# DEVELOPMENT OF A MICROSCOPIC EMISSION MODELING FRAMEWORK FOR ON-ROAD VEHICLES

by

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## Abstarct

The transportation sector has a significant impact on the environment both nationally and globally since it is a major vehicle fuel consumption and emissions contributor. These emissions are considered a major environmental threat. Consequently, decision makers desperately need tools that can estimate vehicle emissions accurately to quantify the impact of transportation operational projects on the environment. Microscopic fuel consumption and emission models should be capable of computing vehicle emissions reliably to assist decision makers in developing emission mitigation strategies. However, the majority of current state-of-the-art models suffer from two major shortcomings, namely; they either produce a bang-bang control system because they use a linear fuel consumption versus power model or they cannot be calibrated using publicly available data and thus require expensive laboratory or field data collection. Consequently, this dissertation attempts to fill this gap in state-of-the-art emission modeling through a framework based on the Virginia Tech Comprehensive Power-Based Fuel consumption Model (VT-CPFM), which overcomes the above mentioned drawbacks. Specifically, VT-CPFM does not result in a bang-bang control and can be calibrated using publicly available vehicle and road pavement parameters. The main emphasis of this dissertation is to develop a simple and reliable emission model that is able to compute instantaneous emission rates of carbon monoxide (CO), hydrocarbons (HC) and nitrogen oxides ($NO_x$) for the light-duty vehicles (LDVs) and heavy-duty diesel trucks (HDDTs). The proposed extension is entitled Virginia Tech Comprehensive Power-Based Fuel consumption and Emission Model (VT-CPFEM). The study proposes two square root models where the first model structure is a cubic polynomial function that depends on fuel estimates derived solely from VT-CPFM fuel estimates, which enhances the simplicity of the model. The second modeling framework combines the cubic function of the VT-CPFM fuel estimates with a linear speed term. The additional speed term improves the accuracy of the model and can be used as a reference for the driving condition of the vehicle. Moreover, the model is tested and compared with existing models to demonstrate the robustness of the model. Furthermore, the performance of the model was further investigated by applying the model on driving cycles based on real-world driving conditions. The results demonstrate the efficacy of the model in replicating empirical observations reliably and simply with only two parameters.

# DEVELOPMENT OF A MICROSCOPIC EMISSION MODELING FRAMEWORK FOR ON-ROAD VEHICLES

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## General audience abstract

The transportation sector places a huge burden on our environment and is one of the major emitters of pollutants. The resulting emissions have a negative impact on human health and could be a concern for national security. Therefore, policymakers are keen to develop models that accurately estimate the emissions from on-road vehicles. Microscopic emission models are capable of estimating the instantaneous vehicle emissions from operational-level projects, and policymakers can use them to evaluate their emission reduction plans and the environmental impact of transportation projects. However, the majority of the current existing models indicate that to achieve the optimum fuel economy, the driver should accelerate at full throttle and full braking for deceleration to minimize the acceleration and deceleration times. This assumption is obviously incorrect since it requires aggressive driving which will result in increasing the fuel consumption rate. Also, the models cannot use publicly accessible and available data to estimate the emissions which require expensive laboratory or field data collection. Consequently, this dissertation attempts to fill this gap in emission modeling through a framework based on the Virginia Tech Comprehensive Power-Based Fuel consumption Model (VT-CPFM), which overcomes the above mentioned drawbacks. Specifically, VT-CPFM does not follow the mentioned assumption of aggressive driving to minimize the fuel consumption as previously explained and can use publicly available vehicle and road pavement variables to estimate the emissions. Also, it utilizes US Environmental Protection Agency (EPA) city and highway the fuel economy ratings to calibrate its parameters. The main emphasis of this dissertation is to develop a simple and reliable emission model that is able to compute instantaneous emission rates of carbon monoxide (CO), hydrocarbons (HC) and nitrogen oxides ($NO_x$) for the light-duty vehicles (LDVs) and heavy-duty diesel trucks (HDDTs). The proposed extension is entitled Virginia Tech Comprehensive Power-Based Fuel consumption and Emission Model (VT-CPFEM). The study proposes two models where the first model structure that depends on fuel estimates derived solely from VT-CPFM fuel estimates, which enhances the simplicity of the model. The second modeling framework combines the VT-CPFM fuel estimates with the speed parameter. The additional speed term improves the accuracy of the model and can be used as a reference for the driving condition of the vehicle. The model framework is consistent in estimating the three emissions for LDVs and HDDTs. Moreover, the performance of the model was investigated in comparison with existing models to demonstrate the reliability of the model. Furthermore, the performance of the model was further evaluated by applying the model on driving cycles based on real-world driving conditions. The results demonstrate the capability of the model in generating accurate and reliable estimates based on the goodness of fit and error values for the three types of emissions.

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# Preface

Prof. Hesham A. Rakha - Ph.D. (Department of Civil Engineering, Virginia Tech) is the primary Advisor and Committee Chair. Prof. Rakha provided extensive guidance toward all the chapters of this dissertation and advice on the research. All the work I performed for my dissertation was done under his advising.

Dr. Kyoungho Ahn is listed as a co-author on the paper presented in Chapter 3 because of his recommendations on model validation. I performed all the analysis, modeling and writing of the paper.

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# Chapter 1: Introduction

## 1.1 INTRODUCTION

The transportation sector plays a vital role all over the world in meeting travel demands, which is a key necessity for human civilization. The resulting emissions have a negative impact on human health and could be a concern for national security. The growing population and increasing car ownership represent a burden as increases in vehicles will result in higher emission rates. The annual rate of vehicles miles traveled (VMT) increased at an average of 3.4 percent between 1985 and 2005 (M.J. Bradley & Associates LLC, 2015).

The transportation sector accounts for approximately 70 percent of petroleum use and 30 percent of greenhouse gas emissions in the United States (US) (Knittel, 2012). The U.S. produces 7.5 million barrels of petroleum per day (M bpd) and consumes 19.15 M bpd (Davis et al., 2011). Additionally, transportation energy use accounts for 28.1% of total U.S. energy use (Davis et al., 2011). In 2012 in the United States, 232 million registered light-duty vehicles traveled 2.7 trillion miles and consumed 124 billion gallons of gasoline. Eleven million heavy trucks registered in the U.S traveled 268 billion miles, burning 42 billion gallons of diesel fuel. From 1973 to 2007, yearly highway fuel consumption, which consisted almost entirely of petroleum-based fuels, rose 59%, from 110.5 to 176 billion gallons (Davis et al., 2009).

Carbon monoxide (CO), hydrocarbons (HC) and oxides of nitrogen ($NO_x$) are the main hazard pollutants that have adverse effects on public health when emitted from vehicles. They could cause severe diseases, including cardiovascular diseases, cancer, respiratory irritation and other hazards. The transportation sector is responsible for producing nearly 70 percent of CO, 45 percent of HC and 45 percent of $NO_x$ emissions (Knittel, 2012). Consequently, public concern has increased and governments are taking action to combat increasing pollution. The Clean Air Act Amendment of 1990 imposed air regulations and emission standards to reduce emission levels and improve air quality. Furthermore, fuel consumption and emission modelling is a noteworthy and primary tool in evaluating the performance of traffic operations projects to sustain the environment. Also, decision and policy makers need the fuel consumption and emission models to estimate emissions resulting from new plans and transportation projects. In this way, they can compare the differences in emission levels before and after implementing plans to evaluate their impact.

## 1.2 PROBLEM STATEMENT

Microscopic fuel consumption and emission models have been widely used as a reliable method to estimate the instantaneous emission rates using second by second explanatory variables (e.g. speed, acceleration, power, etc.) in order to evaluate the impact of transportation operational-level projects on the environment. Moreover, to estimate the fuel consumption and emission rates, the required instantaneous data consider vehicle characteristics and dynamics, roadway conditions and environmental conditions. Fuel consumption and emissions modelling plays a key role in the evaluation of emissions reduction plans through the accurate estimation of motor vehicle emissions. Decision makers can rely on these results to evaluate the consequences of their plans and act accordingly.

Current state-of-the-practice models have experienced two major limitations: the majority of models produce a bang-bang control system and they cannot use publicly available data to calibrate the model parameters. These two shortcomings make these models not ideal for the design of vehicle control systems. The majority of these models utilize extensive and complex data, which costs time and money. Also, data needed to calibrate the parameters and calculate emission rates are collected using special devices that are not widely available.

The Virginia Tech Comprehensive Power-Based Fuel consumption Model (VT-CPFM) is a microscopic fuel consumption model based on instantaneous vehicle power. VT-CPFM meets the requirements of the predictive eco-cruise control systems because it overcomes two of the major shortcomings of existing state-of-the-art models: it does not produce a bang-bang control system, and it utilizes publicly available data to estimate emission levels. VT-CPFM can estimate the vehicle fuel consumption rate (l/s) accurately; however, it does not estimate vehicle emission rates.

## 1.3 RESEARCH OBJECTIVES

According to the above discussion and in light of the mentioned limitations, the research effort presented in this dissertation attempts to extend the VT-CPFM model to capture CO, HC, and $NO_x$ emissions accurately and in a simple framework that could be utilized easily. In order to achieve this goal, the main emphasis of this research is to develop a mathematical model that considers different traffic conditions for vehicles, with acceleration or deceleration incorporated into one scenario for the model. The model should be capable of estimating emissions for light-duty vehicles (LDVs) and Heavy-duty diesel trucks (HDDTs) accurately and in a simple manner to be applied easily. The model will be compared with current state-of-the-art models to evaluate its applicability and accuracy.

## 1.4 RESEARCH CONTRIBUTIONS

This dissertation develops a microscopic emission model that uses the estimated fuel from VT-CPFM and instantaneous speed as explanatory variables to predict instantaneous emissions. Although, the model can estimate LDV emissions using fuel estimates only, the speed term enhances the model accuracy and can be used as a reference of the driving condition of the car at high or low speed. The model is based on the square root formula, which consists of a cubic polynomial function of fuel and linear speed term. The heavy-duty diesel truck emission model consists only of instantaneous fuel and speed variables to estimate the emissions. The structure of the model incorporates the vehicle acceleration and deceleration rates in one equation. The model was validated on different driving cycles to test the model under various ranges of speed and acceleration. Specifically, this research has contributed in:

- Developing a simple and reliable microscopic emission model which overcomes the deficiencies in existing models.
- The mathematical model depends on only two parameters which can be easily calculated or collected.
- The model estimates the emission levels whether the vehicle power is positive or negative in one framework.
- The model is capable of estimating instantaneous emission rates for light-duty vehicles and heavy-duty trucks with two fuel types: gasoline and diesel.
- The model was compared against existing models to evaluate its performance.
- The model was implemented on different driving cycles to ensure its validity on various driving scenarios and behavior.

- Developing a generalized model to save time from calibrating the parameters for each vehicle individually. The coefficients of the model can be generated by inserting the publicly available vehicle parameters only.

## 1.5 DISSERTATION LAYOUT

After the introduction, which describes the problem statement and dissertation objectives, an extensive review of the literature relevant to topics covered in the dissertation is presented in Chapter 2. Thereafter, Chapter 3 includes the light-duty vehicles emission modelling chapter, which describes the data and methodology used to develop the proposed model. Chapter 4 provides the detailed techniques and methods used in the adopted analysis approach to develop the emission model for heavy-duty diesel trucks. Chapter 5 demonstrates the light-duty vehicles emission modeling based on MOVES data to ensure the validity of the model. Finally, the sixth chapter consists of a summary of the dissertation conclusions and recommendations for further research.

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# Chapter 2: Literature Review

**SUMMARY**
This chapter discusses the main topics related to motor vehicle fuel consumption and emission modelling. The first section summarizes the environmental standards and regulations imposed by the government on motor vehicle transportation to reduce vehicle emissions. The second section categorizes the factors affecting emissions levels. The third section demonstrates the hazards of vehicle exhaust pollutants, which this research effort intends to reduce. The fourth section reviews the current state-of-the-art and state-of-practice fuel consumption and emission models. The literature examines the applicability of these models and their limitations in estimating fuel and emission rates. The chapter provides the background of fuel consumption and emission modeling to the significance of the proposed model.

## 2.1 EMISSION STANDARDS AND REGULATIONS

The first state to implement the statewide pollution control act was California. In 1947, the California Air Pollution Control Act (CAPCA) was created to reduce air pollution. Public concern toward air pollution had increased, and the US government decided to act regarding this concern. Therefore, the first federal legislation regarding air pollution in 1955 was the Air Pollution Control Act of 1955 (APCA). All following clean air legislation and other acts evolved from the 1955 Act, which provided funds and technical assistance in air pollution control research (Forswall & Higgins, 2005).

The Clean Air Act (CAA) of 1963 was signed to fund research efforts by state and local governments to decrease air pollution problems. The Act also recognized the impact of motor vehicle exhaust and encouraged the development of emissions standards, as well as standards for stationary sources. There were several amendments to the Act in the following years until 1970. This year witnessed the first major legislation to confront the hazards of air pollution on public health. CAA in 1970 initiated four regulatory programs: National Ambient Air Quality Standards (NAAQS), New Source Performance Standards (NSPS), State Implementation Plans (SIPs), and National Emission Standards for hazardous Air Pollutants (NESHAPs). The Environmental Protection Agency (EPA) was founded in 1971 to implement the CAA (Forswall & Higgins, 2005).

The EPA set NAAQS for six pollutants to protect the public health and welfare. These six pollutants, known as criteria pollutants, are ozone ($O_3$), particulate matter (PM), carbon monoxide (CO), sulfur dioxide ($SO_2$), nitrogen dioxide ($NO_2$), and lead (Pb). This 1970 amendment was intended to achieve clean air by setting standards to be accomplished in 1975. These standards were 3.4 grams per mile of CO and 0.41 grams per mile of HC (EPA, 1994a). However, these standards were not achieved and were thus postponed by the government to be reached in 1980 for HC standard and CO standard was achieved in 1981 according to Clean Air Act of 1977.

The Clean Air Act Amendments of 1990 (CAAA) revolutionized air regulations across the country. Congress executed these amendments to reduce HC, CO, $NO_x$, and particulate emissions. The amendments consisted of mobile source provisions including tighter tailpipe standards, more stringent emission testing procedures, expanded inspection and maintenance (I/M) programs; new vehicle technologies and clean fuels programs, and transportation management provisions (EPA, 1994b).

The CAAA in 1990 defined the geographic areas in the US that did not comply with NAAQS criteria and were classified as nonattainment areas. The severity of air quality conditions compared to NAAQS were classified into marginal, moderate, serious, severe and extreme. The nonattainment areas had to take certain actions within a set time frame to attain NAAQS.

Areas of moderate or worse ozone classifications were required to submit revisions via State Implementation Plans (SIPs). The ozone needed to be reduced by at least 15 percent, with these areas achieving a 3 percent reduction every year until they reached the required level. In addition, severe and extreme areas had to adopt transportation control measures (TCMs). TCMs aim to decrease motor travel, which will consequently reduce vehicle emissions (NRC, 1995).

The SIP has to be approved by the EPA to be included in the Code of Federal Regulations (Title 40, Part 52) and become federally enforceable. Failure to submit SIP to meet the requirements could result in sanctions, such as withholding federal highway funding. Furthermore, the department of transportation (DOT) could only approve single-vehicle trips (NRC, 1995).

## 2.2 FACTORS AFFECTING EMISSION LEVELS

The emission levels produced by motor vehicles are affected by several factors grouped (NRC, 1995) under four main categories: travel-related factors, driver behavior, highway network characteristics, and vehicle characteristics.

*Travel-related factors*

The distance traveled by the vehicle is directly related to the emitted pollutants. Emissions vary, depending on the trip, according to vehicle operating modes (exhaust emissions and evaporative emissions). Also, emissions are a function of speed, acceleration and engine load of the vehicle. Emission rates are highest in low-speed, congested driving conditions. Emissions fall in intermediate-speed, low density traffic conditions. Then, they rise again at higher speeds but do not reach the initial levels. However, $NO_x$ emissions do not follow the same trend, as they rise at relatively low speeds and reach the highest levels at high speeds.

*Driving behavior*

Driving behavior has a significant impact on emissions. Driving at sharp accelerations for passing or changing lanes or other similar scenarios imposes heavy loads on the engine that result in high emission rates. Emissions produced from vehicle accelerations are due to power enrichment, which is an engine operating strategy.

*Highway related factors*

The geometric design is another main factor that has a direct influence on emission levels. Physical characteristics of highways, such as signalized intersections, freeway ramps, weaving sections, rough pavement and other facilities that require engine enrichment from accelerations, increase emission rates.

*Vehicle-related and other factors*

Vehicle characteristics, including weight, engine size, horse power and age, have an effect on emissions. Small engine sizes emit less pollutants than large engine sizes grouped (NRC, 1995). Also, older vehicles emit more pollutants than newer vehicles.

Moreover, temperature is another parameter that affects vehicle conditions and which will result in a variance of emission levels. At cold temperatures, the engine takes longer to warm up, which will increase cold-start emissions. On the other hand, when the temperature increases, evaporative emissions increase.

## 2.3 POLLUTANTS

Exhaust emissions threaten the environment and deteriorate human health. Studying and recognizing these emission levels will be essential to sustain the planning and management of transportaion projects and the environment. The three main pollutants emitted from motor vehicles are carbon monoxide, hydrocarbons and oxides of nitrogen.

Carbon monoxide is a colorless and odorless gas. It is produced by the incomplete combustion of fuel. Carbon monoxide reduces the oxygen carried in the blood because it combines with hemoglobin, resulting in carboxyhemoglobin. In addition, it causes headaches and fatigue (Wark et al. 1998).

Hydrocarbons also result from the incomplete combustion of fuel. It reacts with oxides of nitrogen in the presence of sunlight to form the ozone, which has adverse effects on human health. Hydrocarbons cause respiratory irritation due to lung tissue damage and eye irritation. Furthermore, cancer may be caused by exposure to hydrocarbons (Wark et al. 1998).

Oxides of nitrogen are formed by high temperature chemical processes during the combustion process. As mentioned previously, they react with hydrocarbons to form the ozone. This has a hazardous effect on the respiratory system and forms acid rain (Wark et al. 1998).

The air/fuel (A/F) ratio is the main factor affecting the efficiency of catalytic converters and, consequently, the level of emissions (Johnson, 1988). CO and HC are highest under fuel-rich conditions, and NOx is highest under fuel-lean conditions.

