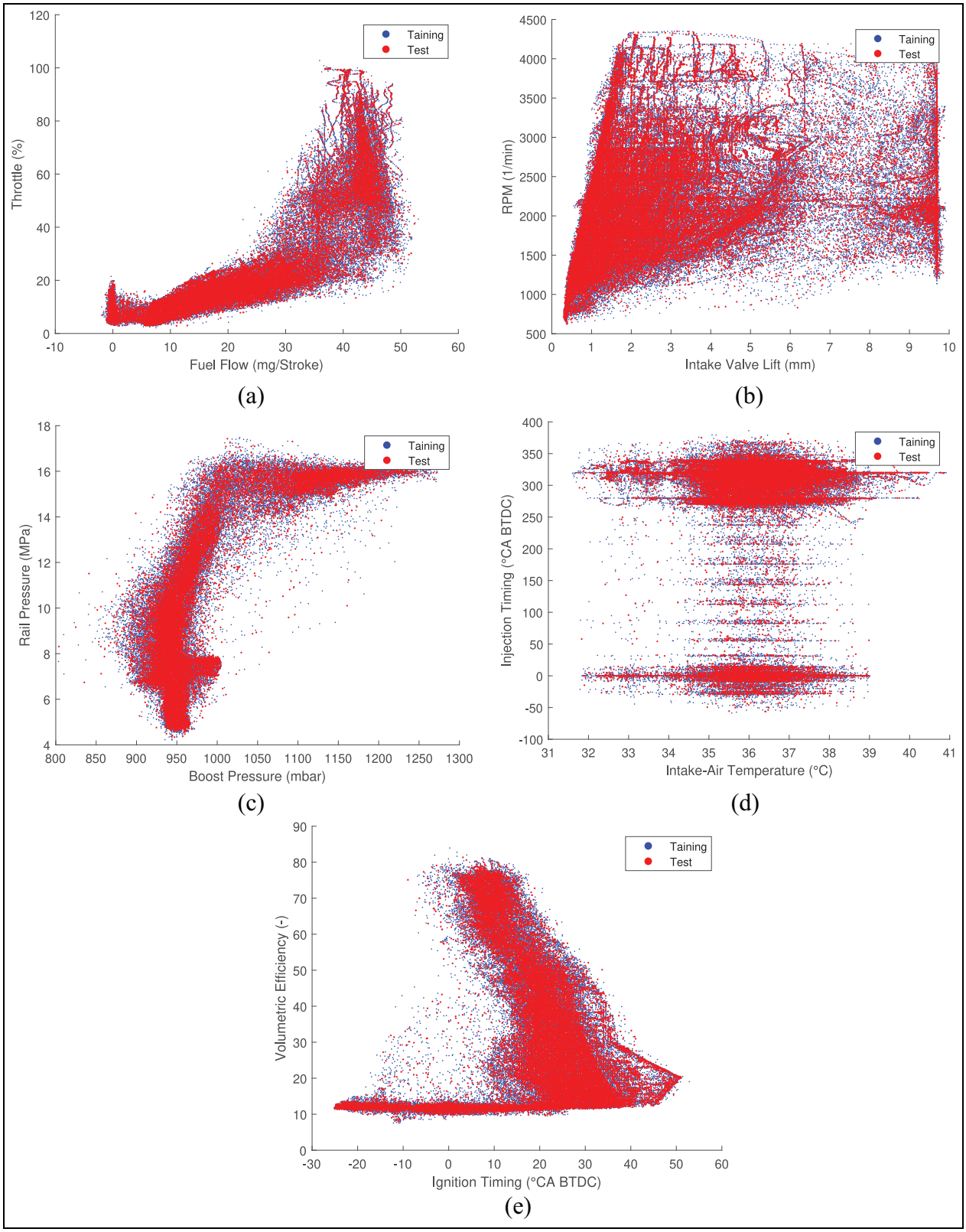

Figure 3. Illustration of training and test data for all input parameters: (a) Throttle (%) over Fuel Flow(mg/Stroke); (b) RPM (1/min) over Intake Valve Lift (mm); (c) Rail Pressure (MPa) over Boost Pressure (mbar); (d) Intejction Timing (°CA BTDC) over Intake Air Temperature (°C) and (e) Volumetric Efficiency ( ) over Ignition Timing (°CA BTDC)

