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Emission Analysis in Data-Driven Model Predictive Control of Hydrogen/Diesel Dual-Fuel Engines

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Abstract

Climate change and global warming concerns have led researchers to alternative fuels, especially zero-carbon fuels like hydrogen. Modifying existing combustion engines for dual-fuel operation can decrease emissions of vehicles that are already on the road. To evaluate the engine performance and emissions of a hydrogen-diesel dual-fuel modified engine a modern controller has been developed and compared to standard diesel operation. This modified engine uses the diesel injection as a pilot to initiate the combustion of the premixed hydrogen-air mixture. To control the injected hydrogen, a nonlinear model predictive controller (NMPC) utilizing a deep neural network (DNN) process model is proposed. This DNN model has eight inputs and four outputs. The model inputs are the previous cycle controller outputs (duration of injection (DOI) main, the duration between the end of the pilot injection and the start of the main injection pre-2-main (P2M), start of injection (SOI) main, and H2 DOI) and four measured engine outputs (indicated mean effective pressure (IMEP), nitrogen oxides (NO_x), soot, and maximum pressure rise rate (MPRR)). The structure and hyperparameters of the DNN are optimized using a Bayesian optimizer. The final DNN model structure has two hidden layers with 31 and 23 neurons, respectively, and a Leaky ReLU activation function. This model has good accuracy, with a mean absolute error (MAE) of 0.18 bar, 7 ppm, 0.04 mg/m^3, and 0.07 bar/CA for the IMEP, NO_x, soot, and MPRR prediction, respectively. This DNN is then integrated into the NMPC using the `acados` NMPC framework which allows for use on the embedded control hardware for experimental testing. The DNN-NMPC is designed to minimize the engine-out emissions while satisfying operating constraints and following an IMEP load trajectory. An average computational time of 2 ms/cycle is observed when the controller is tested, making the control strategy real-time feasible and faster than recurrent networks such as long short-term memory networks (LSTM) and gated recurrent units (GRU). The control performance of the DNN-NMPC for hydrogen-diesel dual fuel showed that an IMEP reference could be followed with an MAE of 0.19 bar and the average H2 utilization of 68%, while also substantially reducing engine-out soot by 87% but increasing engine-out NO_x by 78%.

1 Introduction

Transportation produces about 20% of total carbon dioxide (CO2) emissions [1], with heavy-duty diesel freight trucks producing 3% of total CO2 emissions [2]. While compression ignition (CI) engines have unique characteristics, including higher energy efficiency and torque production than gasoline engines, their combustion process releases a variety of harmful gases, such as hydrocarbons, nitrogen oxides (NO_x), particulate matter (PM) or soot, carbon monoxide (CO), and CO2 [3]. Alternative fuels, especially zero-carbon fuels like hydrogen, have been investigated to reduce GHG emissions from combustion [4]. Performance and emission characteristics at different speeds and hydrogen flow rates were tested in [5]. They revealed that hydrogen flow rates of 21.4 l/min and 42.8 l/min significantly impact engine coefficient of variation and improve CO, CO2, and smoke levels. For a hydrogen ratio of 20% compared with pure diesel conditions, the peak pressure increased by 7.7%, and the cumulative heat release rate increased by 3.7% [6].

Investigation into the control of H2/diesel engines instead of relying on experimental analysis for stationary points for emission analysis has some challenges, and the most significant part is modeling. A combustion model for hydrogen-natural gas/diesel dual fuel engines based on the separation of the different types of combustion modes was developed by first treating the combustion of the pilot fuel by jet modeling, then the combustion of

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the gas mixture by a mathematical model based on the Gaussian function. This model has a maximum error of 2% compared to the conventional Wiebe model and is useful for emission prediction and preliminary design [7], but not for real-time model-based control. Machine learning (ML) based models that are highly accurate and efficient enough to be used in real-time applications after training are being developed [8]. Artificial neural networks (ANN) have been widely used for modeling and controlling IC engines. For instance, [9] used ANN to model performance and exhaust emissions of a gasoline engine with mean relative errors (MRE) values in the range of 0.46–5.57%. Optimization techniques can be used to enhance the effectiveness of ML models [10].