## 2.4 MICROSCOPIC EMISSION MODELING

Microscopic fuel consumption models and emission models have been widely used to estimate instantaneous fuel consumption and emission rates to study the impact of traffic on the environment. This section categorizes the microscopic models into regression-based models, power (load)-based models, emission maps and MOVES to demonstrate their applicability and shortcomings.

### 2.4.1 Regression-based Models

#### VT-Micro

VT-Micro is a regression based model that mainly depends on the instantaneous velocity and acceleration of the vehicle. Rakha et al. developed the model in 2004 based on polynomial combinations of linear, quadratic and cubic terms of acceleration and speed that were collected at the Oak Ridge National Laboratory (ORNL). The fuel consumption and emission models were developed using data that were collected on a chassis dynamometer at ORNL, data gathered by the Environmental Protection Agency (EPA). The ORNL data consisted of nine normal emitting vehicles, including six light-duty automobiles and three light-duty trucks, which resulted in a third-order polynomial regression instantaneous model. Emission rates were estimated at high accuracy with a good fit ($R^2$ in excess of 0.92 for all measures of effectiveness (MOE)). Vehicle speeds ranged from 0-121 km/h (0 to 110 ft/s) at increments of 1 km/h, and vehicle acceleration measurements ranged from -1.5 to 3.7 m/s$^2$ (-5 to 12 ft/s$^2$) at increments of 0.3 m/s$^2$ (Rakha et al., 2004).

The model is expressed mathematically as (Rakha et al., 2004):

$$MOE_e = \begin{cases} e^{\sum_{i=0}^{3}\sum_{j=0}^{3}(L_{ij}^{e} \times u^{i} \times a^{j})} & for\ a \geq 0 \\ e^{\sum_{i=0}^{3}\sum_{j=0}^{3}(M_{ij}^{e} \times u^{i} \times a^{j})} & for\ a < 0 \end{cases} \tag{2-1}$$

Where,
$MOE_e$: Instantaneous fuel consumption or emission rate (CO or HC or $NO_x$) (l/s or mg/s) at e
$L_{ij}^e$: Model regression coefficient for MOE"e" at speed power"i" and acceleration power "j" for positive accelerations
$M_{ij}^e$: Model regression coefficient for MOE "e" at speed power "i" and acceleration power "j" for negative accelerations.
$u$: Instantaneous Speed (km/h)
$a$: Instantaneous acceleration (m/s$^2$)

The logarithmic transformation has been applied to prevent the estimation of any resulted negative values for $MOE_e$. The model evolved into two scenarios, where one accounts for the positive values of acceleration when the vehicle exerts power, while the other estimates the emissions and fuel consumption for the negative acceleration values when there is no power exerted by the vehicle (Rakha et al., 2004).

On the other hand, the models require the calibration of 32 coefficients, including the intercepts, which may overfit the data and be misleading in the results. Moreover, VT-Micro may underestimate the resulted emissions from a malfunctioning engine since it is not capable of considering the vehicle operating conditions.

**POLY**

Similarly, POLY is another regression model that categorized vehicles into 41 classes. The model accounts for instantaneous speed and acceleration and historical values for speed and acceleration (Teng et al., 2002).

$$\begin{aligned} e_i(c,t) = {} & \beta_0 + \beta_1 v(t) + \beta_2 v^2(t) + \beta_3 v^3(t) + \beta_{T'} T'(t) + \beta_{T''} T''(t) + \\ & + \beta_{A_t} A(t) + \cdots + \beta_{A_{t-9}} A(t-9) + \beta_W W(t) \end{aligned} \tag{2-2}$$

Where e accounts for the emission rate for species i, which depends on vehicle category c and time t. v(t) is the speed at time t. T'(t) and T''(t) are the corresponding acceleration and deceleration times since their inception up to the current time t. A(t) and A(t-9) are combined acceleration or deceleration at time t and t−(1,...9), which indicates the emitter type. W(t) is the product of v(t) and A(t). β is the parameter calibrated for each vehicle category c (Teng et al., 2002).

Nevertheless, the models indicate that acceleration and deceleration of previous time periods have more impact on emissions than the current time does (Teng et al., 2002). Also, the model requires a large number of explanatory variables, which indicates overfitting with the data.

### 2.4.2 Power based Models

**CMEM**

CMEM (Comprehensive Modal Emissions Model) is a power-based model that was developed at the University of California at Riverside and the University of Michigan by using the National Cooperative Highway Research Program (NCHRP) vehicle emissions database (Barth et al., 2000). The database consists of the chassis dynamometer of second-by-second speed, and engine-out and tailpipe emission rates data which were collected from 300 automobiles and light trucks in 26 vehicle categories. They were tested with three driving cycles: FTP, US06 and Modal Emission Cycle (MEC) (Barth et al., 2000). The second-by-second tailpipe emissions are estimated as the product of fuel rate (FR), engine-out emission index ($g_{emission}/g_{fuel}$), and catalyst pass fraction (CPF),according to the following equation (Barth et al., 2000):

$$Tailpipe\ emissions = FR\ \times \left(\frac{g_{emission}}{g_{fuel}}\right) \times CPF \quad (2\text{-}3)$$

Where, FR is the fuel rate (g/s) which evolves from the power demand, engine speed and air/fuel equivalence ratio. The engine-out emission index ($g_{emission}/g_{fuel}$) is engine out emissions divided by fuel consumption. CPF is the catalyst pass fraction, which is the ratio of tailpipe to engine-out emissions.

The CMEM model is based on a parameterized physical approach that is related to the physical conditions of vehicle operation and emission productions. It is composed of six modules, which are engine power, engine speed, air/fuel ratio, fuel use, engine-out emissions, and catalyst pass fraction. The model estimates emission rates under different vehicle operating conditions (stoichiometric, cold-start, enrichment, and enleanment conditions) (Barth et al., 2000).

Engine power is expressed as:

$$P_{tract} = A.v + B.v^2 + C.v^3 + M.a.v + M.g.v.sin\theta \quad (2\text{-}4)$$

Where,

$P_{tract}$: Total tractive power (kW),

$v$: Vehicle speed (m/s),

$a$: Vehicle acceleration (m/s2),

$A$: Rolling resistance coefficient (kW/m/s),

$B$: Speed correction to rolling resistance coefficient (kW/(m/s)2),

$C$: Air drag resistance coefficient (kW/(m/s)3),

$M$: Vehicle mass (kg),

$g$: Gravitational constant (9.81 m/s2),

$\theta$: road grade (degrees).

The fuel rate is estimated by CMEM as expressed in Equation (2-5):

$$FR = \left(K.N.V + \frac{P}{\eta}\right)\frac{1}{43.2}.[1 + b_1.(N - N_0)^2] \tag{2-5}$$

Where, $FR$ is the fuel use rate (g/s), $P$ is the engine power output (kW), $K$ is the engine friction factor, $N$ is the engine Speed (revolutions per second),$V$ is the engine displacement (L), $\eta$ is measure of indicated efficiency for diesel engines (0.45), $b_1$ is 10-4, $N_0$is a constant related to engine displacement and 43.2 kJ/g is the lower heating value of typical diesel fuel.

$$EO_i = a.FR + r \tag{2-6}$$

$EO_i$: Engine-out emission species of CO, HC and NOx,

$a\ and\ r$: Equation coefficients,

$FR$: fuel use rate (g/s).

However, the physical approach of the model increases the complexity and may not be simple. In addition, the model is data intensive, which requires physical variables to be collected and/or measured. Also, the data is not publicly available, which increases the difficulty to incorporate the data from many sources and requires recalibration for each data set (Scora and Barth, 2006). Moreover, CMEM may produce a bang-bang type control system, which occurs because the partial derivative of the fuel consumption rate with respect to the engine torque is not a function of torque (Saerens et al., 2010). The bang-bang control system involves accelerating at full throttle to reduce acceleration time and deceleration using full braking to achieve the optimum fuel economy control, which is obviously incorrect, since it requires aggressive driving, in order to minimize fuel consumption rates (Rakha et al., 2011). Furthermore, as long as the same amount of power is applied, CMEM will estimate the same emission levels regardless of whether the vehicle is at a high or low speed, or driving on a flat or steep road, respectively.

**EMIT**

Additionally, EMIT has been developed based on CMEM but developed in simplified concepts for light-duty vehicles. The model integrates two emissions modelling approaches (regression-based and load-based) which incorporates their main advantages. The model captures a satisfactory and reliable estimation level for carbon monoxide and nitrogen oxides but not as high as fuel and carbon dioxide. However, the results for hydrocarbons reached non-desirable levels (Cappiello, 2002).

The model is divided into two parts: engine-out (EO) and tailpipe emission (TP) modules for gas species i. The first module estimates the engine-out emissions based on instantaneous speed (v) and acceleration (a), which is expressed as follows (Cappiello et al., 2002):

$$EO_i = \begin{cases} \alpha_i + \beta_i v + \gamma_i v + \delta v + \zeta_i a v & if\ P_{tract} > 0 \\ \alpha_i' & if\ P_{tract} = 0 \end{cases} \tag{2-7}$$

Where $\alpha_i$, $\beta_i$, $\gamma_i$, $\delta_i$ and $\zeta_i$ are the model coefficients and $P_{tract}$ is the tractive power. Where, the tractive power is calculate by Equation (2-4).

Then, EO is used to estimate tailpipe emissions in the second module and multiplied by $CPF_i$ which is the catalyst pass fraction of gas species i to produce TP, which is expressed as:

$$TP_i = EO_i . CPF_i \tag{2-8}$$

The model should take into consideration other vehicle categories, which means that other databases should be used for model calibration. The model does not represent historical effects, such as cold-start emissions and hydrocarbon enleanment puffs (Cappiello, 2002).

**Virginia Tech Comprehensive Power-based Fuel consumption Model (VT-CPFM)**

VT-CPFM is a power-based model that overcomes the limitations of state-of-the-practice models. Namely, they produce a bang-bang control system and cannot be calibrated using publicly available data. VT-CPFM satisfies the requirements of the predictive eco-cruise control systems.

The power at instant t is developed:

$$P(t) = \left(\frac{R(t)+1.04\,ma(t)}{3600\eta_d}\right) v(t) \tag{2-9}$$

Here *P(t)* is the power exerted by the vehicle driveline (kW) at time *t*, *R(t)* is the resistance force (N) at time *t*, *m* is the vehicle mass(kg), a(t) is the vehicle acceleration ($m/s^2$) at time *t*, *v(t)* is the vehicle speed (km/h) at time *t*, and $\eta_d$ is the driveline efficiency.

The resistance force is computed through combining aerodynamic, rolling, and grade resistance forces using the following formula:

$$R(t) = \frac{\rho}{25.92} C_D C_h A_f v(t)^2 + 9.8066\, m\, \frac{C_r}{1000}(c_1 v(t) + c_2) + 9.8066 m G(t) \tag{2-10}$$

Where $\rho$ is the density of air at sea level at temperature 15°C (59°F) (equal to 1.2256 $kg/m^3$), $C_D$ is the vehicle drag coefficient (unitless); $C_h$ is a correction factor for altitude (unitless) and calculated as 1-0.085 H where H is the altitude (km); $A_f$ is the vehicle frontal area ($m^2$); and $C_r$, $c_1$ and $c_2$ are rolling resistance parameters that depend on the road surface type, road condition and vehicle tire type.

The VT-CPFM framework is a dual regime model to estimate instantaneous fuel, whether power is greater or equal to zero or at negative power. The structure of the model is expressed as:

$$FC(t) = \begin{cases} \alpha_0 + \alpha_1 P(t) + \alpha_2 P(t)^2 & \forall\, P(t) \geq 0 \\ \alpha_0 & \forall\, P(t) < 0 \end{cases} \tag{2-11}$$

Where FC (t) is the instantaneous estimated fuel consumption (l/s), and $\alpha_0$, $\alpha_1$ and $\alpha_2$ are the calibrated coefficients for each specific vehicle.

**PΔP**

The PΔP is one of the most recently developed models. The model utilizes engine power and change in engine power as the main model variables as shown in equation (2-12) expressed by

(Smit, 2013). The model estimates second-by-second fuel consumption, $CO_2$ and $NO_x$ (Smit, 2013).

$$e_t = \begin{cases} \alpha & for\ \ v_t = 0 \\ \beta_0 + \beta_1 P_t + \beta_2 \Delta P_t + \beta_3 P_t^2 + \beta_4 \Delta P_t^2 + \beta_5 P_t \Delta P_t + \varepsilon & for\ \ v_t > 0 \end{cases} \qquad (2\text{-}12)$$

where $e_t$ is the emission or fuel rate at time t, α is the emission rate at idle, $\beta_0$, $\beta_1$, $\beta_2$, β3, $\beta_4$, $\beta_5$ are the model coefficients, ε is the error term, $P_t$ is the engine power at time t, and $\Delta P_t$ is the change in engine power at time t.

The performance of the model was evaluated by Smit through calculating the average coefficient of determination for $NO_x$ and $CO_2$/fuel which had $R^2$ values of 0.65 and 0.93, respectively. However, the model only predicts NOx neglecting the other emissions (HC and CO). The hazards and adverse effects of HC and CO will not be evaluated due to the estimation of $NO_x$ only.

### 2.4.3 Emission maps

Emission maps are look-up tables in the form of matrices. They consist of one dimension for speed ranges and another dimension representing acceleration or power values. For each emission species and vehicle category, instantaneous emission values are assigned to one cell of the matrix according to the corresponding instantaneous speed and acceleration. Emission maps have been used widely due to their simplicity (Cappiello, 2002).

**MODEM**

The MODEM microscopic emission database was developed as a part of the European Comission`s Drive II research program (Jost et al., 1992). The database is derived from testing 150 vehicles on 14 driving cycles based on different operating conditions in urban areas across Europe. The speed ranges were 0-90 km/h, and the product of vehicle and acceleration ranges between -15 and +15 ($m^2/s^3$).

On the other hand, the reliability of the models is affected by the sensitivity of the used driving cycles, which would lead to non-desirable results. Also, these maps are usually not flexible enough to incorporate factors such as road grade, accessory use, or historical effects (Cappiello, 2002).

### 2.4.4 MOVES

In 2010, the U.S. Environmental Protection Agency (EPA) released the MOtor Vehicle Emissions Simulator (MOVES) as its official automobile emissions model (Koupal et al., 2003). The MOVES model estimates vehicle emissions for mobile sources, covers a broad range of pollutants, and allows multiple scale analysis, including project levels. The latest version of MOVES is MOVES2014, which includes the benefits of the Tier 3 rule and NONROAD2008 model, which can estimate both on-road and non-road mobile sources within the MOVES platform. The framework of MOVES is established through four main functions, consisting of an activity generator, a source bin distribution generator, an operating mode distribution generator, and an emissions calculator. These steps are formulated mathematically by (EPA, 2012) as:

$$Total\ Emissions_{UseType} = Total\ Activity_{UseType} \times \sum_{n=1}^{Number\ of\ bins} Emission\ Rate_{UseType,Bin} \times BinDistributer_{UseType,Bin} \quad (2\text{-}13)$$

However, MOVES requires intensive data regarding the geometry of the road and the vehicle parameters which increases its complexity and make it not simple to be used. In addition, running the project level feature of MOVES is too slow for real-time emission modeling. Moreover, it requires an extensive database which needs time and money (Ahn et al., 2015).

## 2.5 SUMMARY

Microscopic Emission Models proved to be significant methods to evaluate the transportation operational-level projects' impact on the environment, which would achieve sustainable development within society. Some of the emission models are similar in concept, like POLY and VT-Micro, and others have evolved from each other, such as CMEM and EMIT. Also, as vehicle technology improves, the models could improve and diminish their shortcomings. However, all the models had both limitations and advantages, which would allow the user to choose among them regarding the compromises between the models and the availability of explanatory variables.

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# Chapter 3: Modeling Light Duty Vehicle Emissions Exploiting VT-CPFM Fuel Estimates

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## ABSTRACT

The Virginia Tech Comprehensive Power-based Fuel consumption Model (VT-CPFM) was designed with the intent of overcoming the limitations of state-of-the-practice models, which produce a bang-bang control system and cannot be calibrated using publicly available data. This paper extends the VT-CPFM to estimate vehicle emissions of hydrocarbons (HC), carbon monoxide (CO), and oxides of nitrogen ($NO_x$) using the estimated fuel consumption level as the sole explanatory variable. A cross validation method was implemented through calibration of the model for nine vehicles, including three light duty trucks and six light duty cars. The quality of fit for the HC and CO emissions was very good, with a coefficient of determination exceeding 0.92 on average for both emissions; however, the quality of fit for $NO_x$ emissions was lower, with a coefficient of determination of 0.80 on average. The proposed emission model produces approximately similar estimates compared to the VT-Micro model, but offers a simplified model, with a reduction in 32 required parameters for the former down to four for the latter. In addition, the model's parameters can be easily calibrated from publicly available data (e.g., speed and acceleration levels can be measured using non-engine instrumentation such as a global positioning system) and do not require any engine data to be collected by special devices. The simplicity of this newly designed model will save time and money.

## 3.1 INTRODUCTION

Air pollution is one of the biggest environmental challenges in the United States and is considered a major environmental threat. The transportation sector is a key player in this area as a result of the increase of cars on the road due to population growth and the correlated increase in car ownership. Specifically, transportation accounts for 67% of the total U.S. petroleum use, and, light-duty vehicles (LDVs) consume 59% of the U.S.'s transportation energy (Davis et al., 2014).

Though the figures in for the U.S. are notable, obviously the problem is also global, since transportation plays a significant role all over the world. The incomplete combustion of fuel from the transportation sector accounts for 70% to 90% of the total carbon monoxide (CO) emissions and results in 40% to 50% of total emissions of hydrocarbons (HC). In addition, of all oxides of nitrogen ($NO_x$) emissions, which are also a by-product of combustion, 45% to 50% are produced by the transportation sector (Rodrigue et al., 2013).

The Virginia Tech Transportation Institute (VTTI) designed the VT-CPFM as an instantaneous power based-model to estimate fuel consumption on the microscopic level (Rakha et al., 2011). VT-CPFM satisfies the requirements of predictive eco-cruise control systems, as it overcomes two major flaws of existing models—use of a bang-bang control system, and an inability to use publicly available data for calibration. Since it does not produce bang-bang control system which occurs because the partial derivative of the fuel consumption rate with respect to the engine torque is not a function of torque (Saerens et al., 2010). The bang-bang control system indicates that upon accelerating at full throttle to reduce acceleration time and deceleration using full braking will achieve the optimum fuel economy control. Which is obviously incorrect, since it requires aggressive driving, in-order to minimize fuel consumption rates (Rakha et al., 2011). Also, the VT-CPFM can be simply calibrated through use of accessible public data from vehicle manufacturers, unlike existing models (Rakha et al., 2011).

