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Predicting Engine Parameters with Cost Efficient AI Models – An Experimental Method Validation

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Abstract

Artificial intelligence (AI) methods have rapidly become a best practice in various industrial applications due to their exceptional predictive abilities. Compared to traditional physical and chemical models, AI-driven approaches typically offer faster computation times without sacrificing accuracy. This makes them well-suited for enhancing or replacing conventional methods in engine technology. Building on this potential, our previous work focused on developing AI-based tools to accelerate the development of novel e-fuels for internal combustion engines. These AI tools require representative training datasets created through expensive engine dyno measurements. To address this challenge, we developed a general methodology to improve the cost-efficiency of dataset creation. This paper presents the experimental validation of this methodology by assessing its performance on seven different predictive tasks. Following the proposed framework, we designed and conducted an engine dyno experiment, then developed AI models to predict seven critical engine performance and emissions parameters: center of heat release, ignition delay, peak combustion temperature, peak pressure rise rate, brake thermal efficiency, exhaust opacity and NO_x emissions. The results demonstrated the effectiveness of the methodology, with five out of seven models achieving excellent predictive performance on unseen test data ($R2 > 0.97$). Peak pressure rise rate and opacity models had slightly lower performance ($R2 > 0.94$), however, given the well-known challenges associated with predicting these parameters, the results are acceptable.

Keywords

artificial neural networks, method validation, e-fuels, internal combustion engines

1 Introduction

Recent research on climate change underscores the significant challenge of meeting the Paris Agreement's target of limiting global warming to 1.5 °C above pre-industrial levels (IPCC, 2023). Current trends suggest a 50% chance of breaching this limit within the next six years (Friedlingstein et al., 2024). In the European Union (EU), transportation accounts for over 25% of total greenhouse gas (GHG) emissions, making the decarbonization of mobility a critical component in meeting climate targets. Carbon-neutral e-fuels offer a promising solution to rapidly reduce the carbon footprint of existing vehicles, therefore the large scale market introduction of these novel fuels have to be accelerated (Koller et al., 2022; Bagdi et al., 2023). Despite the potential, there is no significant progress in the market. The EU missed its own 2020 target to reduce GHG emission intensity of fuels by 6%, achieving only 5.6% decrease primarily through increased biofuel usage. However this reduction is only 4% when the negative effects of the indirect land use change are also considered (European Environment Agency, 2024). The urgent need for CO_2 reduction and the challenges in the market introduction of carbon neutral fuels necessitates new development approaches to increase the cost efficiency of e-fuel development (Cipriano et al., 2022).

Artificial intelligence can be a promising alternative approach to assist e-fuel development. Comparing this technology with conventional methods that utilize physicochemical models, the development process can be simplified. When building physicochemical models, proper knowledge is required on the real processes of the investigated system. Hence, the development can be expensive due to the increased need of computational capacity and professional labor. The AI technology provides a simpler way of model building, since it does not require any

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knowledge on the real principles behind the system's operation, only a sufficient amount of high quality data. During training, the AI maps the input-output relationships of the system and then it is able to provide fast and accurate predictions. Therefore, AI models can replace or supplement conventional physicochemical models to improve the cost efficiency of the e-fuel development process. There are several researches where the AI was effectively applied to predict engine behavior based on fuel properties. Najafi et al. examined, five ethanol-gasoline blends at nine different engine speeds (Najafi et al., 2009). These data were used to train artificial neural networks (ANNs) to predict engine performance and emissions based on engine speed and blend ratio. The models produced strong predictions, with correlation coefficients (R) of 0.981 for brake thermal efficiency (BTE), 0.986 for brake-specific fuel consumption (BSFC), and 0.973 for NO_x emissions. Ismail et al. investigated four fuel types with three different blends, under varying speeds, torques, and fuel flow rates (Ismail et al., 2012). The model successfully predicted NO_x emissions, achieving an R value of 0.981 on unseen data. Besides conventional engine applications, the AI is able to give accurate predictions in the field of molecular fuel design. Our previous research (Virt et al., 2024) demonstrated that AI models outperformed conventional industry methods in predicting the physical properties of fuel molecules based on their atomic structure. These examples demonstrate that the ANNs can accurately forecast engine outputs, offering reliable insights into engine behavior under varying conditions.