Model-based controllers, such as model predictive control (MPC), rely on an embedded model. ML-based MPC is an effective control strategy that is not yet commonly used in automotive applications [11] but is used widely in a range of applications from the chemical process industry to robotics and finance [12]. These applications take advantage of the nonlinear model predictive controller's (NMPC) ability to provide an optimal control solution while incorporating constraints on system states and controller outputs. A deep neural network (DNN) with one long-short-term memory (LSTM) layer has been used as a model for NMPC for real-time experimental control of a diesel engine has been shown in [13]. In [13] where a 7.9% reduction in fuel consumption while decreasing $\mathrm{NO_x}$ and PM by up to 18.9% and 40.8%. There is however still research required on the generalization of the ML-based model and H2/diesel dual fuel engine control. In this paper, a shallow DNN model for an H2/diesel dual-fuel engine is embedded as the model in NMPC in a hydrogen diesel dual-fuel engine to improve the engine's performance and emissions.

The main contributions of this paper are summarized as follows: a model of the indicated mean effective pressure (IMEP), nitrogen oxides (NOx), soot, and maximum pressure rise rate (MPRR), of a dual-fuel H2/diesel engine using a shallow-optimized DNN model is developed; an average computational cost of 2 ms/cycle with high accuracy provides a fast and precise model for NMPC combustion H2/diesel dual-fuel engine control for real-time application; real-time DNN-NMPC for the H2/diesel dual-fuel engine with load control and emissions constraints while significantly reducing soot is experimentally implemented on a 4.5-liter diesel engine on one of the four cylinders.

2 Methodology

Details of the NMPC and a data-driven model are provided below. With an accurate model, the NMPC can control the engine to reduce emissions, increase performance, and satisfy constraints. The controller tracks the desired IMEP and minimizes emissions. ML is used to model the engine for the controller, as an accurate physics-based model is not realtime capable. The DNN model has four outputs and eight inputs.

2.1 Nonlinear Model Predictive Controller

NMPC has a cost function and computes the current control outputs by solving a nonlinear program at each sample instance [14]. The optimization problem involves using a model-based approach to predict the system's behavior based on the current states. Finally, the NMPC algorithm is implemented in real-time on the Raspberry Pi using MATLAB/Simulink for H2/diesel engine control, using `acados` [15] as a solver. `acados` is a free and open-source package to implement the NMPC controller. For the computation of the Hessian in the underlying sequential quadratic programming (SQP) algorithm, the Gauss-Newton approximation has been used in this work. The reference input, the rate of change for controller outputs, and input-output weights (described in Table 1) are:

$$\mathrm{r}_i = \left[\ \mathrm{r}_{\mathrm{IMEP}_i}, \quad 0, \quad 0, \quad 0\ \right]^\top, \tag{1}$$

$$\mathrm{R} = \mathrm{diag}\left(\mathrm{r}_{\Delta \mathrm{u}_{\mathrm{DOI}_{\mathrm{main}}}}, \mathrm{r}_{\Delta \mathrm{u}_{\mathrm{P2M}}}, \mathrm{r}_{\Delta \mathrm{u}_{\mathrm{SOI}_{\mathrm{main}}}} \mathrm{r}_{\Delta \mathrm{u}_{\mathrm{H2DOImain}}}\right), \tag{2}$$

$$\mathrm{Q} = \mathrm{diag}\left(\mathrm{q}_1, \mathrm{q}_2, \mathrm{q}_3, \mathrm{q}_4, \mathrm{r}_1, \mathrm{r}_2, \mathrm{r}_3, \mathrm{r}_4\right) = \mathrm{diag}\left(\mathrm{q}_{\mathrm{IMEP}}, \mathrm{q}_{\mathrm{NO_x}}, \mathrm{q}_{\mathrm{Soot}}, \mathrm{q}_{\mathrm{MPRR}}, \mathrm{r}_{\mathrm{DOI}_{\mathrm{main}}}, \mathrm{r}_{\mathrm{P2M}}, \mathrm{r}_{\mathrm{SOI}_{\mathrm{main}}}, \mathrm{r}_{\mathrm{H2DOI}_{\mathrm{main}}}\right). \tag{3}$$

where the reference r_i and the positive definite matrix weights Q and R are selected to penalize deviations from the requested load while minimizing $\mathrm{NO_x}$ and soot emission concentrations and rate of change in controller outputs. The fuel consumption terms are needed to minimize the amount of injected fuel.