Although the VT-CPFM is capable of estimating vehicle fuel consumption levels accurately, prior to this study, it had not been used to estimate vehicle emissions, which is a critical part of studying climate change and environmental impacts of transportation systems. The estimation of emissions using this model could be of a higher level of accuracy compared to other state-of-the-practice models given the advantages of the VT-CPFM mentioned earlier. As such, this paper extends the VT-CPFM to model vehicle emissions of hydrocarbons (HC), carbon monoxide (CO) and oxides of nitrogen ($NO_x$). The developed model uses the VT-CPFM to estimate fuel rates and then uses those findings to estimates the resulting vehicle emissions.

This paper consists of five sections. The first section is a brief introduction to the project described herein. Section two describes the previously used models along with the VT-CPFM model, which overcomes previous shortcomings and was utilized to develop the proposed modeling approach. The third section describes the data used in constructing the proposed models and highlights how the proposed models were developed and why they were chosen from among other models. The fourth section demonstrates the results of estimated emissions along with validation results. This fourth section also compares the Virginia Tech microscopic energy and emission (VT-Micro) model for estimating emissions with the proposed approach in order to further validate and support the proposed method and to explore the differences between the two models. Finally, a summary of the paper's findings and the paper's conclusions are presented in the fifth section.

## 3.2 BACKGROUND

The proposed emission model described in this paper evolved from the VT-CPFM model, which estimates fuel consumption based on power, and overcomes two main deficiencies of current models: the use of bang-bang control and the inability to use public data for calibration (Rakha et al., 2011). The VT-CPFM estimates fuel consumption level depends on instantaneous power, which is based on the public data for the road and the vehicle to be calibrated. Although the model has been proven to predict accurate fuel level estimates, it has not previously been used to predict vehicle emissions.

The VT-Micro model was developed as a statistical model from experimentation using numerous polynomial combinations of speed and acceleration levels to construct a dual-regime model as expressed by equation (3-1) in (Rakha et al., 2004). These fuel consumption and emission models were developed using data that were collected on a chassis dynamometer at the Oak Ridge National Laboratory (ORNL), data gathered by the Environmental Protection Agency (EPA), and data gathered using an onboard emission measurement device (OBD). These data included fuel consumption and emission rate measurements (CO, HC, and $NO_x$) as a function of the vehicle's instantaneous speed and acceleration levels. The VT-Micro fuel consumption and emission rates were found to be highly accurate compared with the ORNL data, with coefficients of determination ($R^2$) ranging from 0.92 to 0.99 (Rakha et al., 2004).

$$MOE_e \begin{cases} e^{\sum_{i=0}^{3}\sum_{j=0}^{3}(L_{ij}^{e}\times u^i\times a^j)} & for\ a\geq 0 \\ e^{\sum_{i=0}^{3}\sum_{j=0}^{3}(M_{ij}^{e}\times u^i\times a^j)} & for\ a<0 \end{cases} \tag{3-1}$$

$MOE_e$: Measure of effectiveness for nstantaneous fuel consumption or emission rate (CO or HC or $NO_x$) (l/s or mg/s)
$L_{ij}^{e}$: Model regression coefficient for MOE "e" at speed power "i" and acceleration power "j" for positive accelerations
$M_{ij}^{e}$: Model regression coefficient for MOE "e" at speed power "i" and acceleration power "j" for negative
$u$: Instantaneous Speed (km/h)
$a$: Instantaneous acceleration (m/s$^2$)

Despite these capabilities, the VT-Micro requires the calibration of 32 coefficients, including the intercepts, which may overfit the data and be misleading in the results. Also, VT-Micro may underestimate the resulting emissions from a malfunctioning engine since it is not capable of considering a vehicle's operating conditions.
The Comprehensive Modal Emission Model (CMEM) is a power-demand based emission model that was developed at the University of California, Riverside. CMEM estimates the emissions of Light Duty Vehicles (LDVs) and Light Duty Trucks (LDTs) based on the vehicle's operating mode. Chassis dynamometer data were used to develop the model by measuring instantaneous engine out and tailpipe emissions for more than 300 vehicles (automobiles and light trucks) that were tested on three driving cycles: FTP, US06 and Modal Emission Cycle (MEC) (Barth et al., 2000). The CMEM model is based on a parameterized physical approach that is related to the physical conditions of vehicle operation and emission productions. It is composed of six modules: engine power, engine speed, air/fuel ratio, fuel use, engine-out emissions, and catalyst pass fraction

(Barth et al., 2000). Inputs to the model are related to the vehicle and operation variables of the environment, including, for instance, the vehicle speed, acceleration and grade that should be entered at a second-by-second level (Barth et al., 2000).

The drawback of this model's physical approach is its increased complexity. In addition, the model is data intensive, which means that physical variables must be collected and/or measured. Also, the data is not publicly available, which increases the difficulty of incorporating the data from many sources and requires recalibration for each data set (Scora et al., 2006). Moreover, CMEM may produce a bang-bang type control system.

In 2010, the U.S. Environmental Protection Agency (EPA) released the Motor Vehicle Emissions Simulator (MOVES) as its official automobile emission model (Koupal et al., 2003). The MOVES model estimates vehicle emissions for mobile sources, covers a broad range of pollutants, and allows multiple scale analysis, including project levels. The latest version of MOVES is MOVES2014 which includes the benefits of the Tier 3 rule and the NONROAD2008 model, which can estimate both on-road and non-road mobile sources within the MOVES platform. The framework of MOVES is established through four main functions consisting of an activity generator, a source bin distribution generator, an operating mode distribution generator, and an emissions calculator. These steps are formulated mathematically by (EPA, 2012) in equation (3-2) as:

$$Total\ Emissions_{UseType} = Total\ Activity_{UseType} \times \sum_{n=1}^{Number\ of\ bins} Emission\ Rate_{UseType,Bin} \times BinDistributer_{UseType,Bin} \quad (3\text{-}2)$$

However, technical difficulties prevent MOVES from generating a result that provides second-by-second energy and emission rates for all individual vehicles within large transportation networks, and running the project level feature of MOVES is too slow for real-time emission modeling. Moreover, it requires an extensive database to run (Ahn et al., 2015).

VT-CPFM is a microscopic fuel consumption model based on instantaneous vehicle power, which Rakha et al. developed to overcome the major defect for most of the models, which is the bang-bang control through quadratic function of power. Also, the model uses publicly available data for calibration, eliminating the need for extensive data collection (Rakha et al., 2011).

The power at instant t is developed by (Wong, 2001) in equation (3-3):

$$P(t) = \left(\frac{R(t) + 1.04\ ma(t)}{3600\eta_d}\right) v(t) \quad (3\text{-}3)$$

Here $P(t)$ is the power exerted by the vehicle driveline (kW) at time $t$, $R(t)$ is the resistance force (N) at time $t$, $m$ is the vehicle mass(kg), a(t) is the vehicle acceleration (m/s$^2$) at time $t$, $v(t)$ is the vehicle speed (km/h) at time $t$ and $\eta_d$ is the driveline efficiency.

The resistance force is computed through combining aerodynamic, rolling, and grade resistance forces using equation (3-4):

$$R(t) = \frac{\rho}{25.92} C_D C_h A_f v(t)^2 + 9.8066\ m\ \frac{C_r}{1000}(c_1 v(t) + c_2) + 9.8066 mG(t) \quad (3\text{-}4)$$

Where $\rho$ is the density of air at sea level at temperature 15°C (59°F) (equal to 1.2256 kg/m$^3$); $C_D$ is the vehicle drag coefficient (unitless); $C_h$ is a correction factor for altitude (unitless) and calculated as 1-0.085 H where H is the altitude (km); $A_f$ is the vehicle frontal area (m$^2$); and $C_r$, $c_1$ and $c_2$ are rolling resistance parameters that depend on the road surface type, road condition, and vehicle tire type.

The VT-CPFM framework is a dual regime model to estimate instantaneous fuel whether power is greater or equal to zero or at negative power. The structure of the model is formulated by (Rakha et al., 2011) as expressed in equation (3-5):

$$FC(t) = \begin{cases} \alpha_0 + \alpha_1 P(t) + \alpha_2 P(t)^2 & \forall\, P(t) \geq 0 \\ \alpha_0 & \forall\, P(t) < 0 \end{cases} \tag{3-5}$$

Where FC (t) is the instantaneous estimated fuel consumption (l/s) and $\alpha_0$, $\alpha_1$ and $\alpha_2$ are the calibrated coefficients for each specific vehicle.

## 3.3 MATERIAL AND METHODS

### 3.3.1 Data

The emission models were generated from the regression analysis of data from nine normally emitting vehicles. Data were collected at Oak Ridge National Laboratory (ORNL) from six LDVs and three LDTs. Table 3-1 represents these vehicles in terms of engine displacement, vehicle curb weight, and vehicle type (West et al., 1997). In addition, the average engine size was 3.1 L, the average number of cylinders was 5.6, and the average curb weight was 3,219 lbs. (1,460 kg) (West et al., 1997).

The data were gathered from the tested vehicles driven in the field in two opposite directions on the same road, in order to verify their maximum operating boundaries and minimize the grade and wind effects if they were present. Moreover, the testing was never performed under windy, rainy, or snowy conditions (West et al., 1997).

A chassis dynamometer was used to model the vehicle loadings for the measurement of vehicle emission rates for each vehicle in the laboratory within the attainable speed and acceleration range of each vehicle (West et al., 1997). The gathered emission data were hydrocarbon (HC), carbon monoxide (CO) and oxides of nitrogen ($NO_x$). Data sets of speed, acceleration, emission rates, and fuel consumption were generated.

For each vehicle there were between 1,300 and 1,600 individual measurements, where vehicle speeds ranged from 0-121 km/h (0 to 110 ft/s) at increments of 1 km/h, and vehicle acceleration measurements ranged from -1.5 to 3.7 m/s$^2$ (-5 to 12 ft/s$^2$) at increments of 0.3 m/s$^2$. Emissions g/s (mg/s) and fuel consumption l/s (gal/h) for each acceleration and speed measurement were also collected (Ahn, et al., 2002).

**TABLE 3-1 ORNL Test Vehicle Characteristics**

| Year | Make/Model | Engine PFI= Port Fuel Injection TBI= Throttle Body Injection | Transmission M= Manual, L= Automatic with Lockup | Curb Weight kg |
|---|---|---|---|---|
| 1988 | Chevrolet Corsica | 2.8 L pushrod V6, PFI | M5 | 1209 |
| 1994 | Oldsmobile Cutlass Supreme | 3.4 L DOHC V6, PFI | L4 | 1492 |
| 1994 | Oldsmobile Eighty Eight | 3.8 L pushrod V6, PFI | L4 | 1524 |
| 1995 | Geo Prizm | 1.6 L OHC 14, PFI | L3 | 1116 |
| 1993 | Subaru Legacy | 2.2 L DOHC flat 4, PFI | L4 | 1270 |
| 1997 | Toyota Celica | 1.8 L DOHC 14, PFI | L4 | 1143 |
| 1994 | Mercury Villager Van | 3.0 L pushrod V6, PFI | L4 | 1823 |
| 1994 | Jeep Grand Cherokee | 4.0 L pushrod 16, PFI | L4 | 1733 |
| 1994 | Chevrolet Silverado | 5.7 L pushrod V8, TBI | L4 | 1823 |

### 3.3.2 Proposed Models

This paper describes an enhanced VT-CPFM model to estimate emission levels produced from LDVs. The main emphasis is the development of a reliable and simple emissions estimation model, evolved from the VT-CPFM, which uses publicly available data to calibrate parameters and does not result in a bang-bang control system.

A variety of proposed models underwent calibration and validation procedures before we settled on the final model. The models varied between linear, quadratic, cubic, logarithm and exponential functions. The main intention was to develop a robust model that does not generate negative emissions. Accordingly, the broad spectrum of proposed models was quickly narrowed to only five model options: linear, Gaussian, squared root, log, and power.

Model 1: Linear

$$Emission = a.F(t)$$

Model 2: Log

$$Log\ (Emission(t)) = constant + F(t) + F(t)^2 + F(t)^3$$

Model 3: Gaussian

$$E(t) = a.exp - \left(\frac{(F(t) - b)}{c}\right)^2$$

Model 4: Power

$$E(t) = aF(t)^b$$

Model 5: Square Root

$$\sqrt{E(t)} = constant + a.F(t) + b.F(t)^2 + F(t)^3$$

$$\sqrt{E(t)} = constant + v(t) + F(t) + v(t).F(t) + F(t)^2 + F(t)^3 + v(t).F(t)^2 + v(t).F(t)^3$$

$v(t)$= speed of the vehicle at time t.

$F(t)$= estimated fuel from VT-CPFM model at time t.

$E(t)$= CO or HC or $NO_x$ at time t.

$a, b\ and\ c$: Model regression coefficients.

The square root model was ultimately chosen as the best option to satisfy the criteria and the main objective. The square root model is simple due to the low number of coefficients and the straightforward framework. The coefficient of determination was used to test the reliability of the model and the estimated emissions were highly correlated with ORNL in-field measurements. Moreover, the model did not result in any negative emissions, which ensures its reliability. The model also consists of only one scenario to capture various operating conditions by incorporating the positive and negative acceleration and power terms, which highlights its simplicity and simultaneous ability to maintain the robustness of the model implied by the $R^2$ of each emission.

Statistical tools, including stepwise regression, were applied to verify the selected parameters in the model. Power-based and statistical models were integrated, allowing the model to take advantage of the benefits of both. Results showed that VT-CPFM fuel estimates were highly significant in calculating the emission levels. Including the speed parameter slightly elevated the $R^2$ of the model, albeit only at a barely noticeable rate, ranging between 2–2.5%. The benefit of excluding this parameter is that it will allow the model to maintain a greater simplicity and assist in future model generalization. Furthermore, including acceleration and speed parameters may result in multicollinearity between the independent variables. Similarly, inclusion of other parameters may result in a large increase of coefficients, making the model more complex or slightly increasing collinearity, resulting in regression overfitting.

The ORNL data underwent calibration and validation procedures via the k-fold cross validation method. The k-fold cross validation method divides the dataset into k subsets. At each iteration, one of the k subsets serves as the test set and the rest of the subsets execute the training procedure. This method was applied to CO, HC and $NO_x$ data for each vehicle where the average coefficients and coefficient of determination were calculated.

The estimated fuel consumption results from VT-CPFM were first tested against the measured fuel to find the coefficient of determination. Subsequently, the instantaneous estimated fuel consumption result was introduced in each model as the main parameter.

The resulting slope and $R^2$ for each vehicle were generated from linear regression between measured fuel and estimated fuel. All the vehicles had very good fit, with $R^2$ above 0.9 as shown in Table 3-2. The predicted emission levels were processed by utilizing the estimated fuel from the VT-CPFM model after the calibration for each vehicle.

**TABLE 3-2 Results of Estimated Fuel from VT-CPFM**

| Make/Model | Slope | $R^2$ |
|---|---|---|
| Chevrolet Corsica | 1.2 | 0.95 |
| Oldsmobile Cutlass Supreme | 0.92 | 0.93 |
| Oldsmobile Eighty Eight | 1.2 | 0.91 |
| Geo Prizm | 1.4 | 0.89 |
| Subaru Legacy | 1.3 | 0.9 |
| Toyota Celica | 1.2 | 0.95 |
| Mercury Villager Van | 1.29 | 0.9 |
| Jeep Grand Cherokee | 1.5 | 0.94 |
| Chevrolet Silverado | 1.6 | 0.95 |

## 3.4 RESULTS

Figure 3-1 illustrates the significant relationship between fuel consumption and emissions, showing that emissions follow the same behavior as fuel consumption. HC and CO emissions have a direct relationship with fuel consumption—as fuel consumption increases, emissions increase accordingly. This relationship is explained by the fact that HC and CO are the main components of gasoline, which consists of approximately 85% carbon and 15% hydrogen by mass. The proposed model strongly fits the dataset for CO, HC and $NO_x$ relatively. As expected, the highest levels of fuel consumption correspond to the highest levels of HC and CO emissions; this is a result of fuel enrichment at these high levels. Furthermore, $NO_x$ emissions follow a general trend of increasing as they move towards a stoichiometric ratio where they reach a peak level then decrease afterwards during fuel enrichment. The aforementioned results make it evident that vehicle emissions directly relate to fuel consumption levels. Also notable is the significant relation of the fitted model to the emissions data. In addition, the model is consistent with CO, HC and $NO_x$ since it maintains the same structure, using the same number of parameters and coefficients.