Despite the apparent advantages of AI, this technology also has some major challenges, since the creation of high-quality training datasets and the process of model training are difficult and expensive. AI-based predictive models that can estimate different engine parameters require extensive engine dyno measurements. Thus long measurement times and high fuel usage can increase the costs of development. Another problem is the complicated optimization of AI hyperparameters that can significantly prolong model creation and introduce uncertainty in model accuracy. Thus a proper workflow that utilizes the proper state-of-the-art technologies is required to reduce training times and prediction errors.

Our latest works are focusing on these problems (Virt and Zöldy, 2022; Virt and Zöldy, 2024a). We developed a general workflow designed to enhance the cost-effectiveness of AI model generation, specifically for applications related to engine and fuel technologies (Virt and Zöldy, 2022). The developed methodology has two parts: the first determines a proper measurement resolution to minimize fuel costs while maintaining high accuracy, and the second describes best practices that can be applied during training to improve accuracy and accelerate model creation. The methodology was created by analyzing and combining different state-of-the-art methods and applying them on a high resolution dataset. The results revealed that this workflow can be effectively applied to reduce the costs of model generation. However, the method has not yet been tested in a real-world scenario. Therefore, the aim of the current work is to experimentally validate the workflow.

In this paper, the effectiveness of the methodology is demonstrated by applying it on seven predictive tasks. After determining the proper resolution, an engine dyno measurement was performed to create predictive models for the center of heat release (CoHR), ignition delay (ID), peak combustion temperature (T_{max}), peak pressure rise rate (dp_{max}), brake thermal efficiency, exhaust opacity and NO_x emissions of the test engine. The performance of the models is evaluated using three key metrics: mean squared error (MSE), mean absolute error (MAE) and coefficient of determination (R2). These metrics are calculated across the training, validation, and test subsets of the dataset to assess the model's accuracy and generalizability.

2 Materials and methods

2.1 Experimental apparatus

The engine dyno measurements were carried out on a Cummins ISBe 170 30 turbocharged, medium-duty commercial diesel engine. The engine's main properties are listed in Table 1. The test engine has many different added features, such as a low and high pressure EGR system, but for this validation work these were not used. The pressures and temperatures were monitored at multiple points at the inlet and outlet side, while the fuel consumption was measured with an AI 2000 gravimetric device. The combustion was studied with an AVL indicating system based on an AVL 612 IndiSmart, an AVL GH13P piezoelectric pressure sensor and

Table 1 Cummins ISBe 170 30 main parameters

Engine parameters	Dimensions
Displacement	3.922 cm^3
Bore	102 mm
Stroke	120 mm
Compression Ratio	17.3
Rated Effective Power	125 kW

an AVL 365C crank angle encoder. Regarding emissions, a Continental UniNO_x sensor was utilized to measure the oxygen and NO_x concentrations, while an AVL 439 opacimeter was applied to measure exhaust opacity. Since the study focuses on raw emissions, no catalysts or particulate filters were mounted on the engine. This test setup was successfully used for many previous researches (Nyerges and Zöldy, 2020; Nyerges and Zöldy, 2023; Virt and Zöldy, 2024b).

2.2 Cost efficient workflow of AI model creation

The developed workflow is presented in Fig. 1. The upper part describes the cost efficient creation of a representative training dataset, while the lower part demonstrates the steps of fast and accurate AI creation. The process starts by determining the ANN target parameters and the varied measurement parameters. The target parameters are the seven predicted output parameters: the CoHR, ID, T_{max}, dp_{max}, BTE, exhaust opacity and NO_x emissions. The engine dyno software controls the engine with a torque and speed demand, thus these are the varied measurement parameters. The defined operating range is 50-250 Nm and 1.100-1.800 rpm.