overtraining can be ruled out. Considering more or fewer test data (compared to the case when a suitable coverage is available), either by less training data (more test data) the training phase can be worsened or by more training data (fewer test data) the risk of overtraining can be increased. In this work, besides suitable coverage, shown in Figure 3(a) to (e), it will be seen in the next chapter that the calculated errors of training

and test data have a suitable agreement, which shows that the selection of 20% of the data as a test, neither caused the overtraining nor disadvantaged the training phase. Also, all input parameters were standardized before the training phase. This means that the data was adjusted so that the mean value of each input parameter was 0 and its variances were set to 1.[16]

Model validation

To validate the developed Machine Learning models, different parameters were used, namely the coefficient of determination (R^2), the Normalized Root Mean Square Error (NRMSE), and Normalized Mean Absolute Error (NMAE). These parameters are the most important indicators to evaluate the accuracy of the developed models.[5] They are presented in equations (1) to (3).

$$R^2 = 1 - \frac{\sum_{i\ 1}^{num_{data}} (Y_i - \hat{Y}_i)^2}{\sum_{i\ 1}^{num_{data}} (Y_i - Y)^2} \quad (1)$$

$$NMAE = 1 - \frac{\sum_{i\ 1}^{num_{data}} |Y_i - \hat{Y}_i|}{num_{data} \times Y} \quad (2)$$

$$NRMSE = \frac{\sqrt{\frac{\sum_{i\ 1}^{num_{data}} (Y_i\ \ \hat{Y}_i)^2}{num_{data}}}}{Y} \quad (3)$$

Results and discussion

Different architectures of neural networks were evaluated and after the optimization of hyperparameters, the ANN models for HC and NO_x emissions were developed. The developed ANN models for HC and NO_x emissions have two hidden layers in addition to input and output layers. The first and the second hidden layers for the developed model for NO_x prediction have 40 and 30 neurons respectively, whereas in the HC model each of the hidden layers has 25 neurons. Sigmoid was selected as the activation function for both hidden layers and both models. The activation function for the input and output layer was Linear as mentioned before. Furthermore, the Levenberg-Marquardt algorithm was used for weight optimization of the networks.

In the case of LSTM models, in addition to the sequence layer as input, the developed LSTM models have two LSTM layers and each layer has 250 hidden units. To avoid overtraining, each LSTM layer is followed by a drop-out layer with a drop-out probability of 20%.[22] The processed data is transferred after the second drop-out layer through a fully connected layer to the regression layer (output layer). A batch size of 40 was selected for the training. Furthermore, to optimize the weight, the Adam method was used, with the advantage of adjusting the learning rate according to the loss function.[17] It was parameterized with an initial learning rate of 0.001 and a gradient threshold of 1.

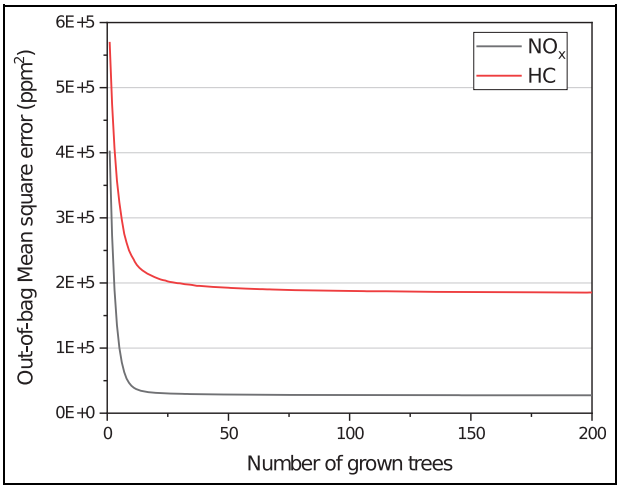

Figure 4. Out of bag error over the number of grown trees.

Table 5. The errors of diffrent models for HC and NO_x emissions prediction.