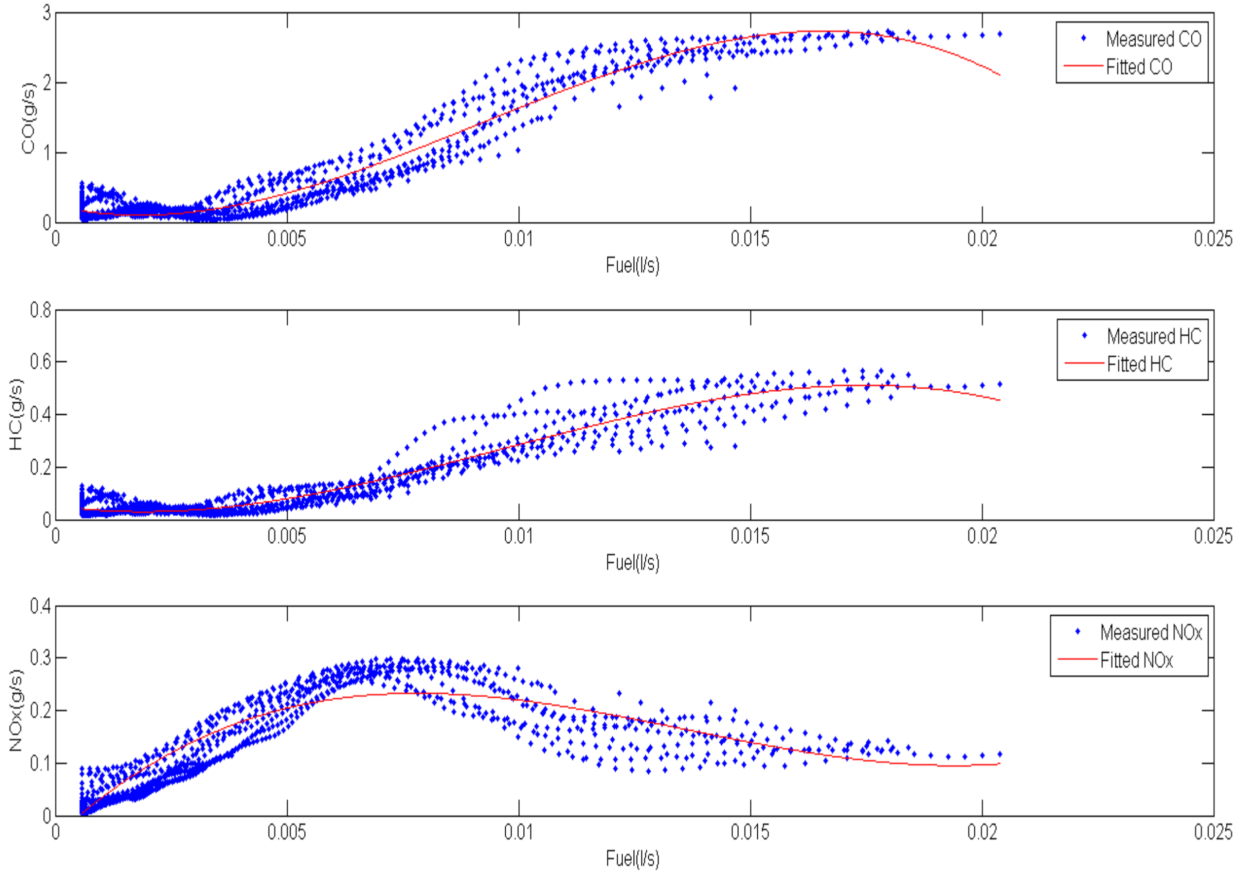



**Figure 3-1 Fitting the Model to Oldsmobile Eighty Eight Emission Data**

Regression analysis was implemented on the nine vehicles in the study to investigate the model's performance in estimating emissions. Table 3-3 demonstrates the coefficient of determination ($R^2$) for each vehicle's emissions. The model showed a good fit for CO and HC, both when using the speed parameter and when excluding it. $NO_x$ also had a relatively good fit for the model both with and without the speed parameters ($R^2$=0.802 and 0.828 respectively), as shown in Table 3-4. Table 3-4 also summarizes the average $R^2$ for CO and HC values, showing that including speed parameters ($R^2$ = 0.923 and 0.921 respectively) resulted in a slightly better fit than not using the speed parameters ($R^2$= 0.944 and 0.942 respectively). As these results show, there is only a slight increase in $R^2$ between the simpler model, which does not use the speed parameter, and the model that includes the speed parameter, indicating the negligible effect of speed on the model. Table 3-5 and Table 3-6 summarize sample model coefficients for estimating CO, HC and $NO_x$ rates for the Oldsmobile Eighty-Eight.

**TABLE 3-3 Coefficient of determination according to adding or excluding speed variable**

| Make/Model | Without Speed parameter | | | With Speed parameter | | |
|---|---|---|---|---|---|---|
| | CO | HC | NOx | CO | HC | NOx |
| Toyota Celica | 0.917 | 0.913 | 0.538 | 0.929 | 0.931 | 0.591 |
| Geo Prizm | 0.936 | 0.933 | 0.886 | 0.960 | 0.961 | 0.890 |
| Subaru Legacy | 0.939 | 0.939 | 0.837 | 0.957 | 0.960 | 0.841 |
| Chevrolet Corsica | 0.924 | 0.904 | 0.627 | 0.957 | 0.935 | 0.677 |
| Oldsmobile Eighty Eight | 0.950 | 0.922 | 0.895 | 0.958 | 0.936 | 0.902 |
| Oldsmobile Cutlass Supreme | 0.941 | 0.949 | 0.808 | 0.956 | 0.955 | 0.863 |
| Mercury Villager Van | 0.867 | 0.878 | 0.737 | 0.914 | 0.916 | 0.762 |
| Jeep Grand Cherokee | 0.942 | 0.956 | 0.930 | 0.952 | 0.963 | 0.951 |
| Chevrolet Silverado | 0.889 | 0.897 | 0.962 | 0.910 | 0.921 | 0.973 |

**TABLE 3-4 Regression Model Comparison**

| Model | CO | HC | NOx |
|---|---|---|---|
| With Speed | 0.923 | 0.921 | 0.802 |
| Without Speed | 0.944 | 0.942 | 0.828 |

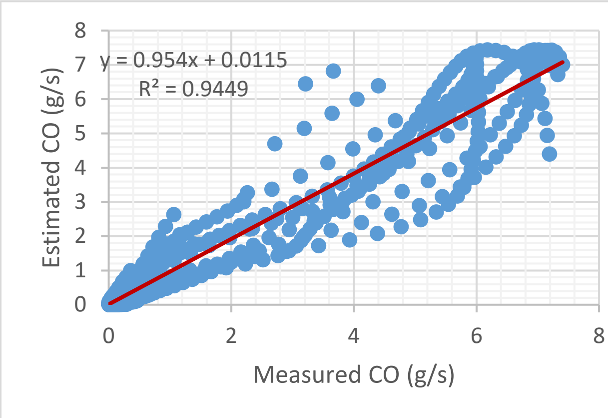
The performance of the model was further evaluated by comparing the instantaneous emission estimates to in-field measurements to examine their relationship and behavior. Figure 3-2 illustrates the fitted regression to the scattered data points used to estimate $R^2$. The predicted emission levels were highly correlated with the in-field measured data. Moreover, the $R^2$ values were approximately the same when the speed parameter was added and when only the fuel parameter was used. The two models follow similar trends for each emission, which implies that introducing the speed parameter into the model will produce approximately the same emission estimates based on fuel consumption.

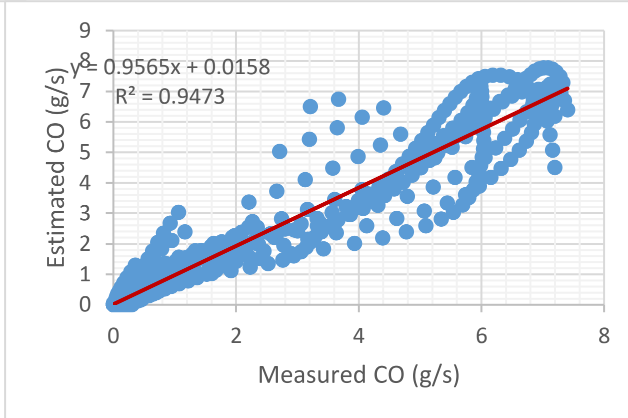
**TABLE 3-5 Sample Coefficients for Oldsmobile Eighty Eight Emissions (with speed parameters)**

| Old | Constant | $v$ | $F$ | $v.F$ | $F^2$ | $v.F^2$ | $F^3$ | $v.F^3$ |
|---|---|---|---|---|---|---|---|---|
| CO | 0.092 | 0.003 | -70.712 | -1.888 | 42790.00 | 141.752 | -1.80E+06 | -1727.70 |
| HC | 0.014 | 0.001 | 4.008 | -0.549 | 3505.80 | 74.384 | -1.55E+05 | -2205.30 |
| NOx | -0.0505 | 2.20E-04 | 89.4688 | -0.2207 | -7661.00 | 21.5654 | 1.50E+05 | -282.71 |

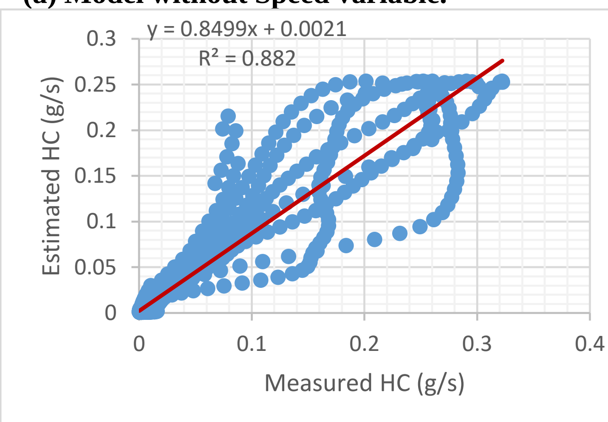
**TABLE 3-6 Sample Coefficients for Oldsmobile Eighty Eight Emissions (without speed parameters)**

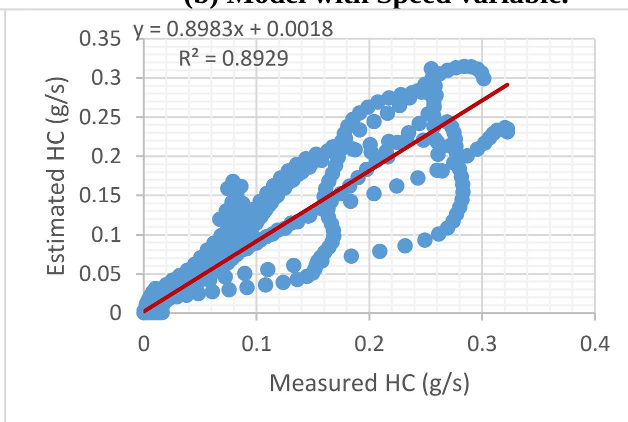
| Old | Constant | $F$ | $F^2$ | $F^3$ |
|---|---|---|---|---|
| CO | 0.234 | -150.551 | 45499.00 | -1.65E+06 |
| HC | 0.053 | -25.599 | 7430.80 | -2.56E+05 |
| NOx | -0.040 | 80.696 | -7237.90 | 1.77E+05 |



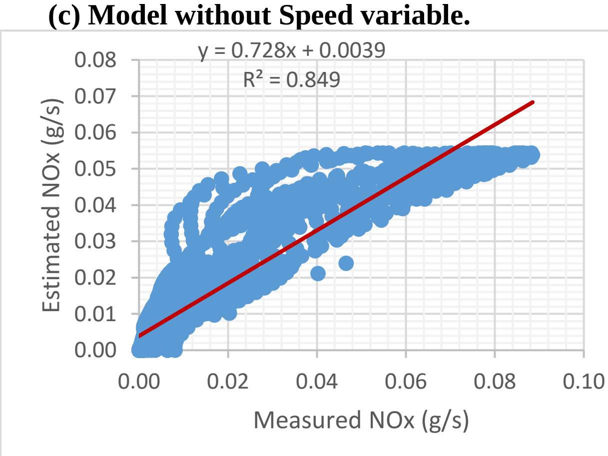



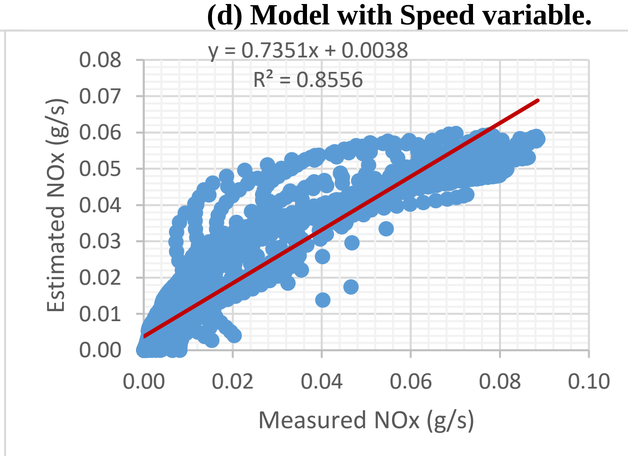

**(a) Model without Speed variable.** **(b) Model with Speed variable.**




**(c) Model without Speed variable.** **(d) Model with Speed variable.**




**(e) Model without Speed variable.** **(f) Model with Speed variable.**

**Figure 3-2 Correlation between Measured estimated emission rates (Oldsmobile Eighty Eight)**

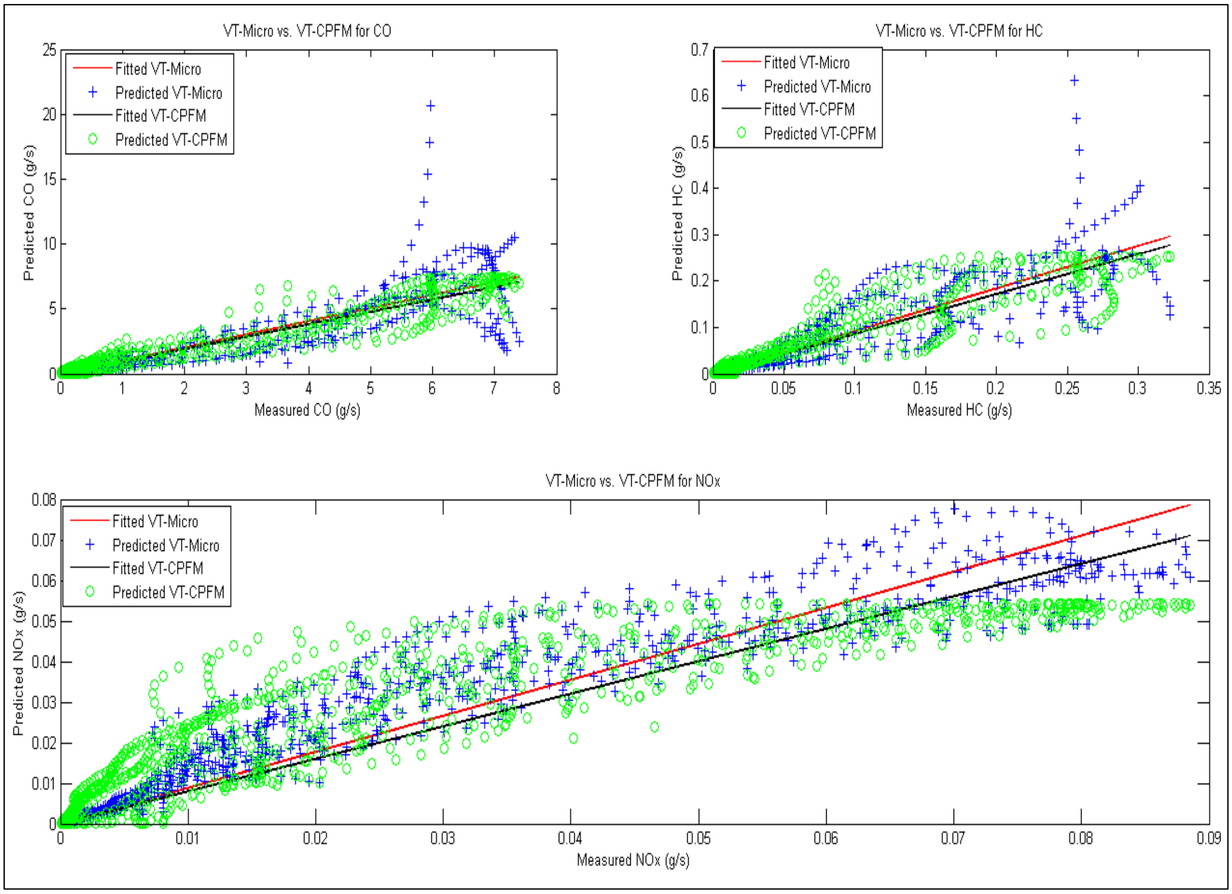



**FIGURE 3-3 VT-Micro Vs. VT-CPFM**

Moreover, the performance of the model was further evaluated by comparing its estimates to the VT-Micro model. Figure 3-3 demonstrates the correlation between a sample of the Oldsmobile Eighty-Eight's instantaneous in-field measurements and estimated emissions from VT-Micro and VT-CPFM models. Figure 3-3 shows, the VT-CPFM emission model follows the same trend in predicting the emissions. The fitted regression lines for both models reveal the goodness of fit of the resulting estimates. VT-CPFM had a better fit for CO compared to VT-Micro for the Oldsmobile Eighty-Eight ($R^2 = 0.945$ and 0.82 respectively) as well as better estimates for HC ($R^2 = 0.882$ and 0.84 respectively). However, VT-Micro estimated $NO_x$ with a higher $R^2$ of 0.922 compared to the VT-CPFM model's $R^2$ of 0.85. Note, though, that VT-Micro utilizes 32 coefficients incorporated within two boundary conditions to predict emission levels as compared to the VT-CPFM model, which uses only four calibrated coefficients at approximately the same level of accuracy. From these results, we can conclude that, overall, VT-CPFM returns good regression fit results for HC and CO over $NO_x$, which affirms the applicability of the VT-CPFM model to estimate emissions alongside fuel consumption.

The performance of the model was further investigated by calculating the mean absolute percentage error (MAPE) for the 9 vehicles for 16 driving cycles. Table 3-7 illustrates the error in trip emissions across 16 driving cycles for CO, HC and $NO_x$. Specifically, the error did not exceed 16.5% for almost the 16 driving cycles.

**Table 3-7 Error in Trip Emissions**

| Driving Cycle | Error (%) | | |
|---|---|---|---|
| | CO | HC | NOx |
| The City Test (LA04) | 9.80% | 10.35% | 10.76% |
| Arterial LOS A (ARTA) | 6.55% | 8.90% | 14.44% |
| Arterial LOS C (ARTC) | 10.28% | 10.33% | 12.70% |
| Arterial LOS E (ARTE) | 13.49% | 11.35% | 15.14% |
| Freeway High Speed (FWYSP) | 8.57% | 8.51% | 20.23% |
| Freeway LOS A (FWYA) | 9.15% | 7.48% | 16.50% |
| Freeway LOS D (FWYD) | 7.04% | 6.27% | 16.46% |
| Freeway LOS E (FWYE) | 5.17% | 6.70% | 11.20% |
| Freeway LOS F (FWYF) | 5.25% | 9.54% | 9.00% |
| Freeway LOS G (FWYG) | 13.73% | 11.94% | 10.26% |
| Local (LOCL) | 12.26% | 10.10% | 11.19% |
| RAMP | 5.17% | 2.41% | 8.68% |
| ST01 | 6.42% | 8.50% | 10.95% |
| AREA | 7.54% | 7.35% | 11.49% |
| LA92 | 4.23% | 4.06% | 8.19% |
| New York Cycle (NYC) | 5.55% | 6.61% | 15.65% |
| Average | 8.14% | 8.15% | 12.68% |

## 3.5 CONCLUSIONS

This paper discusses the enhancement of the VT-CPFM model to capture CO, HC and $NO_x$ emissions based on instantaneous fuel estimates as an explanatory variable. The model was applied to nine light duty vehicles consisting of three light duty trucks and six light duty cars. Regression analysis was implemented to evaluate the performance of the model. HC and CO had very good fit with an $R^2$ value exceeding 0.92, and were highly correlated against the in-field measured data. The model estimated $NO_x$ with a lower accuracy than HC and CO, but still had a relatively good fit at $R^2 = 0.802$. The performance of the model was further validated by comparing its estimation results to VT-Micro estimates, with results showing approximately similar fits.