The cost function, J, for the NMPC is defined as:

$$
\begin{aligned}
\mathrm{J} = \sum_{i=0}^{N} & \underbrace{\left\|\mathrm{r}_{\mathrm{IMEP}_i} - \mathrm{y}_{\mathrm{IMEP}_i}\right\|_{\mathrm{q}_1}^2}_{\text{Load Tracking}} + \underbrace{\left\|\mathrm{y}_{\mathrm{NO}_{\mathrm{x}_i}}\right\|_{\mathrm{q}_2}^2 + \left\|\mathrm{y}_{\mathrm{Soot}_i}\right\|_{\mathrm{q}_3}^2}_{\text{Emission Reduction}} + \underbrace{\left\|\mathrm{y}_{\mathrm{MPRR}_i}\right\|_{\mathrm{q}_4}^2}_{\text{Combustion Stability}} + \underbrace{\left\|\mathrm{u}_{\mathrm{H2DOI}_{\mathrm{main}_i}}\right\|_{\mathrm{r}_4}^2}_{\text{Hydrogen Reduction}} + \\
& \underbrace{\left\|\mathrm{u}_{\mathrm{DOI}_{\mathrm{main}_i}}\right\|_{\mathrm{r}_1}^2 + \left\|\mathrm{u}_{\mathrm{P2M}_i}\right\|_{\mathrm{r}_2}^2 + \left\|\mathrm{u}_{\mathrm{SOI}_{\mathrm{main}_i}}\right\|_{\mathrm{r}_3}^2}_{\text{Diesel Reduction}} + \underbrace{\left\|\Delta \mathrm{u}_i\right\|_{\mathrm{R}}^2}_{\text{Oscillation Reduction}} + \underbrace{\left\|\mathrm{W}_i\right\|_{\mathrm{S}}^2}_{\text{Constraint Violation}}
\end{aligned} \tag{4}
$$

where W contains slack variables and S is the penalty for constraint violation.

The chosen cost function Equation (4) aims to minimize NO_x and soot concentrations while reducing diesel and hydrogen consumption and maintaining the requested output torque in stable combustion.

Table 1: MPC weights, constraints and rate of the change on inputs and outputs of the engine.

	Variable			Rate of Variable Change		
Variable	Weight (Q*)	Min	Max	Weight (R**)	Min	Max
IMEP [bar]	10	0	9	-	-	-
NO_x [ppm]	0.0001	0	1000	-	-	-
Soot [mg/m^3]	0.0001	0	2	-	-	-
MPRR [bar/°CA]	0.5	0	3	-	-	-
DOI_{main} [ms]	1	0.17	0.5	1	-1000	1000
P2M [ms]	0.0001	0.43	0.80	1	-1000	1000
SOI_{main} [°CAbTDC]	0.0001	-2	3	1	-1000	1000
$H2DOI_{main}$ [ms]	0.5	1	5.5	5	-1000	1000

* the positive definite matrix weights which selected to penalize deviations from the requested load while minimizing NO_x and soot emission concentrations, ** the positive definite matrix weights which selected to penalize rate of change in controller outputs.

2.2 Data-driven Engine Model

The experimental testing is performed on amodified four-cylinder Cummins QSB 4.5-liter diesel engine equipped with emission measurement equipment. This is a direct-injected diesel engine without external after-treatment or exhaust gas recirculation (EGR). The hydrogen is injected into the intake air manifold. To measure NO_x emission from the engine, a Bosch sensor with ECM electronics (P/N: 06-05) is used, whereas a Pegasor particle sensor (PPS-M) is utilized to measure soot. Additional details regarding the experimental setup can be found in [13].