First, two parameter sensitivity measurements have to be carried out in the defined operating range. Following the methodology, the first measurement holds engine speed at the middle value of the speed range, which is 1.450 rpm, and the torque is varied on the defined range with 20 Nm resolution, since at least 10 measurement points are required for a parameter sensitivity measurement. The second measurement is similar, the defined speed range is measured with a 50 rpm resolution at a constant 100 Nm load. From these measurements, the correlation coefficients (R_{pair}) between the seven output parameters, and the two varied measurement parameters can be

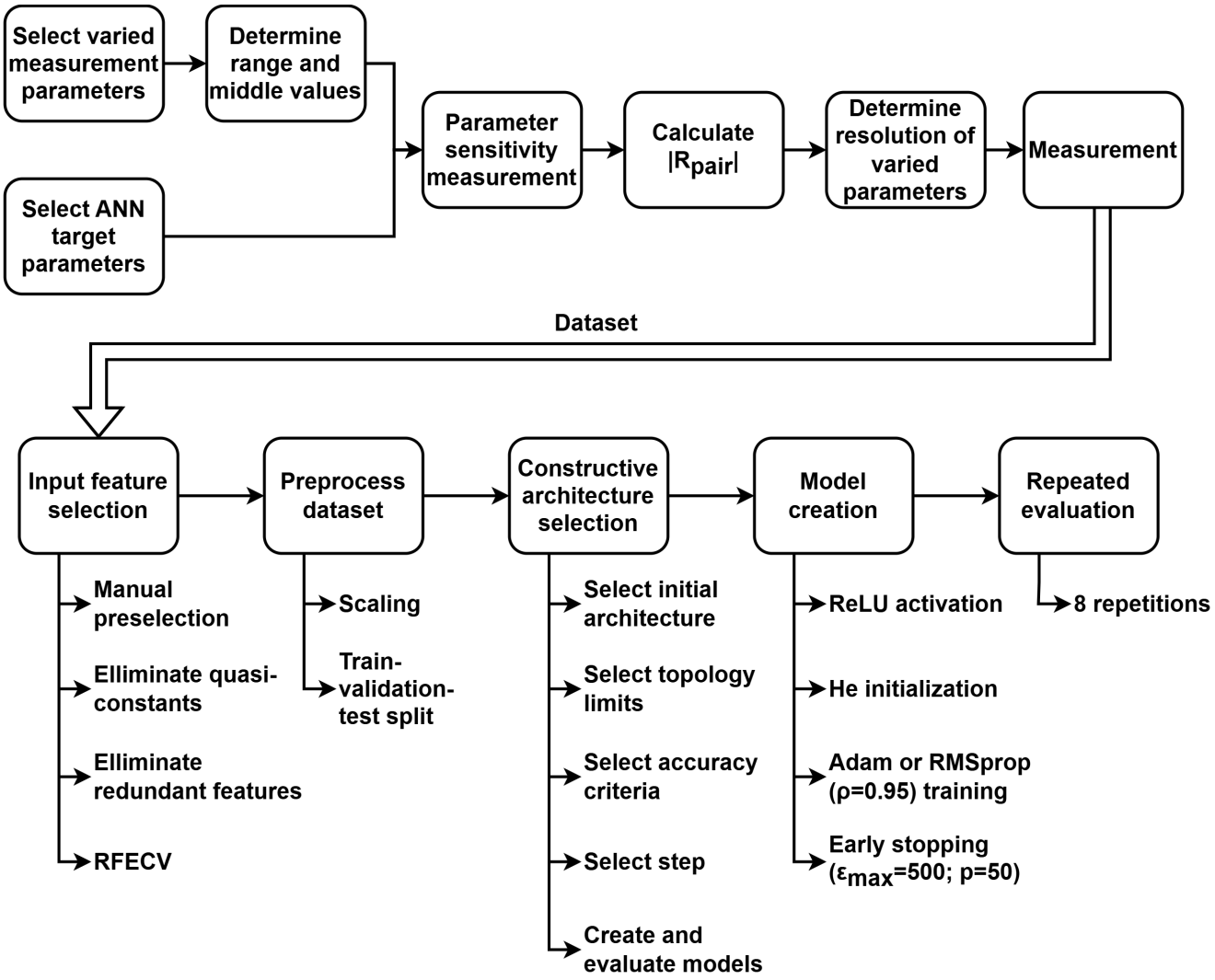

Fig. 1 Cost efficient method of fast and accurate AI engine model creation (Virt and Zöldy, 2024a)