		NO_x		HC	
		Train	Test	Train	Test
ANN	NMAE	0.132	0.132	0.214	0.218
	NRMSE	0.211	0.211	0.518	0.535
	R^2	0.935	0.934	0.614	0.603
LSTM	NMAE	0.09	1.02	0.092	0.095
	NRMSE	0.161	0.17	0.261	0.284
	R^2	0.957	0.942	0.9	0.893
RF	NMAE	0.060	0.063	0.1	0.101
	NRMSE	0.116	0.118	0.294	0.297
	R^2	0.98	0.97	0.877	0.871

For the Random Forest models out-of-bag Method was used for the validation. As already mentioned, the higher number of trees in this method always leads to improvement of the results, whereas after a certain number of trees, no further significant improvement happens, and in this case, the increasing number of trees only slows down the calculation. For this reason, a total number of 200 trees were used in this work. As described in Figure 4, the error of developed models (for both HC emission and NO_x emission) tends to a constant value and an increasing number of trees does not bring any significant advantage anymore.

Table 5 shows the errors of different methods. The results show that all three models developed to predict NO_x emissions have suitable accuracy. Otherwise, the ANN models are not competitive with Random Forest or LSTM regarding predicting HC emission in transient operation. For the prediction of NO_x, the RF method gives the best results with R^2 equal to 0.98 and 0.97 for training and test samples, respectively. The NMAE is almost 0.6 and NRMSE is 0.12. In the case of HC prediction, the LSTM model has the best results. The R^2 for the developed model is 0.9 and 0.89 for the test and training data. Moreover, NMAE is 0.92 and

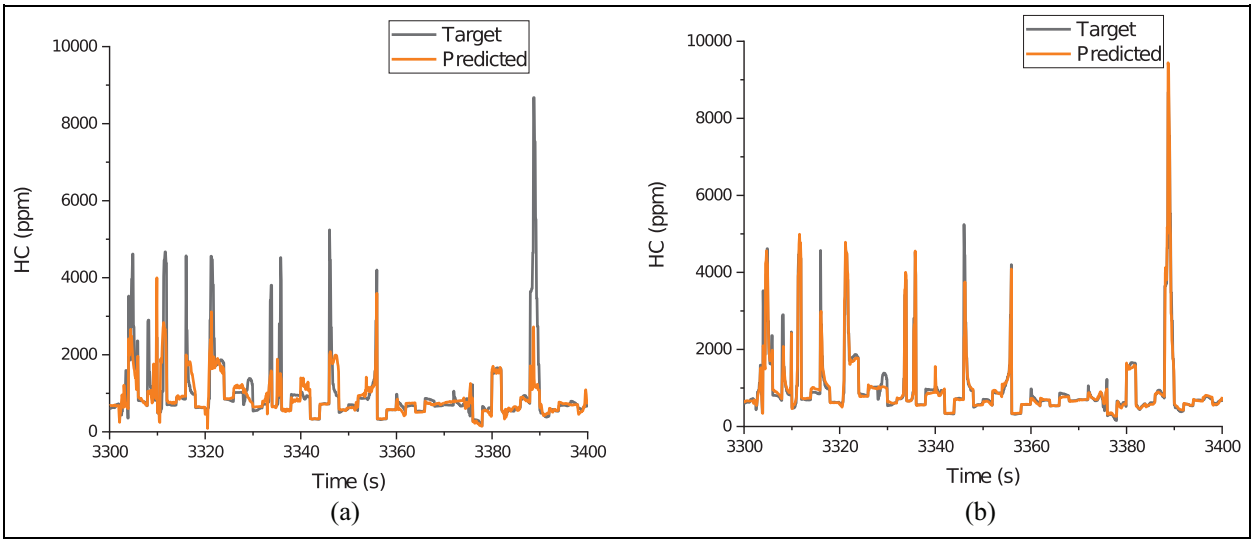

Figure 5. Target value and predicted value by: (a) ANN model and (b) LSTM model.