The data-driven model is a DNN model, which has been optimized using the Bayesian optimizer [16]. The resulting DNN model for the H2/diesel engine has two hidden layers with 31 and 23 neurons and uses a Leaky ReLU as an activation function. The structure of the DNN is shown in Figure 1. The inputs of the model are: the duration of injection (DOI) for main injection (DOI_{main}), start of main injection (SOI_{main}), the duration between the end of the pilot injection and the start of the main injection pre-2-main (P2M), DOI for hydrogen ($H2DOI_{main}$) and the measured outputs of the engine from the previous cycle to capture the dynamic of the system. The outputs of this model are IMEP, NOx, Soot, and MPRR. The dataset for training this model is collected by varying the engine inputs with a pseudo-random generator for all of the controlled variables: DOI_{main} ms, P2M ms, SOI_{main} °CAbTDC, and $H2DOI_{main}$ ms. The mean value of the training dataset is 6.5, 641, 0.5, and 0.9, with standard deviations of 1.9, 369, 0.04, and 0.9 for IMEP bar, NO_x ppm, soot mg/m^3, and MPRR bar/°CA, respectively. In Table 2, the statistics of the dataset and the results of our prediction in different datasets can be seen.

To achieve cycle-by-cycle control, all the calculations must be within one engine cycle time - approximately 20 ms at 1500 rpm. The computational cost of the developed model is 2-3 ms on realtime hardware, making it suitable for embedded in NMPC and then running the online optimization.

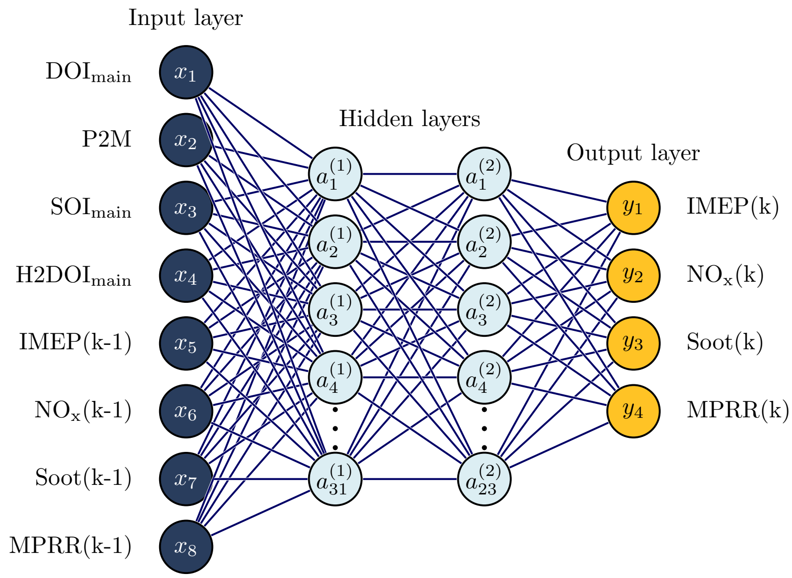

Fig. 1: Structure of the proposed deep neural network (DNN) model for engine performance and emission concentration modeling with eight inputs and four outputs. DOI: duration of injection, SOI: start of injection, P2M: the duration between the end of the pilot injection and the start of the main injection pre-2-main, main: main injection, H2: hydrogen, IMEP: indicated mean effective pressure, NO_x: nitrogen oxides, MPRR: maximum pressure rise rate and k-1 indicates the previous cycle.

Table 2: Training dataset characteristics and DNN model results of the H2/diesel dual-fuel engine. IMEP: indicated mean effective pressure, NO_x: nitrogen oxides, MPRR: maximum pressure rise rate.