The proposed model is advantageous in that it can be easily calibrated using publicly available data, obviating the need for extensive data use and reducing complexity. Furthermore VT-CPFM will be a valuable addition to exiting emissions models as a result of its reliability and simplicity, which will save time and money when predicting emissions.

**ACKNOWLEDGEMENTS**

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# Chapter 4: HEAVY DUTY DIESEL TRUCK EMISSION MODELING

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## ABSTRACT

Heavy-duty vehicles (HDVs) are the second largest source of greenhouse gas (GHG) emissions and energy use within the transportation sector even though they represent only a small portion of on-road vehicles. Heavy-duty diesel vehicles (HDDVs) emit around half of on-road nitrogen oxide ($NO_x$) emissions. However, due to the limited amount of HDDV emissions data, research has focused on light-duty vehicle (LDV) emissions. The majority of these microscopic models suffer from two major limitations: they result in a bang-bang control system and the calibration of the model parameters is not possible using publicly available data. This paper proposes to extend the Virginia Tech Comprehensive Power-Based Fuel consumption Model (VT-CPFM) to overcome the two shortcomings in state-of-the-practice HDDV emission models of carbon monoxide (CO), hydrocarbons (HCs), and nitrogen oxides ($NO_x$). The University of California Riverside heavy-duty diesel truck (HDDT) data were used for the calibration and validation processes. The results were satisfying, especially for $NO_x$, which is the main concern in HDDV emissions. Model validity and performance were evaluated by comparing the correlation of measured field data and estimated emissions between VT-CPFM and the Comprehensive Modal Emissions Model (CMEM). The results demonstrate the efficacy of VT-CPFM in replicating empirical observations producing better accuracy compared to other state-of-the-practice models (e.g. CMEM). Moreover, unlike CMEM, which requires extensive data collection for calibration purposes, the VT-CPFM only needs Global Positioning System (GPS) and publically accessible data for calibration.



*Keywords*: Diesel engine, microscopic emission modeling, Virginia Tech Comprehensive Power Based Fuel Consumption Model (VT-CPFM)

## 4.1 INTRODUCTION

In 2011, NHTSA and the EPA jointly declared federal regulations and standards to reduce the fuel consumption and greenhouse gas (GHG) emissions of heavy-duty vehicles (HDVs) (The white House, 2016). Although HDVs were only 4% of registered vehicles in 2010, they accounted for approximately 25% of on-road energy use and GHG emissions (The white House, 2016) and approximately 6% of total U.S. GHG emissions (EPA, 2011). More narrowly, heavy duty diesel vehicles (HDDVs) produce around 50 percent of on-road $NO_x$ emissions (Yanowitz et al., 2000). HDVs are the second largest source for GHG emissions and energy use within the transportation sector and are expected to exceed the level of emissions from passenger vehicles by 2030 globally (EPA, 2015). Moreover, an average passenger car's original purchase price is similar to the lifetime fuel cost for this vehicle, but the lifetime fuel of HDVs costs are around five times that of the original purchase price for the vehicle (EPA, 2009).

Transportation consumes about 72% of the total U.S. domestic oil use. HDVs are responsible for 17% of the transportation oil use and 12% of all U.S. oil consumption (EPA, 2011). In 2013, 2.7 million barrels of oil-derived fuels per day were consumed by the on-road truck fleet, which emitted 530 million metric tons of carbon pollution (NRDC, 2014).

Despite the extent of HDV emissions, because light-duty vehicles (LDVs) greatly outnumber HDVs, transportation researchers and engineers have focused more on modeling fuel consumption and emissions for LDVs. Consequently, HDV vehicle emission models are less developed than their LDV counterparts due to the limited amount of HDDV emissions data available compared with LDVs (Barth et al., 2004).

Fuel consumption and emission models play a vital role in evaluating GHG reduction plans because they inform the actions of decision makers, and accurate estimations of HDV emissions are needed. This paper addresses that need by extending the Virginia Tech Comprehensive Power-Based Fuel Consumption Model (VT-CPFM) to estimate HDDV emissions for nitrogen oxides ($NO_{x)}$, carbon monoxide (CO), and hydrocarbons (HC) using readily available data.

## 4.2 BACKGROUND

Various microscopic models have been developed to estimate the fuel consumption and emissions of HDVs. One of the models that is considered to be reliable in its estimates is MOVES (EPA, 2009). MOVES covers a broad range of pollutants for mobile sources and allows multiple scale analysis (Koupal et al., 2003). However, MOVES is too slow for real-time emission modeling for a project-level feature and requires an extensive database to run (Ahn and Rakha, 2015).

The Comprehensive Modal Emissions Model (CMEM) is based on a parameterized physical approach that is related to the physical conditions of vehicle operation and emission production. It is composed of six modules: engine power, engine speed, air/fuel ratio, fuel use, engine-out emissions, and catalyst pass fraction. The model estimates emission rates under different vehicle operating conditions (stoichiometric, cold-start, enrichment, and enleanment conditions) (Barth et al., 2000).

CMEM estimates second-by-second tailpipe emissions as the product of fuel rate (FR), engine-out emission index ($g_{emission}/g_{fuel}$), and catalyst pass fraction (CPF) using Equation (4-1) (Barth et al., 2000):

$$Tailpipe\ emissions = FR\ \times \left(\frac{g_{emission}}{g_{fuel}}\right) \times CPF \qquad (4\text{-}1)$$

The CPF for all heavy-duty diesel trucks (HDDTs) is considered to be 100% (Barth et al., 2004). FR is estimated as shown in Equation (4-2):

$$FR = \left(K.N.V + \frac{P}{\eta}\right)\frac{1}{43.2}.[1 + b_1.(N - N_0)^2] \qquad (4\text{-}2)$$

where

$FR$ is the fuel use rate (g/s),

$P$ is the engine power output (kW),

$K$ is the engine friction factor,

$N$ is the engine speed (revolutions per second),

$V$ is the engine displacement (L),

$\eta$ is measure of indicated efficiency for diesel engines (0.45),

$b_1$ is $10^{-4}$, and

43.2 kJ/g is the lower heating value of typical diesel fuel.

The engine out emissions for CO, HC, and $NO_x$ are modeled according to the following linear equation as shown in Equation (4-3), with $a$ and $r$ as equation coefficients:

$$Engine\ out = a.FR + r \qquad (4\text{-}3)$$

However, the physical approach used by CMEM increases its complexity and may not be simple. The model is data intensive and requires physical variables to be collected and measured. The data required are not publicly available, which increases the difficulty of incorporating data from many sources and requires recalibration for each data set, which costs time and money (Scora and Barth, 2006). Furthermore, as long as the same amount of power is applied, CMEM will estimate the same emission level regardless of whether the vehicle is driving at a high or low speed or on a flat or steep road. CMEM may also produce a bang-bang type control system, which occurs because the partial derivative of the fuel consumption rate with respect to the engine torque is not a function of torque (Saerens et al., 2010). The bang-bang control system relies upon accelerating at full-throttle to reduce acceleration time and braking at full deceleration to achieve optimum fuel economy control, which is obviously incorrect since it requires aggressive driving in order to minimize fuel consumption rates (Rakha et al., 2011).

VT-Micro is a regression-based model that mainly depends on the instantaneous velocity and acceleration of the vehicle (Rakha et al., 2004). It overcomes the bang-bang control problem but requires the calibration of 32 coefficients, including the intercepts, which costs time. Also, it may overfit the data and be misleading in its estimates.

VT-CPFM is a microscopic fuel consumption model based on instantaneous vehicle power, which Rakha et al. developed to overcome the major defect for most models, which is the bang-bang control system resulting from the quadratic function of power. The model uses publicly accessible data for calibration (Rakha et al., 2011).

The power at instant *t* is shown in Equation (4-4) (Wong, 2001):

$$P(t) = \left(\frac{R(t)+1.04\, ma(t)}{3600\eta_d}\right) v(t) \tag{4-4}$$

where

*P(t)* is the power exerted by the vehicle driveline (kW) at time *t*,
*R(t)* is the resistance force (N) at time *t*,
*m* is the vehicle mass (kg),
*a(t)* is the vehicle acceleration (m/s$^2$) at time *t*,
*v(t)* is the vehicle speed (km/h) at time *t*, and
$\eta_d$ is the driveline efficiency.

The resistance force is computed by combining aerodynamic, rolling, and grade resistance forces:

$$R(t) = \frac{\rho}{25.92}\, C_D C_h A_f v(t)^2 + 9.8066\, m\, \frac{C_r}{1000}(c_1 v(t) + c_2) + 9.8066 m G(t) \tag{4-5}$$

Where

$\rho$ is the density of air at sea level at temperature 15°C (59°F) (equal to 1.2256 kg/m$^3$),
$C_D$ is the vehicle drag coefficient (unitless),
$C_h$ is a correction factor for altitude (unitless) and calculated as $1 - 0.085H$, where $H$ is the altitude (km),
$A_f$ is the vehicle frontal area (m$^2$), and

$C_r$, $c_1$, and $c_2$ are rolling resistance parameters that depend on the road surface type, road condition, and vehicle tire type. Vehicle coefficient values can be retrieved from (Rakha et al., 2001).

The VT-CPFM framework as shown in Equation 6 is a dual regime model to estimate instantaneous fuel consumption based on whether power is greater than or equal to zero or negative. The structure of the model is expressed in Equation (4-6) (Rakha et al., 2011):

$$FC(t) = \begin{cases} \alpha_0 + \alpha_1 P(t) + \alpha_2 P(t)^2 & \forall\, P(t) \geq 0 \\ \alpha_0 & \forall\, P(t) < 0 \end{cases} \tag{4-6}$$

Where $FC(t)$ is the instantaneous estimated fuel consumption (L/s) and $\alpha_0$, $\alpha_1$, and $\alpha_2$ are the calibrated coefficients for each specific vehicle.

Given the complexities of MOVES, CMEM, and VT-Micro, this paper applies the VT-CPFM model to capture the instantaneous HDDT vehicle emissions for CO, HC, and $NO_X$. The advantages of VT-CPFM for this purpose are that it overcomes the bang-bang control problem and that publicly available data can be used for model calibration. Because VT-CPFM requires only eight coefficients and two primary inputs, speed and fuel, it is also easier to implement.

### 4.3 DATA

The data used to calibrate and validate the proposed extension to the VT-CPFM model were provided by The University of California, Riverside (Barth et al., 2004). Data from eight HDDVs were used in this study (Table 4-1). Vehicles were recruited randomly within test categories by engine and model year. A balance between different horsepower and between manufacturers was attempted (Barth et al., 2004).

**TABLE 4-1 University of California, Riverside, Test Vehicle Characteristics**

| Test Vehicle ID Number | Make/ Model | Truck Year | Odometer (mi) | Engine Make | Engine Model | Engine Year | Rated Power (hp) | Engine Size (L) |
|---|---|---|---|---|---|---|---|---|
| HDDT 1 | Freightliner/FLD 120 | 2001 | 8,000 | CAT | C-15 | 2000 | 475 | 14.6 |
| HDDT 2 | International/ 9800 SBA | 1997 | 442,674 | Cummins | M11-330 | 1997 | 330 | 10.8 |
| HDDT 3 | Freightliner/ D120 | 1997 | 545,700 | DDC | C-60 | 1996 | 360/400 | 12.7 |
| HDDT 4 | Freightliner/ D120 | 1997 | 512,786 | Cummins | N14 | 1997 | 370/435 | 14 |
| HDDT 5 | Freightliner/ C-120 | 1997 | 353,953 | Cummins | N14 | 1997 | 370/435 | 14 |
| HDDT 6 | Freightliner/ C-120 | 1998 | 449,404 | DDC | C-60 | 1997 | 370/430 | 12.7 |
| HDDT 7 | Freightliner/ FDL 120 | 1999 | 489,310 | DDC | C-60 | 1998 | 470 | 12.7 |
| HDDT 8 | Freightliner/ FDL 120 | 1999 | 469,801 | DDC | C-60 | 1998 | 360 | 12.7 |

The University of California, Riverside, Center for Environmental Research and Technology tested the recruited vehicles using their Mobile Emissions Research Laboratory (MERL). MERL was developed to measure on-road, real-world emissions accurately and reliably (Barth et al., 2004). The laboratory weighs approximately 45,000 lb and serves as the truck's load. It contains all the instrumentation normally found in a conventional vehicle emissions laboratory.

The tested vehicles used fuel from the same source to ensure consistency. The testing was conducted on long and uninterrupted stretches of roadways in California's Coachella Valley at zero grade, approximately at sea level (Barth et al., 2004). The testing procedure for each truck measured the fuel rate, CO, HC, $NO_x$, velocity, engine speed, and elevation. A total of 238,893 seconds of data were collected and recorded at a 1-Hz frequency.

The scattering of emissions data was the primary check to reveal if any of the data were invalid. CO data for Vehicle 5 were out of the normal range of the other vehicles by more than 10 times the normal value. The HC data for Vehicle 8 had too many negative values, which prevented the model from undergoing the calibration and validation processes for this vehicle due to the insufficient remaining data points.

However, the model does not estimate particulate matter (PM) because PM data were not available to develop models. PM is dependent on vehicle operating conditions. Also, it can be a function of vehicle parameters and emission rates of CO and HC.

## 4.4 METHODOLOGY

This study proposes to extend the VT-CPFM to estimate emission levels for HDDVs. The main focus is to develop a simple and accurate model to overcome the limitations of other models. The proposed model parameters could be generated from publicly available data on websites or manufacturer and Global Positioning System (GPS) data.

The fuel estimates were generated from the calibrated coefficients of the VT-CPFM model for HDDVs using Wang and Rakha's convex model (Wang & Rakha, 2016) due to the lack of fuel economy data. Then, the VT-CPFM model was applied to generate the instantaneous estimated fuel consumption along with the other data. HDDT 1 generated coefficients $\alpha_0, \alpha_1$ and $\alpha_2$ are 1.56E-03, 8.10E-05 and 1.00E-08, respectively. These coefficients vary according to the characteristics of each vehicle. The correlation between the estimated and measured fuel data provides a measure for the performance of the model in estimating vehicle emissions.

Different models were tested to determine which parameters would be used. Stepwise regression was applied to choose the proposed model that would meet the required criteria. The square root model uses fuel estimates and speed along with coefficients as shown in Table 4-2 to generate the emissions of the vehicles as expressed in Equation (4-7):

$$\sqrt{E(t)} = a + b.v(t) + c.F(t) + d.v(t).F(t) + e.F(t)^2 + f.F(t)^3 + g.v(t).F(t)^2 + h.v(t).F(t)^3 \tag{4-7}$$

where

$v(t)$= speed of the vehicle at time $t$,
$F(t)$= estimated fuel from VT-CPFM model at time $t$, and
$E(t)$= CO or HC or $NO_x$ at time $t$.
$a, b, c, d, e, f, g, h$= regression model coefficients.

**TABLE 4-2 Sample Model Coefficients for HDDT 1**

| Emission | *a* | *b* | *c* | *d* | *e* | *f* | *g* | *h* |
|---|---|---|---|---|---|---|---|---|
| CO | -0.023 | 0.003 | 58.967 | -1.089 | -3201.70 | 70.879 | 47595 | -1209.50 |
| HC | 0.035 | 0.001 | 11.219 | -0.216 | -796.41 | 16.847 | 22888 | -456.31 |
| $NO_x$ | 0.049 | 0.002 | 100.098 | -1.017 | -10536.00 | 161.68 | 339250 | -5640.50 |

This polynomial formula combines the cubic function of VT-CPFM fuel with the linear speed term. The square root model guarantees that the emission results will always be positive. Fuel is an essential parameter because vehicle emissions result from the combustion of fuel. Furthermore, speed can be used as a reference for the driving condition of the car, whether it is at a high or low speed or even idling at zero speed. Moreover, these parameters will not result in multicollinearity. These two parameters; estimated fuel and instantaneous speed had better results than other vehicle parameters while maintaining the simplicity of the model. Addition of other parameters did not produce significant improvements in the results and may cause regression overfitting. The generated coefficients vary from one vehicle to another according to the collected data and vehicle parameters.

The hold-out method was applied, where a random portion of the data was split into a training set and a testing set. For each vehicle, 70% of the data were used for the training set and 30% for the testing. This process was applied for each vehicle and for each emission, and the average coefficients and a coefficient of determination ($R^2$) were calculated.

The calibrated coefficients were applied to the model to predict CO, HC, and $NO_x$ emissions. Results were compared with field-measured data to ensure the validity of the model. In addition, the model was compared with the CMEM model structure in Equation (4-3) to ensure its accuracy. Where, the coefficients in CMEM were calibrated from the same dataset that was used for the calibration of the developed model. Then, the coefficients were applied on the testing sets to generate the results.

Randomization of data was performed, and the data split was executed to separate the training data from the testing data. The same randomized training and testing data sets were applied to the CMEM and VT-CPFM emissions models. The removal of outliers was implemented based on each model to ensure impartiality in comparing the two models.

## 4.5 RESULTS AND DISCUSSION

The HDDT 1 data set is illustrated in Figure 1 to represent the behavior of emissions as a function of VT-CPFM fuel consumption and speed.