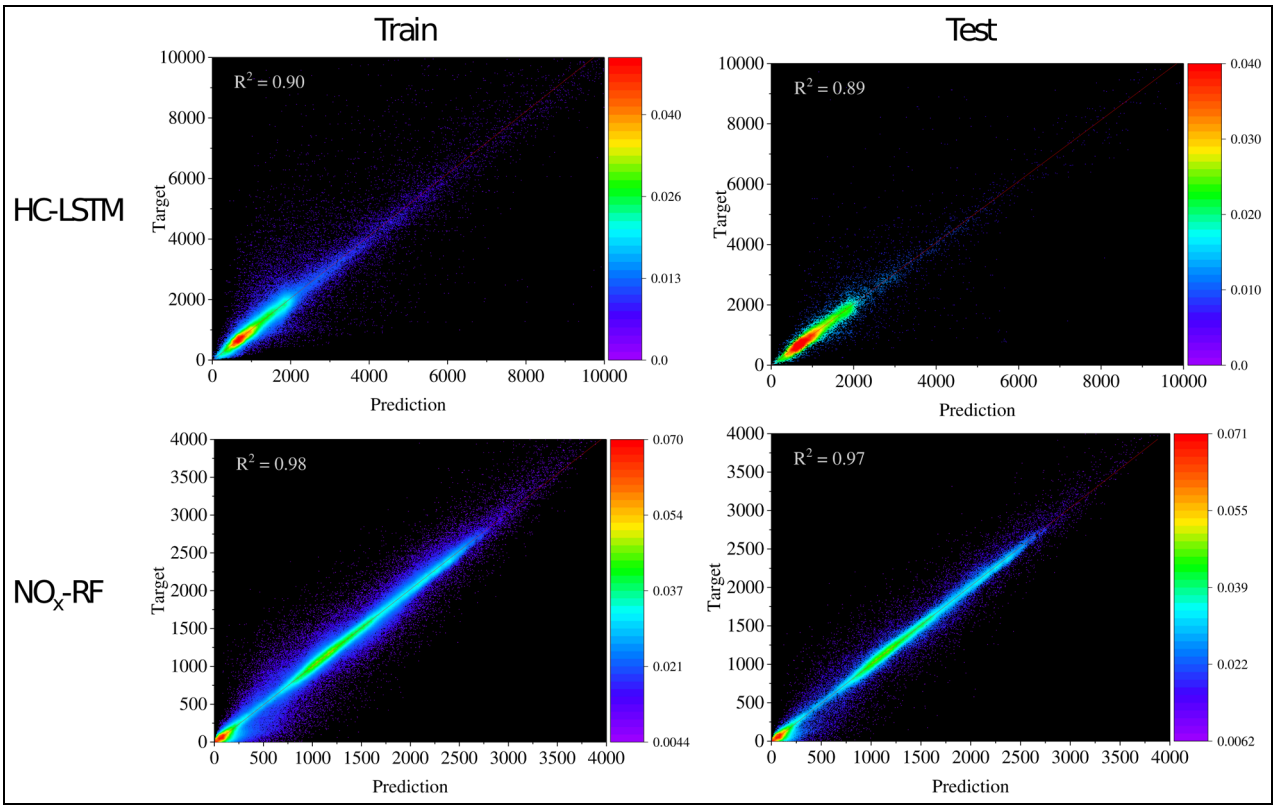

Figure 6. Density diagram for the most accurate models.

0.95, and NRMSE is 0.261 and 0.284 for training and test data, respectively. As already mentioned, the developed ANN models are not accurate enough, especially regarding HC emissions prediction. LSTM is equipped with memory characteristics, which can lead to a more accurate model. In gasoline engines and transient operation by load change, high HC emission peaks, due to the delay in mixture control, can happen. The prediction of these peaks is not possible by ANN models (Figure 5(a)). On the other hand, the LSTM model, which can utilize information from the previous time-series, offers a great advantage. As described in Figure 5(b), the HC peaks were detected and correctly predicted by the LSTM method. Additionally, in Figure 6, the density diagram for R^2 in the most accurate models (RF for NO_x and LSTM for HC) are shown. Based on these figures, the models can provide suitable results for the whole range of output parameters.