calculated. These R_{pair} values can be used to determine the minimal resolution that is required to obtain representative datasets. If $|R_{pair}|$is between 0.4 and 0.9, thirteen equidistant measurements are required on the defined range, while when the value is lower or higher than this range, seven or eleven measurement points are required, respectively. Table 2 contains the $|R_{pair}|$ values and the required engine speed resolutions for the seven output parameters, while Table 3 presents these values for the torque.

It is discernable that the maximal resolution is 13 for both the engine speed and torque. Since all the parameters are recorded from one engine dyno measurement, both the engine speed and torque will be recorded with a resolution of 13 samples per variable, thus a dataset with 169 samples is recorded.

After the measurements, the dataset is created. The features are scaled between 0 and 1 to avoid overflows. The dataset is divided into training (126 samples), validation (25 samples), and test (18 samples) subsets. The training dataset is used to optimize the weights of the neural networks. The validation dataset is applied during hyperparameter optimization, and the test dataset is used to assess the final performance of the models during the evaluation.

First, an input feature selection is applied on the dataset. This step starts with the manual preselection of all possible measured parameters that can influence the output parameters. These are the inlet pressure (p_{in}) and temperature (T_{in}), engine speed (n), torque (M), inlet and outlet oxygen concentrations (O_{2_in} and O_{2_out}), rail pressure (p_{rail}), dose (m_{fuel}), air-fuel ratio (AFR), start of injection (SoI), end of injection (EoI) and the ratio of the main injection (γ_{main}).

Table 2 $|R_{pair}|$ values and the required engine speed resolutions

	CoHR	ID	T_{max}	dp_{max}	BTE	opacity	NO_x
$\|R_{pair}\|$	0.935	0.799	0.718	0.777	0.725	0.930	0.933
Resolution	11	13	13	13	13	11	11

Table 3 $|R_{pair}|$ values and the required torque resolutions

	CoHR	ID	T_{max}	dp_{max}	BTE	opacity	NO_x
$\|R_{pair}\|$	0.421	0.710	0.988	0.665	0.905	0.621	0.964
Resolution	13	13	11	13	11	13	11

Then a recursive feature elimination (RFE) process is performed on the dataset. This automatically eliminates the least important features from the dataset to improve model performance. After the RFE, a manual fine tuning may be performed with a trial and error method.

Next, the final network architecture has to be selected with a constructive architecture selection method. This technique starts with a small network capacity that is not able to properly map the system behavior. Then the capacity is increased by adding new neurons and layers to the architecture until an accuracy criterion is reached. The current methodology for this specific engine-related predictive problem operates with minimum 30 neurons in the architecture. The maximal number of hidden layers is 3, and the maximal number of neurons in a layer is 50. The target validation accuracy of the networks is $R2_{val} = 0.98$ (Dey et al., 2021). If the networks are unable to reach the target accuracy, the architecture is selected manually from the investigated possibilities. In this case it is possible that higher network capacities are resulting in overfitted models, thus the manual selection have to consider the generalization of the models by comparing the training and validation accuracies, and the learning curves.

During training, the Adam algorithm (Kingma and Ba, 2018) is applied that can optimize the network's weights in a fast and adaptive way. The training also applies an early stopping method to avoid overfitting. This method investigates the learning curves, and if the validation accuracies are showing a decreasing tendency for a 50 epoch long patience time, the training is stopped. Otherwise the training can last up to maximum 500 epochs. To avoid the vanishing gradients problem, rectified linear unit (ReLU) activation functions are used in neurons of the hidden layer. Since all the presented predictive models are solving regression problems, linear activation functions are used in the output layer. The random nature of the training process is handled by repeated training and evaluation. The reported accuracies of the networks are the averages of 8 repeated training and evaluation processes. With this methodology, seven different multiple input single output ANNs were created to predict the seven output parameters.