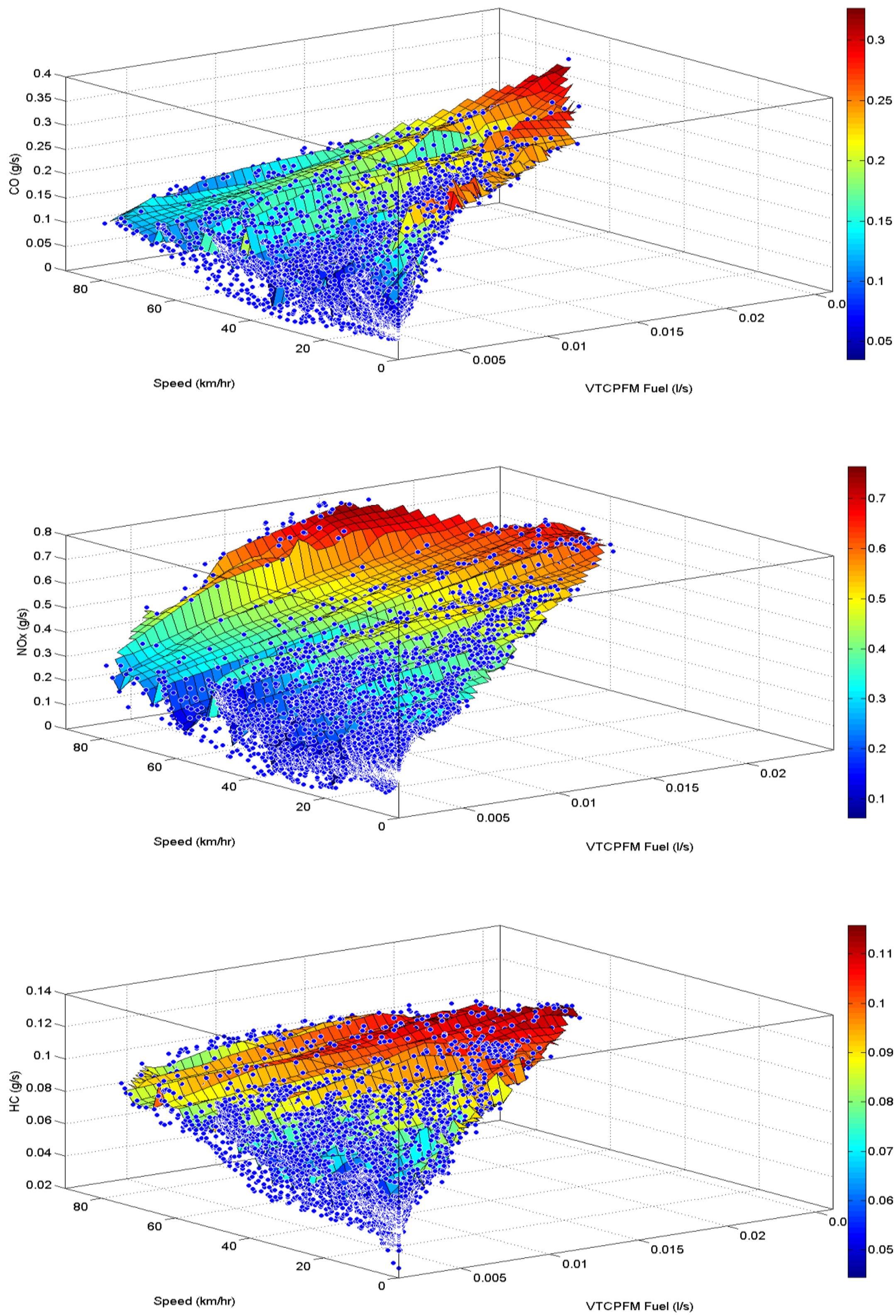



**FIGURE 4-1 Sample of the randomized emission data with speed and VT-CPFM fuel consumption (HDDT 1).**

Figure 4-1 clearly demonstrates that the highest emission levels occur at the highest level of fuel estimates; as fuel consumption increases, emissions increase. $NO_x$ has the highest level of emissions and is the most well-distributed emission compared with CO and HC. $NO_x$ makes up the largest portion of diesel emissions at more than 50% because diesel engines are lean combustion engines and the concentration of CO and HC is lower (Reşitoğlu, 2015).

The VT-CPFM emission model maintains consistency by using the same model to predict the three emissions. The accuracy of the model was evaluated by estimating the coefficient of determination ($R^2$) of CO, HC, and $NO_x$ for the eight trucks. Table 4-3 shows $R^2$ values for each truck across the three emissions and the average values for each emission. $NO_x$ has the highest $R^2$ values, followed by CO then HC, which has the lowest $R^2$ values. Figure 1 illustrates this by showing the well-distributed data for $NO_x$, which were measured more easily and captured more accurately than CO and HC for some trucks. Diesel engines emit low levels of HC (Reşitoğlu, 2015), making it more difficult to predict accurately compared with $NO_x$. Consequently, $NO_x$ has the highest average $R^2$ of 0.857, followed by CO then HC (0.749 and 0.582, respectively).

**TABLE 4-3 Coefficient of Determination for Each Vehicle**

| Vehicle ID | CO | HC | $NO_x$ |
|---|---|---|---|
| HDDT 1 | 0.821 | 0.626 | 0.929 |
| HDDT 2 | 0.752 | 0.753 | 0.898 |
| HDDT 3 | 0.749 | 0.226 | 0.821 |
| HDDT 4 | 0.710 | 0.583 | 0.897 |
| HDDT 5 | NA | 0.651 | 0.915 |
| HDDT 6 | 0.721 | 0.440 | 0.676 |
| HDDT 7 | 0.752 | 0.796 | 0.858 |
| HDDT 8 | 0.739 | NA | 0.862 |
| Average | 0.751 | 0.582 | 0.856 |

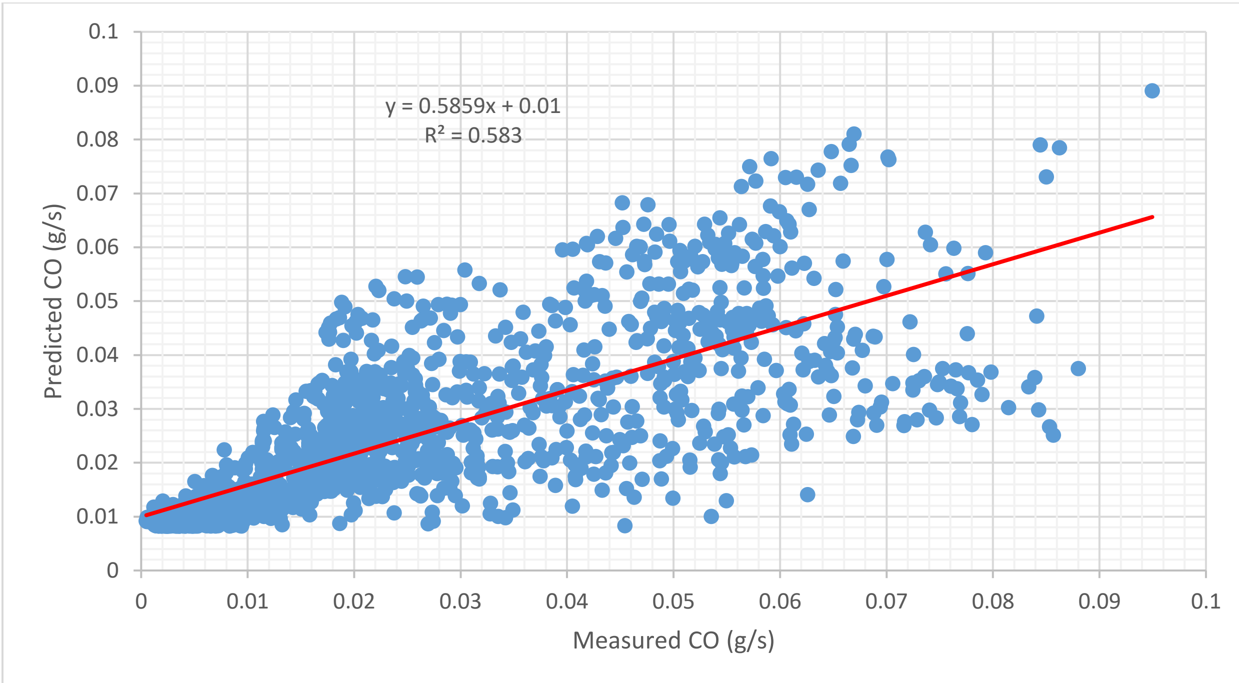
The performance of the VT-CPFM emission model was further evaluated and validated by comparing it with CMEM's model structure (Table 4-4). The predicted emission values were plotted against measured field data to fit the regression line to estimate $R^2$ for each model (Figures 4-2, 4-3, and 4-4; Table 4-4). Table 4-4 summarizes the individual and average $R^2$ values, revealing the robustness of the model based on its goodness of fit. It is evident that the average $R^2$ values of the VT-CPFM emission model are higher than those for the CMEM model, demonstrating the superior performance of the model. In general, the VT-CPFM model has higher $R^2$ values for almost all the vehicles compared to CMEM.

**TABLE 4-4 $R^2$ Values for Emission Field Data vs. Estimates for CMEM and VT-CPFM**

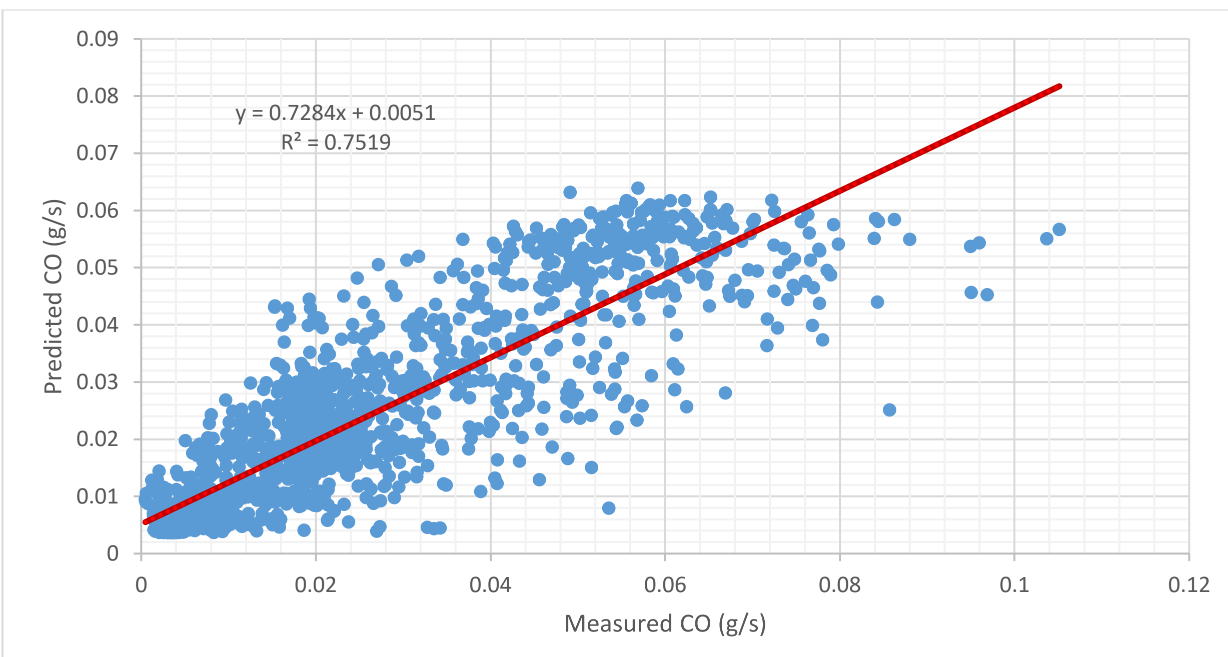
| Vehicle ID | VT-CPFM (CO) | CMEM (CO) | VT-CPFM (HC) | CMEM (HC) | VT-CPFM ($NO_x$) | CMEM ($NO_x$) |
|---|---|---|---|---|---|---|
| HDDT 1 | 0.836 | 0.613 | 0.578 | 0.392 | 0.955 | 0.939 |
| HDDT 2 | 0.728 | 0.586 | 0.745 | 0.695 | 0.924 | 0.904 |
| HDDT 3 | 0.779 | 0.708 | 0.172 | 0.148 | 0.832 | 0.820 |
| HDDT 4 | 0.665 | 0.487 | 0.566 | 0.525 | 0.925 | 0.951 |
| HDDT 5 | NA | NA | 0.658 | 0.512 | 0.934 | 0.938 |
| HDDT 6 | 0.707 | 0.594 | 0.423 | 0.404 | 0.700 | 0.661 |
| HDDT 7 | 0.789 | 0.645 | 0.162 | 0.107 | 0.880 | 0.866 |
| HDDT 8 | 0.743 | 0.510 | NA | NA | 0.896 | 0.824 |
| Average | 0.750 | 0.592 | 0.472 | 0.397 | 0.881 | 0.863 |

The two models are similar in terms of the order of goodness of fit for $NO_x$ emissions. Table 4-4 shows that the average coefficient of determination ($R^2$) $NO_x$ emission values for the two models are the highest. Alternatively, the coefficient of determination is the lowest for HC emission estimates. The values imply that $NO_x$ has the best fit. VT-CPFM has a slightly higher $R^2$ value than CMEM (0.881 versus 0.863). On the other hand, the average $R^2$ values for HC demonstrate the relatively poor fit between the predicted and measured field data, which is due to the low HC emission levels as mentioned before. Nevertheless, VT-CPFM has better HC estimates than CMEM as expressed in the average $R^2$ values (0.472 versus 0.397). Finally, the VT-CPFM model has a relatively average fit of $R^2 = 0.750$ compared to CMEM with a relatively poor fit of $R^2 = 0.592$ for CO emissions.

The VT-CPFM model is simple, with only eight coefficients and two main parameters, speed and fuel. CMEM requires extensive and complicated data to estimate emissions. For instance, CMEM requires engine speed data, which would require installation of onboard diagnostics to measure. On the other hand, the data used by VT-CPFM are publicly available except for the speed data, which can be collected using a GPS device.