Moreover, the occurrence probability for the test data in different ranges of relative error is shown in

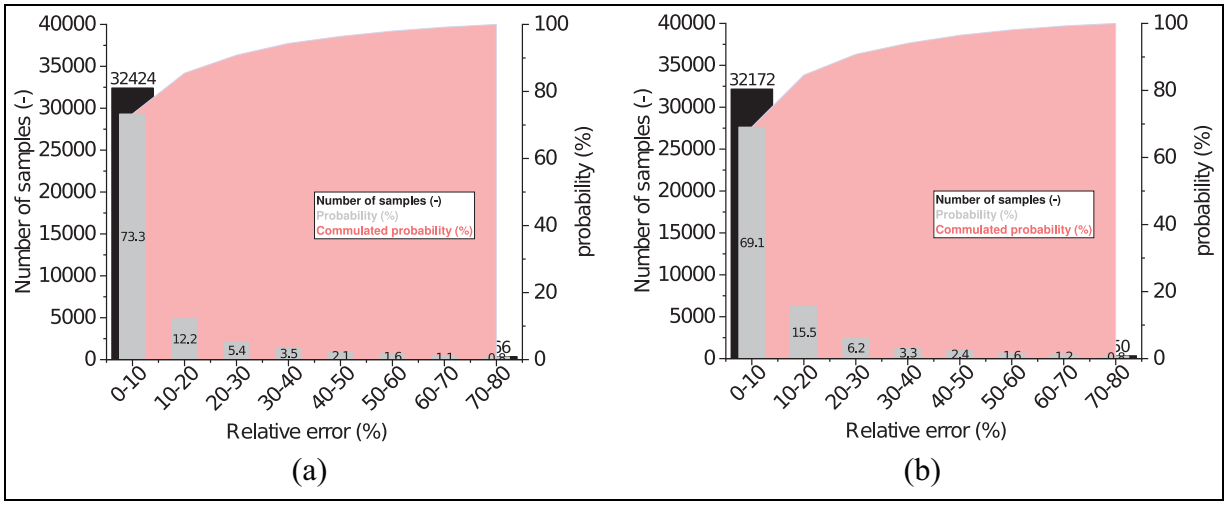

Figure 7. Occurrence probability for different ranges of relative error for the test data: (a) NO_x and (b) HC.

Figure 7(a) and (b) for NO_x and HC, respectively. It can be seen that for the prediction of both emissions, around 70% of the data samples show a relative error of less than 10%. Furthermore, in both cases, more than 85% of the data show an error of less than 20%, which shows a highly accurate model for the prediction of emissions in high transient engine operations.

Conclusion

The modeling of HC and NO_x raw emissions for a six-cylinder gasoline engine using machine learning methods was performed. To the best of the authors' knowledge, the models have one of the highest accuracies among so far developed machine learning models for emissions prediction by the highly transient operation. Moreover, according to the results, the ANN model has a shortcoming in the prediction of HC. The reason for this is the very higher HC peak, which can happen in a gasoline engine during load changes. In this case, the LSTM model, which uses data from earlier time steps, offers advantages concerning accuracy. For the prediction of NO_x emission, the developed RF model has the best accuracy, and the R^2, NMAE, and NRMSE values for the test data are, 0.97, 0.063, and 0.118, respectively. These values are 0.98, 0.06, and 0.116 for training data. For the prediction of HC emission, the LSTM model is the most accurate, and the R^2, NMAE, and NRMSE values for the test data are 0.89, 0.095, and 0.284, respectively. These values are 0.9, 0.092, and 0.261 for training data.

Outlook

An important benefit of these models is the evaluation of exhaust aftertreatment systems while driving on the road. The modeling of the raw emissions could be performed on the test bench (as in this study) and the trained models used in RDE driving. By comparing the predicted raw emissions from the developed models and measured tailpipe emissions from the PEMS measurement system, a meaningful evaluation of the efficiency of exhaust aftertreatment systems in real driving conditions could be obtained. Furthermore, the use of ANN in model-based reinforcement learning (RL) would be relevant. ANN can be used to provide real-time information to the RL agent. RL could be applied in various applications, such as power split optimization, etc.

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Appendix

Notation

NUM_{data}	number of data
R^2	coefficient of determination
v_{mean}	mean value of vehicle speed
$va_{pos,95}$	characteristic dynamic value
Y	observed value
$\overline{Y}$	average of observed values
$\hat{Y}$	predicted data

Abbreviations

ANN	artificial neural network
ECU	engine control unit
EiL	Engine-in-the-Loop
HC	hydrocarbon
LSTM	long short-term memory
NMAE	normalized mean absolute error
NO_x	nitrogen dioxide + Nitrogen monoxide
NRMSE	normalized root mean square error
PEMS	portable emissions measurement system
ppm	parts per million
RDE	real driving emission
RF	Random Forest