Metrics	Data (Number of Data)	IMEP [bar]	NO_x [ppm]	Soot [mg/m^3]	MPRR [bar/°CA]
Max	All Training Data (82,348)	10.5	1862	0.8	10.0
Mean		6.5	641	0.5	0.9
Min		1.0	66	0.3	0.2
STD*		1.9	369	0.04	0.9
MAE**	Training (59,495)	0.125	7	0.020	0.204
	Validation (10,500)	0.119	7	0.022	0.173
	Testing (12,353)	0.138	8	0.022	0.232
	Real-time Prediction (5,025)	0.182	7	0.037	0.065
RMSE***	Training	0.234	13	0.025	0.432
	Validation	0.208	11	0.027	0.349
	Testing	0.272	16	0.027	0.506
	Real-time Prediction	0.243	9	0.047	0.082
R2-score	Training	0.998	0.999	0.997	0.878
	Validation	0.999	0.999	0.997	0.890
	Testing	0.998	0.999	0.997	0.854
	Real-time Prediction	0.998	0.999	0.878	0.941

* standard deviation, ** mean absolute error, *** root mean square error.

3 Results and Discussion

The DNN-NMPC for IMEP tracking while minimizing emission concentration (NO_x and soot) and fuel consumption while meeting constraints on inputs and outputs has been experimentally tested. The controller is subjected to step and smooth changes in IMEP reference to check the command following. The controller is also compared with the production diesel engine ECU, which serves as a benchmark (BM) for comparison with the NMPC. The Cummins production ECU is duplicated on our prototyping ECU (dSPACE MABX) to provide a BM. The results of controlling the IMEP load with this controller and its constraints can be seen in

Figure 2. The IMEP follows the reference trajectory (dashed line) with a mean absolute error (MAE) of 0.19 bar. The reference load, IMEP, and tracking error are shown in Figure 2 (a). IMEP tracking errors tend to increase when the reference is changed quickly and sharply. Since the optimized DNN model has no memory, unlike LSTM models, making fast transient prediction difficult. In Figure 2 (b), the NO_x emission of the engine slightly exceeds the upper limit constraint because it is implemented as a soft constraint in the NMPC. The average NO_x per cycle is 470.34 ppm/cycle. The cumulative soot emissions in Figure 2 (c) are 413.03 mg/m^3. In Figure 2 (d), the MPRR is less than 1 bar/°CA during the test. The engine inputs (controller outputs) are shown in Figure 2 (e,f,g,h). In Figure 2 (h), by increasing the DOI of H2, IMEP is increased. As the IMEP reference is increased, the controller increases the H2 with the main diesel injection. At 300-350 seconds, the controller increases the H2 instead of diesel to produce a higher load. This experimental test shows the negative correlation between H2 and soot and the positive correlation between H2 and NO_x. There, increasing H2 over diesel to generate more power reduces soot and increases NO_x. At 100-150 seconds, the controller increased H2 and diesel to produce a higher load. Resulting in both soot and NO_x increasing. However, the NO_x increased proportionally less than the 300-350 seconds case. As the IMEP reference is increased, the controller increases the H2 with the main diesel injection. In Figure 2 (h), the average H2 utilization is 68%, which varied from 29% to 95% during the test.