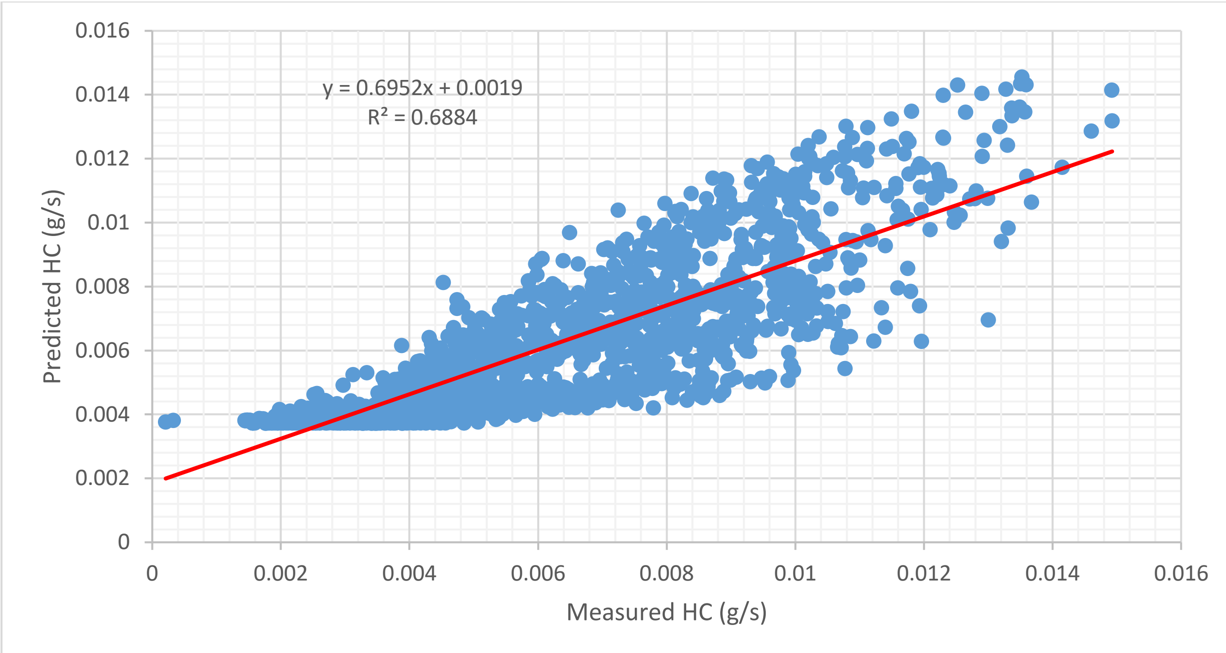



(a) CMEM

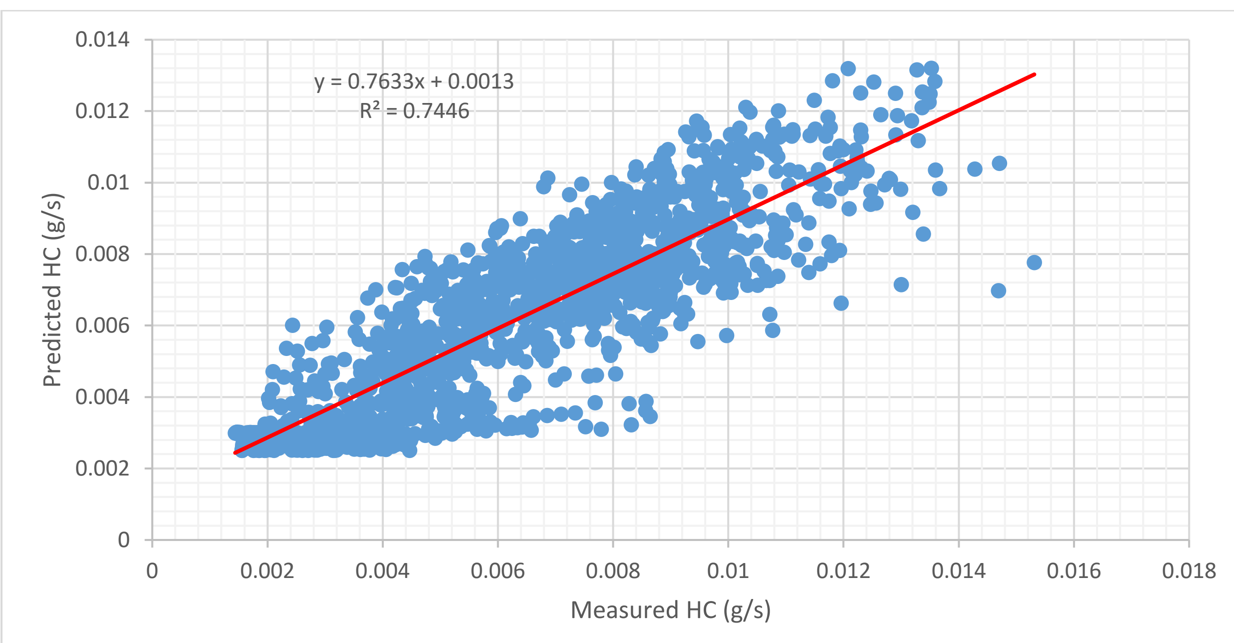



(b) VT-CPFM

**FIGURE 4-2 Comparison between (a) CMEM and (b) VT-CPFM of CO estimates for HDDT 1.**

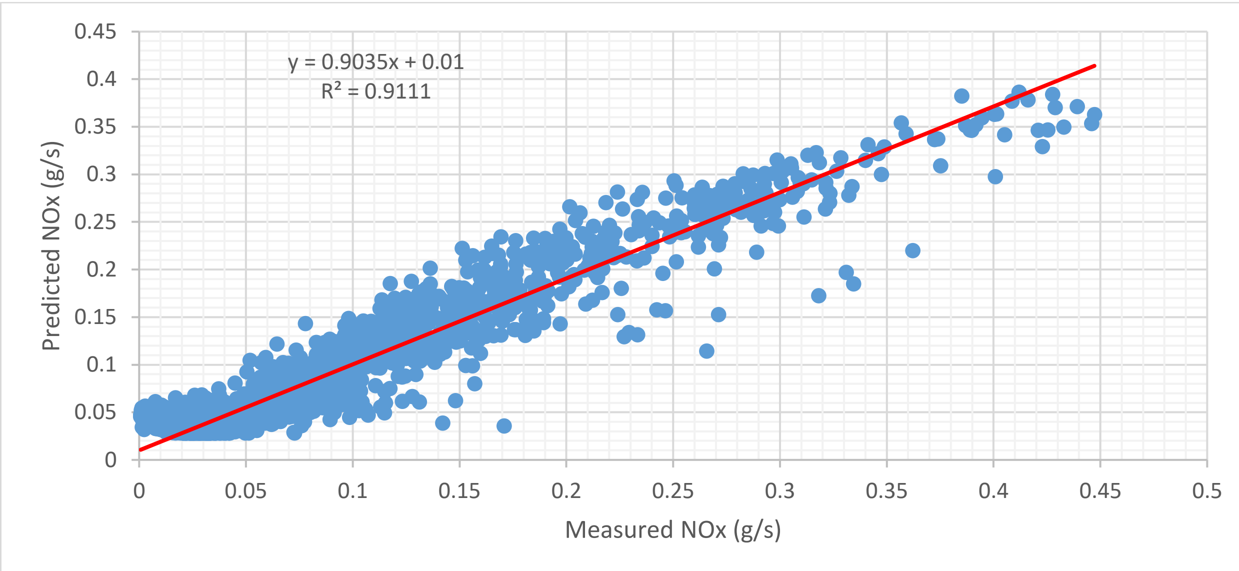



(a) CMEM

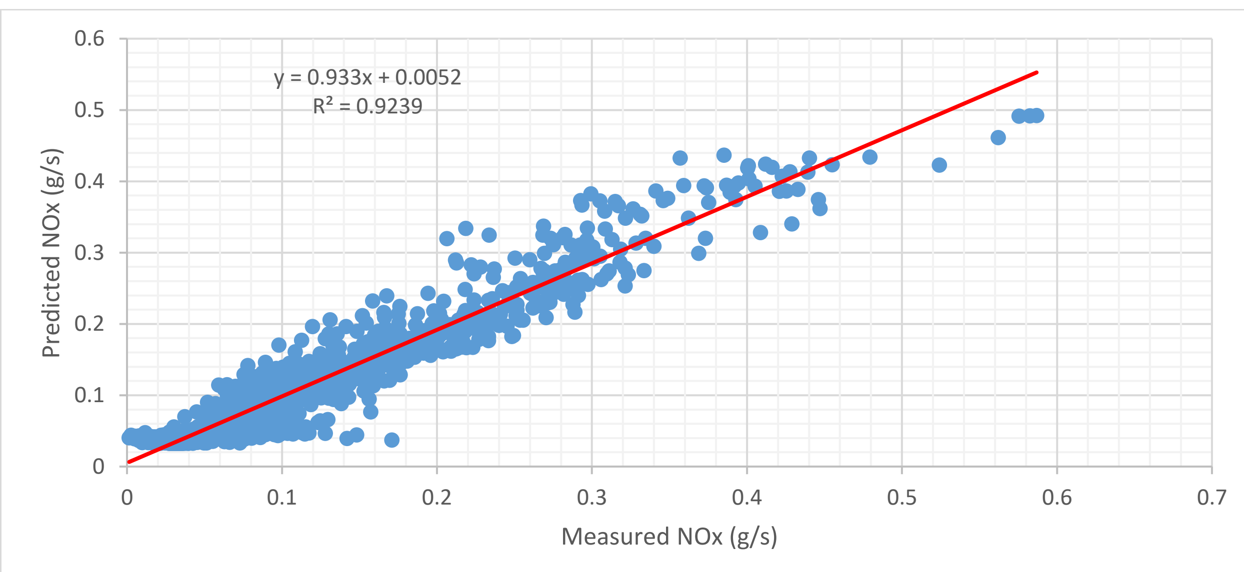



(b) VT-CPFM

**FIGURE 4-3 Comparison between (a) CMEM and (b) VT-CPFM of HC estimates for HDDT 1.**




(a) CMEM




(b) VT-CPFM

**FIGURE 4-4 Comparison between (a) CMEM and (b) VT-CPFM of $NO_x$ estimates for HDDT 1.**

Figures 4-2, 4-3, and 4-4 illustrate the correlation of estimated emissions from CMEM and VT-CPFM with in-field measurements from HDDT 1. $NO_x$, the key target emission and the main concern in HDDT emissions, is highly correlated compared with CO and HC emissions. Moreover, VT-CPFM had better estimates for $NO_x$, CO, and HC compared to CMEM based on the $R^2$ values. The VT-CPFM estimated emissions are uniformly scattered and have better distribution around the regression line than CMEM. This is additional evidence that VT-CPFM provides better fuel estimates than CMEM. In addition, VT-CPFM offers the two additional benefits, namely: it does not produce a bang-bang control system and it can be calibrated and run much easier given that it is a simpler model.

**TABLE 4-5 Average MAE and SMAPE for CMEM and VT-CPFM**

| Emissions | CMEM | | VT-CPFM | |
|---|---|---|---|---|
| | MAE | SMAPE | MAE | SMAPE |
| CO | 0.021786 | 0.54016 | 0.017014 | 0.455586 |
| HC | 0.000888 | 0.21699 | 0.000732 | 0.193229 |
| $NO_x$ | 0.023443 | 0.24979 | 0.022614 | 0.246200 |

The performance of the model was further investigated and analyzed by estimating mean absolute error (MAE) and symmetric mean absolute percentage error (SMAPE) for CO, HC, and $NO_x$ estimates (Table 4-5). MAE and SMAPE were calculated for vehicle trips estimated by the VT-CPFM and CMEM model structure to compute the difference in estimates against in-field measured data. SMAPE can be used as an alternative to mean absolute percentage error (MAPE) when there are zero or near-zero values in the data, which could result in infinitely high error rates that will increase the average error rate and will not represent the correct value (Makridakis, 1993). SMAPE was used as benchmark for the two models since some of the emissions values were near-zero. SMAPE yields higher error rates than usual due to the near-zero values but it limits the error to 200% as shown in Equation 4-8:

$$SMAPE = \left|\frac{A_t - F_t}{(A_t + F_t)/2}\right| \tag{4-8}$$

where $A_t$ is the actual value and $F_t$ is the forecast value at time $t$.

$NO_x$ had an approximately similar SMAPE for both models, although SMAPE and MAE for CMEM were slightly higher than for VT-CPFM. The HC and CO error rates were higher for CMEM than for VT-CPFM, which corroborates the evident goodness of fit of VT-CPFM over CMEM.

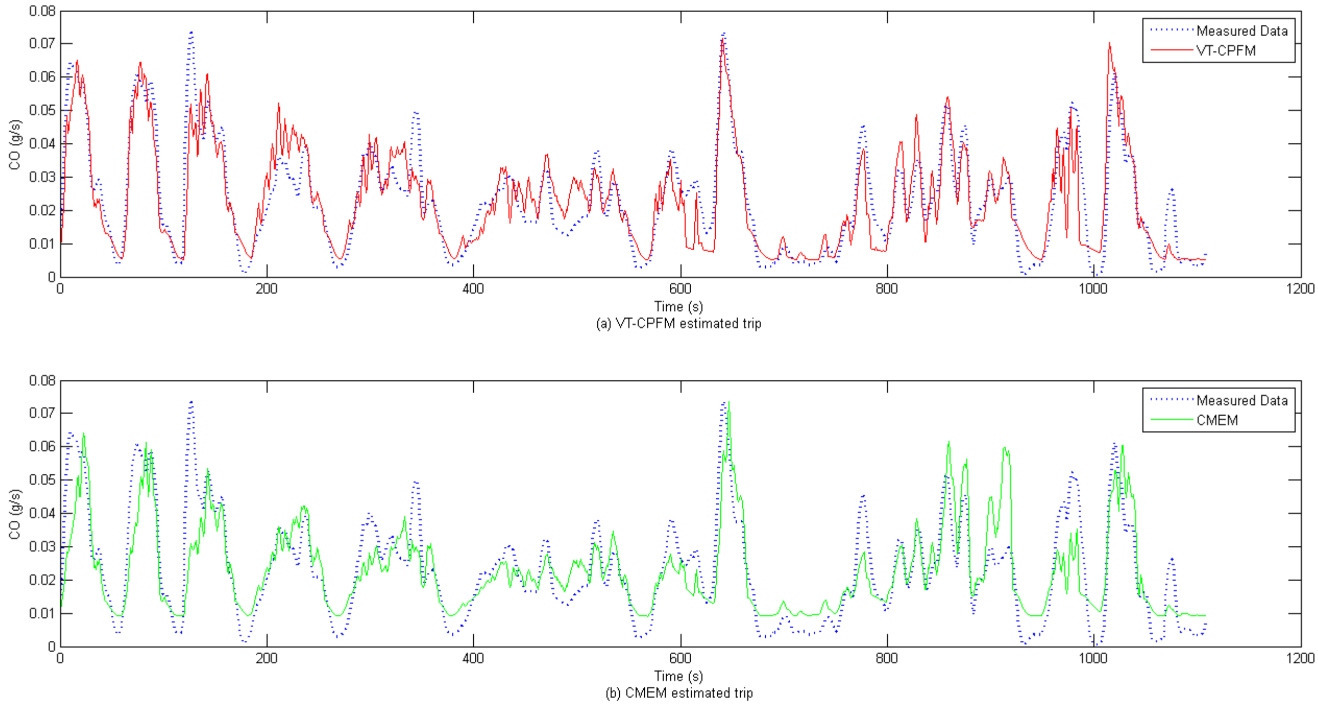



**Figure 4-5 Model validation and comparison of VT-CPFM with CMEM for CO.**

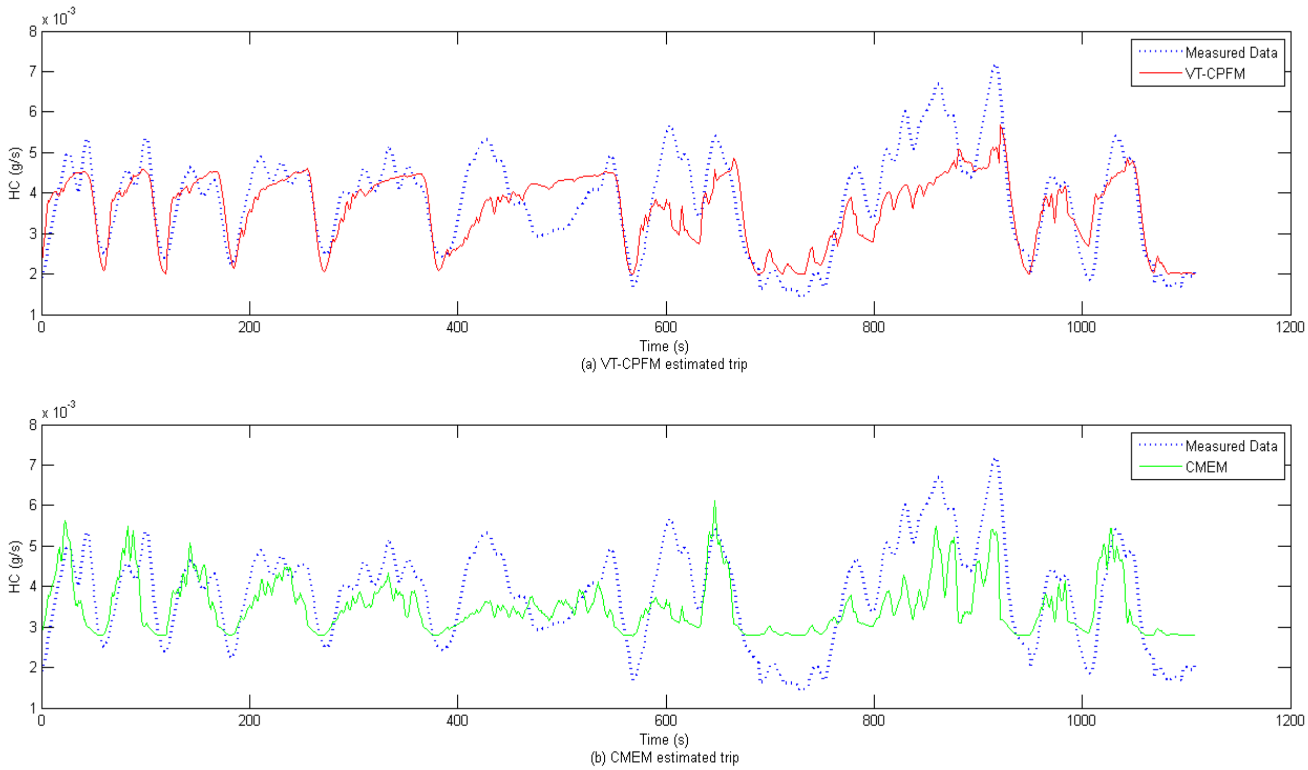



**Figure 4-6 Model validation and comparison of VT-CPFM with CMEM for HC.**

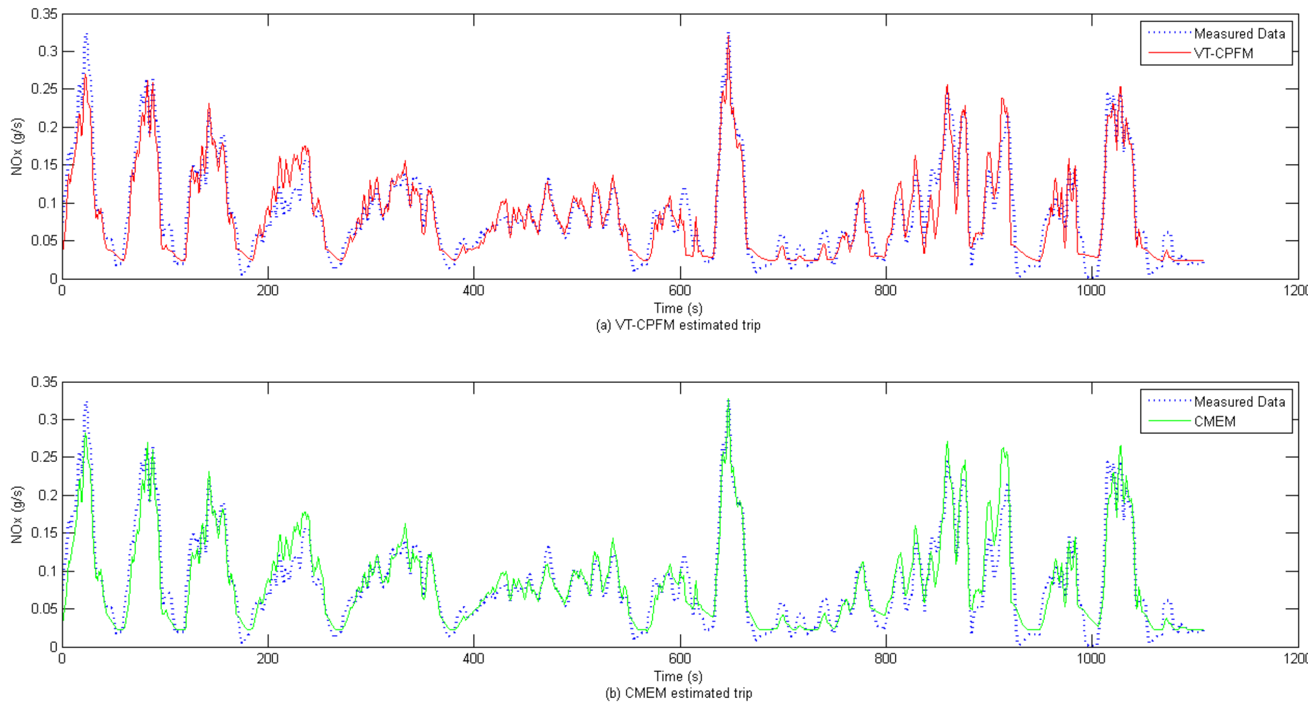



**Figure 4-7 Model validation and comparison of VT-CPFM with CMEM for $NO_x$.**

Figures 4-5, 4-6, and 4-7 show sample estimated trip emissions of the two models along with in-field measured data. The figures illustrate the ability of the models to capture the transient behavior of the three pollutants. The high error rates, which correspond to near-zero values are interpreted by the figures showing the large drops in empirical data. For $NO_x$, the two models were similar and fit the measured data well. The VT-CPFM model had better estimates for CO and HC, especially at lower values, where CMEM overestimates the emissions at these values. The VT-CPFM estimates were more consistent with in-field measured data for the three pollutants, specifically for HC and CO, which was expected from the demonstrated goodness of fit of the VT-CPFM model in previous tables and figures.

