Abstract

Given an on-board diagnostics (OBD) dataset and a physics-based emissions prediction model, this paper aims to develop an accurate and computational-efficient AI (Artificial Intelligence) method that predicts vehicle emissions. The problem is of societal importance because vehicular emissions lead to climate change and impact human health. This problem is challenging because the OBD data does not contain enough parameters needed by high-order physics models. Conversely, related work has shown that low-order physics models have poor predictive accuracy when using available OBD data. This paper uses a divergent window co-occurrence pattern detection method to develop a spatiotemporal variability-aware AI model for predicting emission values from the OBD datasets. We conducted a case-study using real-world OBD data from a local public transportation agency. Results show that the proposed AI method has approximately 65% improved predictive accuracy than a non-AI low-order physics model and is approximately 35% more accurate than a baseline model.

1 Introduction

On-board diagnostics (OBD) data is multi-attribute trajectory data obtained from sensors in vehicles. It contains time series of engine and vehicle performance parameters. Guided by a low-order combustion-physics-based model, this paper aims to develop an OBD-data-driven AI model to predict vehicle emissions values.

This problem is of significant societal importance because transportation is the biggest worldwide contributor to greenhouse gases such as $CO_2$ (Carbon dioxide) and toxic gases like $NO_x$ (Oxides of Nitrogen like $NO$, $NO_2$, etc.). These emissions impair people’s health (Thakrar et al. 2020) and global climate. An understanding of vehicle and engine behavior in the real world is essential for tracking and eventually mitigating these emissions by aiding the design of cleaner and more efficient vehicle systems.

This problem is challenging because the processes by which they are produced are complex and dependent on many parameters. Traditional laboratory experiments conducted to measure emissions values are usually based on engine-specific steady-state measurements. However, data collection inside a laboratory is expensive compared to low-cost sensor data from vehicles on the road.

Two types of related work are relevant: purely phenomenological methods or purely AI approaches. (He, Durrett, and Sun 2008) introduced a low-order physics (LOP) model that uses a purely phenomenological method for predicting the emission index of $NO_x$ ($EI-NO_x$, grams of $NO_x$ per kilogram fuel) of a diesel engine. It assumes that $EI-NO_x$ depends on the intake oxygen concentration, duration of combustion, and the peak adiabatic (i.e. without heat loss) flame temperature, which was validated using engine testing observations in laboratory conditions. To show its performance in the real world, we evaluated it using an OBD dataset from transit buses in the Metro Transit (local public transportation agency), which showed that the LOP method had poor accuracy (Figure 1).

![Figure 1: Comparing Observed and Predicted $NO_x$ values using LOP phenomenological model](image)

An example of a purely AI approach is (Obodeh 2009), which evaluates the performance of an artificial neural network (ANN) on data from a laboratory test rig for an engine. However, it provides no understanding of $NO_x$ formation and had spurious non-physical results. Instead, engine scientists prefer an approach to predicting emissions that is interpretable using domain knowledge (Karpatne et al. 2018).
We first introduce a baseline physics-aware AI model to pre-
vehicles, thus other vehicular emissions are not considered.
The extended Zeldovich Mechanism (Mellor et al. 1998):
This paper focuses on the prediction of
of public availability of proprietary engine calibration data.
Other AI models such as neural networks fall outside
the scope of this work. Proprietary manufacturers’ physics-
model. Other AI models are also outside the scope, due to lack
of public availability of proprietary engine calibration data.
This paper focuses on the prediction of \( NO_x \) emissions from
vehicles, thus other vehicular emissions are not considered.

## 2 Proposed Baseline Approach

We first introduce a baseline physics-aware AI model to predict \( NO_x \) emission values. The emission index for \( NO_x \)
\( EI - NO_x \) is given by a chemical kinetic equation for the extended Zeldovich Mechanism (Mellor et al. 1998):
\[
EI - NO_x(k + \delta) = a * T_{adiab}(k)^b * t_{comb}(k)^c
\] (1)
where, \( EI - NO_x(k + \delta) \) is the \( EI - NO_x \) in grams \( NO_x \)
per kilogram fuel at time ‘k+\( \delta \)’; \( T_{adiab}(k) \) is the adiabatic
flame temperature in kelvin at time ‘k’; \( t_{comb} \) is the duration
of combustion in seconds at time stamp ‘k’, which is
approximately equal to the fuel injection duration; \( a, b, c \) are
constants; and \( \delta \) is the time lag between the adiabatic flame
temperature \( T_{adiab} \) and duration of combustion \( t_{comb} \) with
the corresponding \( NO_x \) emission index \( EI - NO_x \). More
details of the physics calculations are provided in the Appendix Sections of (Panneer Selvam et al. 2020)