3 Results and discussion

3.1 Predicting combustion parameters

The first model predicts the CoHR and its performance is reported in Table 4. During input feature selection p_{in}, n, O_{2_in}, O_{2_out}, AFR, SoI, EoI and γ_{main} were identified as

Table 4 Prediction accuracies of the center of heat release model

	Train	Validation	Test	All
MSE [-]	1.183e-4	3.813e-4	2.842e-4	1.731e-4
MAE [°CA]	0.0941	0.1658	0.1447	0.1101
R2 [-]	0.9987	0.9945	0.9957	0.9979

important input parameters. The constructive architecture selection method resulted in a simple network structure: 8-35-1. Since the ANN has only one hidden layer and 35 neurons inside the hidden layer is a low number in the current context, it can be concluded that the prediction of CoHR is an easier mathematical problem. This is logical, since Table 2 shows that this parameter would require measurements at only 11 different engine speeds. The engine speed was directly selected as an input, while the torque is only indirectly represented by the AFR, oxygen concentrations and injection parameters, thus engine speed has higher impact on the prediction than the torque. The model accuracy is really high. The coefficient of determination is well above 0.99, and the MAE is only 0.14 °CA. All subsets of the dataset have similarly high accuracy, thus the generalization of the model is also good.

The next is the ignition delay model. All of our previous studies showed that this is one of the most challenging parameters, since the exact value of the ignition delay depends on many factors, including cyclic variations and other non-measured parameters. After applying the methodology, the network structure of 9-50-50-50-1 was selected along with p_{in}, n, O_{2_in}, O_{2_out}, m_{fuel}, AFR, SoI, EoI and γ_{main} as input features. The outcome of the optimization is logical, since the mathematical problem is challenging, thus high model capacity is required. As shown in Table 5, the created ANN has an excellent accuracy with 0.97 R2 and 0.24 °CA MAE for the test dataset. The ignition delay values are ranged between 4 and 18 °CA (mostly around 10 °CA) in the dataset thus this MAE value corresponds to approximately 2% prediction error, which is outstanding compared to our previous ID estimation attempts (Virt and Zöldy, 2022; Virt and Zöldy, 2024a). The performance of the model is similarly good on all subdatasets, thus the generalization can also be considered good. The improvement in the prediction accuracy of this parameter is a strong proof that supports the effectiveness of the developed methodology.

Table 5 Prediction accuracies of the ignition delay model

	Train	Validation	Test	All
MSE [-]	3.718e-2	6.488e-2	1.589e-1	5.313e-2
MAE [°CA]	0.129	0.205	0.243	0.152
R2 [-]	0.9917	0.9832	0.9770	0.9882

Peak combustion temperature is the following predicted feature. The selected architecture is 6-50-15-1, while the selected inputs are p_{in}, n, O_{2_in}, m_{fuel}, AFR and SoI. From Table 6, it is discernible that the model is highly accurate, since R2 is well above 0.99 and MAE is around 20K for all subsets of the dataset. This means that the model can operate with an error around 1%, since the combustion temperatures are around 2000 K. Such low errors in case of all subsets suggests an excellent generalization.

Another important engine parameter is the peak pressure rise rate that should be limited in order to increase engine lifetime. The optimization resulted in a network structure of 6-45-40-1, and the applied input features are n, O_{2_in}, m_{fuel}, SoI, EoI and γ_{main}. The main accuracy measures are presented in Table 7. This engine parameter is also hardly predictable, although the performance of the created AI is acceptable. The R2 of the test dataset is 0.94, while the MAE is 0.49 °CA which corresponds to approximately 5% prediction error. The performance difference between the subdatasets is somewhat higher than for the previous models, however, the generalization can also be considered acceptable.