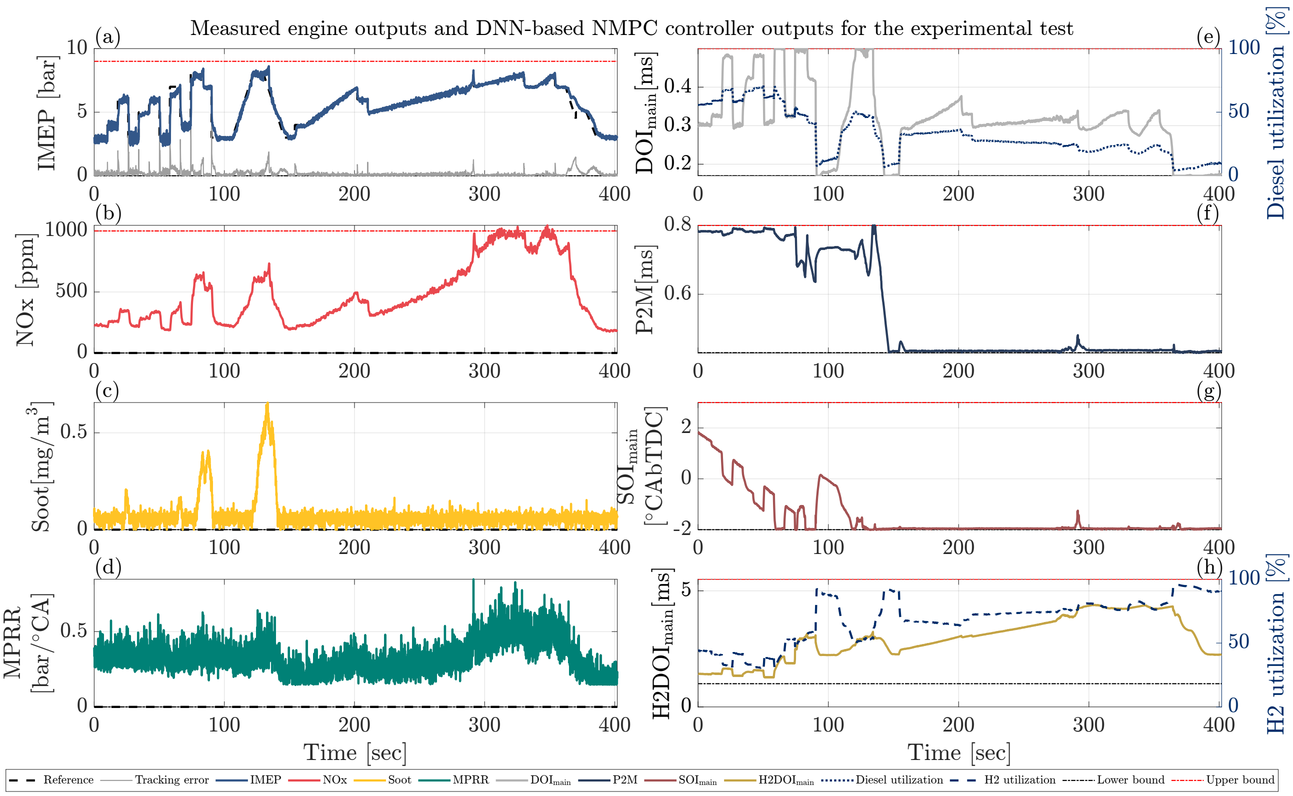

Fig. 2: IMEP tracking results for real-time NMPC with measured engine outputs and DNN-NMPC controller outputs for the experimental test with their limitation bounds—(a) indicated mean effective pressure (IMEP), its reference trajectory and error, (b) nitrogen oxides (NO_x), (c) Soot (upper limit for Soot is 2 mg/m^3), (d) maximum pressure rise rate (MPRR) (upper limit for MPRR is 3 bar/°CA), (e) duration of injection (DOI) of main injection, (f) the duration between the end of the pilot injection and the start of the main injection pre-2-main (P2M), (g) start of injection (SOI) of main-injection, (h) DOI of hydrogen injection.

The BM diesel was implemented in the same reference for IMEP tracking and followed the trajectory with MAE 0.3 bar. The BM's average NOx and soot emissions are 263 ppm and 0.64 mg/m^3, respectively.

4 Conclusions

Using an NMPC allows for control of both hydrogen and diesel injection to track IMEP subject to engine-out emissions, and pressure rise rates. An optimized DNN model has been created with the help of Bayesian optimization, which has two hidden layers of 31 and 23 neurons that can represent the engine dynamics: IMEP, NO_x, soot, and MPRR. The DNN model used has 1,111 learnable parameters to model the emissions and performance characteristics of a modified 4.5-liter Cummins compression ignition engine. The DNN is embedded within an NMPC and implemented in real-time to minimize H2/diesel dual fuel engine-out emissions and fuel consumption while enforcing constraints on engine inputs and outputs. With an average H2 utilization of 68%, the controller reduced soot concentrations by up to 87% compared to the Cummins-calibrated production controller. The mean controller computational time is 2 ms, 10 times smaller than 20 ms available calculation time at 1500 rpm. However, the controller tracking error in transient dynamics was too high due to the DNN reliance on only one previous cycle. More past cycles will be added in future work to help improve the controllers transient response. Furthermore, using hydrogen to increase the IMEP led to a predictable increase in chamber temperature and a 78% increase in NO_x concentrations compared to the Cummins-calibrated production controller.

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