![Figure 2: Comparing Observed and Predicted \( NO_x \) values using baseline physics-aware AI model](image)

We evaluated the baseline physics-aware AI model using
the same OBD dataset as the one used for the LOP method. First, we used six engine attributes (i.e.
intake air flowrate(kilograms per hour), fuel consumed (kilograms per
hour), rail pressure (pascal), intake pressure (pascal), intake
temperature (kelvin), engine speed (revolutions per minute))
to calculate \( T_{adiab} \) and \( t_{comb} \). Then, we applied a nonlinear
regression method from Python Scikit-Learn package (Pedregosa et al. 2011) to estimate the values of \( a, b \) and \( c \) in
Equation [1].
The value of \( \delta = 1 \) was derived using hand
computation and data visualization.

Figure 2 shows the \( NO_x \) values predicted using baseline
model compared with the actual values. The baseline model
is an improvement over the low-order physics (LOP) model
(Figure 1), however, there is room for further improvement.

## 3 Proposed Variability-Aware Approach

To overcome the limitations of the baseline method, we propose
a spatiotemporal (ST) variability-aware AI approach.
Since one group of estimated parameters (e.g., \( a, b, c \)) values
in Equation [1] does not fit all scenarios well, it may be
beneficial to initially partition the data into multiple homogeneous
groups, and estimate parameter values group-wise.
The top half of Figure 3 shows our proposed ST variability-aware AI framework. First, we test in-coming
OBD data to identify \( NO_x \) emissions that diverge from the
predictions made by the baseline model. We define divergence as
the large (i.e. above a given threshold) absolute error between the observed and predicted \( NO_x \) values. In
general, when a vehicle exhibits divergence, there are two
potential pathways for understanding the issues and improving
the model: (1) using AI to improve the prediction results,
or (2) using physics-based methods to develop new and refined
process-based mechanistic models.

This paper focuses on AI model refinement based on data
partitioning and fitting separate models to each partition.
The partitioning is based on ST correlates of divergent
observations, thus we call it an ST variability-aware AI
approach. This approach can potentially reduce prediction
errors as illustrated in Figure 3 (lower half).

![Figure 3: Proposed ST Variability-aware AI framework. The figure in the bottom half is for illustration purpose only.](image)
except for the use of spatial statistical interest measure, i.e., temporal form of Ripley’s cross-k function $\epsilon$ (Ali et al. 2017; Ripley 1976). These pattern represents those subsets of engine attributes with their specific value ranges, which are present together in many divergent (time-) windows and have cross-k function values above a given threshold $\epsilon$. Engine scientists review and group co-occurrence patterns into scenarios (for example, cold start of an engine, sudden acceleration, etc.) for physically interpreting situations where the baseline model performs poorly.

Given the co-occurrence pattern groups formed in the first step, the original OBD data is split into multiple subsets corresponding to different pattern groups. Within each subset, we use the baseline approach to calculate the values of $T_{attab}$ and $\epsilon_{comb}$, and then estimate the parameter $(a, b, c)$ values in Equation (1) by fitting nonlinear regression models independently. Since the scenarios when the baseline approach does not perform well are handled separately, the ST variability-aware AI model is expected to yield better predictive accuracy by lowering errors.

4 Experimental Evaluation and Discussion

We conducted experiments to compare predictive accuracy of the proposed approaches with the low-order physics (LOP) approach detailed in Section 1 (He, Durrett, and Sun 2008) to address the following questions: (1) How do the predictions of the proposed approaches compare with those from the low-order physics approach? (2) How sensitive is the proposed spatiotemporal variability-aware AI approach to the number of partitions, input divergence threshold, and window length?

Data: The dataset used in the experiments is the Metro Transit OBD dataset that was used to evaluate the LOP approach and the proposed baseline approach in the earlier sections. It contains 99,895 data entries containing measurements of 90 engine and vehicle attributes. The OBD data was obtained from transit buses traversing 3 different routes for 16 different runs in the Minneapolis-St.Paul region. We used 8 runs for training sample and the remaining 8 runs for testing, ensuring each route is represented in both samples. More details are provided in (Panneer Selvam et al. 2020).

Candidate methods and metrics: The methods evaluated in the experiments include low-order physics model (LOP), the proposed baseline (P-Base), and the proposed spatiotemporal variability-aware AI approach (P-STVA).