3.2 Predicting engine emissions and efficiency

Table 8 presents the performance of the brake thermal efficiency model. The model operates with an architecture of 5-50-10-1 and with the following input features: n, O_{2_in}, m_{fuel}, AFR and γ_{main}. The 0.97 test R2 and 0.52% test MAE

Table 6 Prediction accuracies of the peak combustion temperature model

	Train	Validation	Test	All
MSE [-]	2.571e-4	4.125e-4	7.409e-4	3.308e-4
MAE [K]	14.52	17.53	25.98	16.19
R2 [-]	0.9940	0.9964	0.9923	0.9964

Table 7 Prediction accuracies of the peak pressure rise rate model

	Train	Validation	Test	All
MSE [-]	1.879e-1	1.012	6.701e-1	3.598e-1
MAE [°CA]	0.261	0.595	0.487	0.335
R2 [-]	0.9633	0.9330	0.9457	0.9529

Table 8 Prediction accuracies of the brake thermal efficiency model

	Train	Validation	Test	All
MSE [-]	5.783e-4	3.566e-3	1.536e-3	1.112e-3
MAE [%]	0.320	0.828	0.524	0.416
R2 [-]	0.9908	0.9669	0.9729	0.9843

is a fine accuracy, however, similarly to the peak pressure rise rate model, the difference between the accuracies over the subsets of the dataset are also higher. Overall, this model is also acceptable to further predictive tasks.

Next, the NO_x emission model is presented in Table 9. The model operates with relatively low number of input features. These are the n, O_{2_in}, m_{fuel}, and SoI. The resulted network architecture is 4-50-40-1. The model shows a good behavior with a test R2 well above 0.99 and 29 ppm test MAE. The accuracy is similarly high for each of the training, validation and test datasets, thus the generalization of the network is good.

The last model predicts the exhaust opacity. The only selected input features are the pin, mfuel, and SoI, while the network structure is 3-50-15-1. According to Table 10, this model has the worst performance from the presented ones. The R2 of the test dataset is 0.94, while the MAE is only 0.568, which corresponds to approximately 10% prediction error. The inaccuracy of the model can be attributed to multiple aspects. Similarly to the ID and dp models, the mathematical problem is also complicated in this case, since the sooting of the engine is influenced by many physical and chemical processes. Since higher network capacities led to overfitted models, the problem is attributed to the training dataset. During measurements, the opacity had a high fluctuation even in steady state conditions, thus the measurements may not be reliable enough. Despite this, the methodology could provide an acceptable model that may be used to estimate exhaust opacity in later investigations.

Table 9 Prediction accuracies of the NO_x emission model

	Train	Validation	Test	All
MSE [-]	1.453e-4	4.595e-4	2.625e-4	1.974e-4
MAE [ppm]	19.70	36.39	29.93	23.26
R2 [-]	0.9969	0.9837	0.9941	0.9952

Table 10 Prediction accuracies of the opacity model

	Train	Validation	Test	All
MSE [-]	4.866e-3	6119e-3	4.986e-3	5.052e-3
MAE [%]	0.579	0.649	0.568	0.588
R2 [-]	0.9405	0.9302	0.9451	0.9398

4 Conclusion

This study provided an experimental validation of our previously developed methodology aimed at enhancing the cost-effectiveness of AI-based engine model generation. The methodology focused on reducing measurement times and offering a structured framework for fast and accurate model creation. By following the outlined steps, a dataset with optimized resolution was produced, and seven multiple-input single-output ANNs were trained to predict the seven target parameters.

The results showed strong model performance, with five out of seven models achieving R2 values above 0.97 on unseen test data. The remaining two models, for peak pressure rise rate and exhaust opacity, achieved R2 values above 0.94. While further optimization of hyperparameters, such as increasing model capacity, led to overfitting and did not improve these models, their accuracy is sufficient for predictive tasks. These parameters are inherently challenging to model due to their dependence on complex physico-chemical processes and the noise in measurement signals.

Overall, the methodology enabled straightforward and efficient model development, producing accurate results with minimal engine dyno measurements. The successful demonstration of the framework supports its application in similar research and development tasks.

Our future work will focus on extending the methodology to predict parameters as a function of crank angle, such as heat release rates and cylinder temperatures. This extension will be a base for the development of our AI-based fuel designer tool, which aims to support the creation of novel e-fuels.

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