Predictive accuracy was measured using $R^2$ values, root mean square error (RMSE) and mean absolute error (MAE).

Experimental results: Figure 4 shows a comparison of the refined $NO_x$ prediction using the P-STVA method with the observed $NO_x$ values in the training data. Compared with Figure 2, the dots in Figure 4 are closer to the $y = x$ line, and the number of green and yellow dots in the upper-left part of Figure 4 reduces dramatically, which indicates improved predictive accuracy.

How do the predictions of the proposed approaches compare with those from the low-order physics approach? Tables 1 and 2 summarize predictive accuracy metrics for the candidate methods on training and testing data respectively with $n = 4$ and $\text{summationThreshold} = 30$ ppm (parts per million). The proposed physics-aware AI methods outperformed the low-order physics model. For the training data, the P-Base method provides about 50% improvement in RMSE and 35% improvement in MAE when compared to the LOP method, while RMSE and MAE of the P-STVA method with $n = 4$ are both around 35% smaller than the P-base method. For the testing data, the P-base method provides about 50% improvement in RMSE and 40% improvement in MAE when compared to the LOP method, while RMSE and MAE of the P-STVA method with $n = 4$ are both around 35% smaller than the P-base method.

Table 1: $NO_x$ predictive accuracy for training data

| Prediction method | $R^2$ | RMSE | MAE |
|-------------------|-------|------|-----|
| LOP               | 0.1264 | 311.76 | 258.87 |
| P-Base            | 0.4464 | 196.39 | 155.17 |
| P-STVA n = 4      | 0.3900 | 132.60 | 102.13 |

Table 2: $NO_x$ predictive accuracy for testing data

| Prediction method | $R^2$ | RMSE | MAE |
|-------------------|-------|------|-----|
| LOP               | 0.1260 | 368.67 | 238.23 |
| P-Base            | 0.4607 | 183.52 | 144.69 |
| P-STVA n = 4      | 0.4769 | 117.39 | 92.99 |

How sensitive is the proposed spatiotemporal variability-aware AI approach to the number of partitions, input divergence threshold, and window length? Figures A, B, and C show the sensitivity of predictive accuracy metrics of the P-STVA method to number of patterns $n$ (number of partitions is $n + 1$), $\text{summationThreshold}$, and window Length $L$ respectively for training and testing data. Optimum values are found at $n = 4$, $\text{summationThreshold} = 30$ ppm and $L = 3$ s.

Domain interpretation of partitions: The P-STVA method uses $n + 1$ partitions including the non-divergent case (and divergent cases not covered by the patterns) and $n$ partitions of divergent cases, one for each co-occurrence.

Table 3: Four most significant divergent co-occurrence patterns in the training data

| Pattern | Co-occurrence | Scenario |
|---------|---------------|----------|
| Pattern2 | EngEq: $E_g$ $E_N$ $E_{EGR}$ | High Engine Load |
| Pattern3 | EngEq: $R_1$ $R_2$ $R_3$ | High Engine Idling |
| Pattern4 | EngEq: $R_1$ $R_2$ $R_3$ | Low Engine Speed |

Figure 4: Refined $NO_x$ prediction using P-STVA method, number of partitions $n = 4$, $L = 3$ seconds, $\text{summationThreshold} = 30$ ppm, min$\text{Supp} = 0.003$, $\epsilon = 2$
pattern. Table 3 shows 4 co-occurrence patterns for the case $n = 4$, $\text{summationThreshold} = 30$ ppm and $L = 3$ seconds along with their domain interpretation in terms of different scenarios.

5 Conclusions and Future Work

We proposed a novel physics-aware AI emission prediction model and evaluated it with an on-board diagnostics dataset. The experimental evaluation shows the proposed models outperform the non-AI low-order physics model. Furthermore, the resultant models were interpreted using domain concepts as different vehicle scenarios.

In the future, we will explore other AI models such as neural networks guided by combustion physics. We will characterize the sensitivity of the computation time of the proposed P-STVA model to parameters such as the number of partitions. We will also investigate physics-aware AI models to predict vehicle emissions other than $NO_x$ as well as to predict energy use. This will assess the applicability of the Co-Occurrence Pattern Based Approach (Shown in top half of Figure 3) to other problems. Currently, engine scientists review and group co-occurrence patterns into scenarios for domain interpretation. For the future work, we will explore building a machine learning model for grouping the patterns to assist human experts and reduce manual labor.

6 Acknowledgments

This material is based upon work supported by the National Science Foundation under Grant No. 1901099. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

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