**Table 4-6 MAPE of emissions for VT-CPFM and CMEM**

| Model | VT-CPFM | | | CMEM | | |
|---|---|---|---|---|---|---|
| Emission | CO | HC | $NO_x$ | CO | HC | $NO_x$ |
| HDDT 1 | 0.16% | 0.99% | 0.29% | 5.65% | 1.51% | 6.52% |
| HDDT 2 | 3.44% | 2.11% | 0.99% | 1.31% | 1.09% | 3.17% |
| HDDT 3 | 1.00% | 0.53% | 0.73% | 3.72% | 1.32% | 2.02% |
| HDDT 4 | NA | 2.02% | 0.87% | NA | 0.20% | 2.29% |
| HDDT 5 | 5.01% | 3.14% | 3.11% | 2.60% | 4.41% | 4.34% |
| HDDT 6 | 5.50% | 3.46% | 0.28% | 3.42% | 5.91% | 6.92% |
| HDDT 7 | 3.67% | NA | 1.37% | 6.99% | NA | 3.15% |
| HDDT 8 | 1.97% | 2.26% | 0.57% | 3.29% | 1.06% | 0.70% |
| Average | 1.97% | 2.26% | 0.57% | 3.29% | 1.06% | 0.70% |

Moreover, the mean absolute percentage error (MAPE) was calculated over the trip for each truck to evaluate the performance of the model over the whole trip. Table 4-6 represents the calculated MAPE of CO, HC and NOx for each truck based on each model. VT-CPFM had lower error rates than CMEM for CO and HC for the majority of the tested trucks. However, VT-CPFM had lower MAPE for NOx which is the key target emission for all the trucks. VT-CPFM will generate better estimates based on the goodness of fit and the error rates.

## 4.6 CONCLUSIONS AND FUTURE RESEARCH

The research presented in this paper extends the VT-CPFM model to capture HDDT emissions using calibrated model parameters. An additional advantage of this model is that it does not result in a bang-bang control system. The proposed VT-CPFM emission model is consistent in its structure for CO, HC, and $NO_x$ estimation using only two parameters: speed and fuel consumption. Results show good estimates of $NO_x$—the key target of HDDVs—which have the best fit compared to CO and HC. The model was tested against CMEM's model structure to evaluate its performance and robustness. The models' estimated emission rates were compared with in-field measurements. The results demonstrate that VT-CPFM estimates are more accurate than those from CMEM based on the coefficient of determination. Moreover, the VT-CPFM model is simpler and more cost-effective, requiring vehicle parameters and the collection of instantaneous GPS data.

With regards to future work, emission models should be developed for later HDDV models to capture the impact of emerging technologies, including after treatment devices such as selective catalytic reduction (SCR) on vehicle emissions. Given that VT-CPFM models the tailpipe emissions directly, the specifics of the engine and the exhaust system is not needed to develop the model. Consequently, there do not appear to be any foreseeable problems in calibrating VT-CPFM to different truck technology platforms.

## ACKNOWLEDGMENTS

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# Chapter 5: Developing VT-CPFM Emission Modeling using MOVES Data

This paper to be submitted at Transportation Research, Part D: Transport & Environment.

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**ABSTRACT**
The current state-of-practice fuel consumption and emission models suffer from two limitations: they produce a bang-bang control system and cannot be calibrated using publicly available data. The Virginia Tech Comprehensive Power Based Fuel Consumption Model (VT-CPFM) was developed to overcome those two shortcomings. It does not result in bang-bang control and can be calibrated by using U.S. Environmental Protection Agency (EPA) city and highway fuel economy ratings. This research focuses on developing a simple and reliable microscopic emission model based on VT-CPFM. The proposed model was calibrated and validated using the MOtor Vehicle Emissions Simulator (MOVES) data to estimate the carbon monoxide (CO), hydrocarbon (HC), and oxides of nitrogen ($NO_x$) emissions of light-duty vehicles (LDVs). The model framework is consistent in estimating the three emissions using instantaneous estimated fuel using VT-CPFM and instantaneous speed measurements. The model was calibrated and validated against MOVES data. The coefficient of determination was a measure of performance for the model, and exceeded 0.9 for all the emissions. $NO_x$ had the best fit at over 0.95. Furthermore, the model was implemented on 16 driving cycles to evaluate its performance. The prediction errors varied between approximately 1% and 18% according to the Mean Absolute Percent Error (MAPE). The model's simplicity in estimating the emissions reliably may save time and money compared with other existing models.

*Keywords*: microscopic emission modeling, Virginia Tech Comprehensive Power Based Fuel Consumption Model (VT-CPFM), MOtor Vehicle Emissions Simulator (MOVES)

## 5.1. INTRODUCTION

The transportation sector places a huge burden on our environment and is one of the major emitters of pollutants. In particular, transportation is considered to be one of the largest sources of greenhouse gases (GHGs), which increase the level of pollution and have an impact on climate change. Therefore, policymakers are keen to develop models that accurately estimate the emissions from on-road vehicles. Microscopic emission models are capable of estimating the instantaneous vehicle emissions from operational-level projects, and policymakers can use them to evaluate their emission reduction plans and the environmental impact of transportation projects.

Nevertheless, the majority of the existing fuel consumption and emission models suffer from two major deficiencies. They produce a bang-bang control system and require extensive calibration through in-field or laboratory data, which costs time and money. Models that result in bang-bang control systems suggest that optimum fuel economy is achieved by accelerating at full throttle or decelerating at full braking to reach a desired speed. These models imply that using full throttle will reduce the acceleration time, which will reduce the fuel consumption rate. However, this is obviously incorrect since it means that aggressive driving is required to minimize the fuel consumption rate (Rakha et al., 2011).

The Virginia Tech Comprehensive Power Based Fuel Consumption Model (VT-CPFM) overcomes those two shortcomings: it does not result in a bang-bang control system and can be easily calibrated by using publicly available data to calculate fuel consumption. However, VT-CPFM does not capture vehicle emissions levels. Consequently, the objective of this paper is to extend the VT-CPFM model to estimate emission rates for CO, HC, and $NO_x$. This study outlines the development of a simple and reliable emission model evolved from VT-CPFM. The model was implemented on recent light-duty vehicle (LDV) models, and calibrated and validated for 12 best-selling vehicles. Sixteen different driving cycles with various speed and acceleration ranges were used to evaluate the model's capability in estimating the emissions.

## 5.2. LITERATURE REVIEW

VT-Micro is a regression-based model that estimates fuel rate, CO, HC, and NOx (Rakha et al., 2004). VT-Micro is a dual regime model that consists of polynomial combinations of instantaneous speed and acceleration (Rakha et al., 2004). The model predicts emission and fuel rates based on whether the vehicle is accelerating or decelerating, as shown in Equation (5-1):

$$MOE_e \begin{cases} e^{\sum_{i=0}^{3}\sum_{j=0}^{3}(L_{ij}^{e}\times u^{i}\times a^{j})} & for\ a\geq 0 \\ e^{\sum_{i=0}^{3}\sum_{j=0}^{3}(M_{ij}^{e}\times u^{i}\times a^{j})} & for\ a<0 \end{cases} \tag{5-1}$$

where

$MOE_e$ is instantaneous fuel consumption or emission rate (l/s or mg/s);

$L_{ij}^{e}$ is the model regression coefficient for MOE $e$ at speed power $i$ and acceleration power $j$ for positive accelerations;

$M_{ij}^{e}$ is the model regression coefficient for MOE $e$ at speed power $i$ and acceleration power $j$ for negative accelerations;

$u$ is instantaneous speed (km/h); and

$a$ is instantaneous acceleration (m/s$^2$).

The results from VT-Micro were verified by comparing the fuel and emission estimates to measured data from the chassis dynamometer at the Oak Ridge National Laboratory (ORNL), resulting in coefficient of determination ($R^2$) ranges from 0.92 to 0.99. However, the model requires 32 coefficients to be calibrated, which may over fit the data.

One recently developed microscopic fuel consumption and emission model is PΔP (Smit, 2013), which utilizes power and engine power as the main model variables. The model estimates second-by-second fuel and emission rates based on whether the vehicle is at idle or moving, as shown in Equation (5-2):

$$e_t = \begin{cases} \alpha & for \;\; v_t = 0 \\ \beta_0 + \beta_1 P_t + \beta_2 \Delta P_t + \beta_3 P_t^2 + \beta_4 \Delta P_t^2 + \beta_5 P_t \Delta P_t + \varepsilon & for \;\; v_t > 0 \end{cases} \quad (5\text{-}2)$$

where $e_t$ is the emission or fuel rate at time $t$; α is the emission rate at idle; $\beta_0$, $\beta_1$, $\beta_2$, β3, $\beta_4$, and $\beta_5$ are the model coefficients; ε is the error term; $P_t$ is the engine power at time $t$; and $\Delta P_t$ is the change in engine power at time $t$.

The PΔP model estimates instantaneous fuel consumption, $CO_2$, and $NO_x$. Smit used the coefficient of determination to evaluate the model's performance in estimating fuel/$CO_2$ and $NO_x$, resulting in $R^2$ values of 0.93 and 0.65, respectively. However, the model neglects the other main emissions, HC and CO, which precludes studying the hazards of HC and CO and evaluating their impacts on the environment.

The Comprehensive Modal Emissions Model (CMEM) was developed at the University of California to estimate on-road vehicle emissions based on the vehicle's operating mode. CMEM consists of six modules: engine power, engine speed, air/fuel ratio, fuel use, engine-out emissions, and catalyst pass fraction (Barth et al., 2000).

CMEM estimates second-by-second tailpipe emissions as the product of fuel rate (FR), the engine-out emission index ($g_{emission}/g_{fuel}$), and catalyst pass fraction (CPF), as shown in Equation (5-3):

$$Tailpipe\ emissions = FR \times \left(\frac{g_{emission}}{g_{fuel}}\right) \times CPF \quad (5\text{-}3)$$

The CMEM model first estimates the power demand to calculate FR as expressed in Equation (5-4), then applies Equation (5-3) to estimate the tailpipe emissions.

$$FR = \left(K.N.V + \frac{P}{\eta}\right)\frac{1}{44} \quad (5\text{-}4)$$

where

$FR$ is the fuel use rate (g/s),

$P$ is the engine power output (kW),

$K$ is the engine friction factor,

$N$ is the engine speed (revolutions per second),

$V$ is the engine displacement (L),

$\eta$ is measure of indicated efficiency (0.44).

However, CMEM is not simple to use due to its physical approach. Massive and detailed data inputs are required, which consume time and money to be collected and measured. The lack of publicly available data also increases the difficulty of calibrating each data set since many sources are needed. In addition, the CMEM model may result in a bang-bang control system.

The MOtor Vehicle Emissions Simulator (MOVES), developed by the U.S. Environmental Protection Agency (EPA), covers a broad range of pollutants from mobile sources. MOVES estimates GHG emissions, criteria pollutants, and energy consumption (EPA, 2016). The model assigns emission factors to each specific combination of instantaneous speed and acceleration rates. MOVES relates vehicle operation to emission behavior based on vehicle specific power (VSP), and deploys a binning approach with 23 operating mode bins representing the operating conditions listed in Table 5-1 (EPA, 2009). The bins include scenarios of vehicle dynamics data assimilated into speed and VSP data. Therefore, vehicles in the same operating mode bin based on instantaneous speed and VSP data will have the same emission rate (Liu et al., 2016).

**Table 5-1**
Definition of MOVES operating modes for running energy consumption.

| Operating Mode Bin ID | Operating Mode Description | VSP | Speed ($v$) (mph) | Acceleration ($a$) (mph/s) |
|---|---|---|---|---|
| 0 | Deceleration/Braking | | | ($a \le -2$) or ($a \le -1$ and $a - 1 \le -1$ and $a - 2 \le -1$) |
| 1 | Idling | | $-1 \le v < 1$ | |
| 11 | Coast | VSP < 0 | $1 \le v < 25$ | |
| 12 | Cruise/Acceleration | 0 ≤ VSP < 3 | $1 \le v < 25$ | |
| 13 | Cruise/Acceleration | 3 ≤ VSP < 6 | $1 \le v < 25$ | |
| 14 | Cruise/Acceleration | 6 ≤ VSP < 9 | $1 \le v < 25$ | |
| 15 | Cruise/Acceleration | 9 ≤ VSP < 12 | $1 \le v < 25$ | |
| 16 | Cruise/Acceleration | 12 ≤ VSP | $1 \le v < 25$ | |
| 21 | Coast | VSP < 0 | $25 \le v < 50$ | |
| 22 | Cruise/Acceleration | 0 ≤ VSP < 3 | $25 \le v < 50$ | |
| 23 | Cruise/Acceleration | 3 ≤ VSP < 6 | $25 \le v < 50$ | |
| 24 | Cruise/Acceleration | 6 ≤ VSP < 9 | $25 \le v < 50$ | |
| 25 | Cruise/Acceleration | 9 ≤ VSP < 12 | $25 \le v < 50$ | |
| 27 | Cruise/Acceleration | 12 ≤ VSP < 18 | $25 \le v < 50$ | |
| 28 | Cruise/Acceleration | 18 ≤ VSP < 24 | $25 \le v < 50$ | |
| 29 | Cruise/Acceleration | 24 ≤ VSP < 30 | $25 \le v < 50$ | |
| 30 | Cruise/Acceleration | 30 ≤ VSP | $25 \le v < 50$ | |
| 33 | Cruise/Acceleration | VSP < 6 | $50 \le v$ | |
| 35 | Cruise/Acceleration | 6 ≤ VSP < 12 | $50 \le v$ | |
| 37 | Cruise/Acceleration | 12 ≤ VSP < 18 | $50 \le v$ | |
| 38 | Cruise/Acceleration | 18 ≤ VSP < 24 | $50 \le v$ | |
| 39 | Cruise/Acceleration | 24 ≤ VSP < 30 | $50 \le v$ | |
| 40 | Cruise/Acceleration | 30 ≤ VSP | $50 \le v$ | |

MOVES requires extensive data regarding vehicle operation and road parameters, which are not always available and cost time and money to collect. Averaging the data over many vehicles may also lead to errors in emission estimation (Alkafoury et al., 2013). The detailed data and information required increase the complexity of MOVES, making it less easy to use.

As previously mentioned, Rakha et al. developed VT-CPFM to overcome the two main shortcomings of the majority of current state-of-the-art models. VT-CPFM does not produce a bang-bang control system and can be calibrated by using publicly accessible data (Rakha et al., 2011). The model estimates fuel consumption using instantaneous vehicle power, based on Equation (5-5) (Wong, 2001).

$$P(t) = \left(\frac{R(t) + 1.04\, ma(t)}{3600\eta_d}\right) v(t) \tag{5-5}$$

Here, *P(t)* is the power exerted by the vehicle driveline (kW) at time *t*, *R(t)* is the resistance force (N) at time *t*, *m* is the vehicle mass (kg), *a*(*t*) is the vehicle acceleration (m/s$^2$) at time *t*, *v(t)* is the vehicle speed (km/h) at time *t*, and $\eta_d$ is the driveline efficiency.

The model does not require calibration through laboratory or field testing. The vehicle parameters can be retrieved from the manufacturer's website and used as the inputs to a Matlab script that calibrates the coefficients of the model. VT-CPFM is a dual regime model that estimates second-by-second fuel consumption based on whether vehicle power is negative or non-negative, as expressed in Equation (5-6):

$$FC(t) = \begin{cases} \alpha_0 + \alpha_1 P(t) + \alpha_2 P(t)^2 & \forall\, P(t) \geq 0 \\ \alpha_0 & \forall\, P(t) < 0 \end{cases} \tag{5-6}$$

where *FC*(*t*) is the instantaneous estimated fuel consumption (l/s), and $\alpha_0$, $\alpha_1$ and $\alpha_2$ are the calibrated coefficients for each specific vehicle.

The same proposed model in this study was used to estimate the emissions for heavy-duty diesel trucks (Abdelmegeed and Rakha, 2017). Also, Abdelmegeed et al. developed an emission model based on VT-CPFM in 2016 to estimate CO, HC and $NO_x$ which had relatively good fit compared with in-field data. However the vehicles were manufactured from 1988 to 1997 which represented a concern if the model can capture the emerging technologies and if it can be applied on recent models. Therefore, this paper expands VT-CPFM to capture the emissions of recent vehicles models while overcoming the limitations of existing models. Moreover, the developed model will be implemented on various driving conditions to test it's capability in estimating the emissions reliably.

## 5.3 DATA

The EPA has approved the use of MOVES to validate emissions. Consequently, this study used MOVES data as the basis of comparison for emission profiles generated by the proposed model for a list of the best-selling cars in 2011. Table 5-2 lists the selected vehicle models and each vehicle's characteristics, including curb weight, engine size, and horsepower.

**Table 5-2**
Test vehicle characteristics.

| Class | Make/Model | Curb Weight (Kg) | Engine Size (L) | Rated Power (hp) |
|---|---|---|---|---|
| Compact | Honda Civic | 1212 | 1.8 | 140 |
| | Ford Focus | 1341 | 2.0 | 160 |
| | Toyota Corolla | 1270 | 1.8 | 132 |
| | `Mazda 3 | 1329 | 2.0 | 148 |
| Mid-Size | Toyota Camry | 1447 | 2.5 | 178 |
| | Nissan Altima | 1442 | 2.5 | 175 |
| | Ford Fusion | 1490 | 2.5 | 175 |
| | Chevrolet Cruze | 1435 | 1.8 | 138 |
| | Chevrolet Malibu | 1557 | 2.4 | 169 |
| Full-Size | Honda Accord | 1487 | 2.4 | 177 |
| | Hyundai Sonata | 1451 | 2.4 | 198 |
| | Chrysler 300 | 1814 | 3.6 | 292 |

Sixteen different driving cycles were used to compare the VT-CPFM estimates with MOVES data based on the mean absolute percentage error (MAPE) of the model. Some of these cycles were developed by the EPA based on real-world driving studies. These driving cycles were also used in the development of the MOBILE6 model (Brzezinski et al., 1999) and VT-Micro (Rakha et al., 2004). The cycles consist of various speed-acceleration profiles with different ranges based on various roadway types to incorporate various driving behavior scenarios. The cycles include four roadway types: freeways, arterials, freeway ramps, and local roadways. These roads were classified based on level of service (LOS) from A to G. Four EPA vehicle emission testing cycles were also used: the Urban Dynamometer Driving Schedule (UDDS) cycle or LA-4, the California Air Resources Board (CARB) area-wide unified cycle (LA92), the New York City (NYC) cycle, and the ST01 cycle. Table 5-3 provides the characteristics of each cycle that were used in the validation process.

**Table 5-3**
EPA driving cycle characteristics.

| Cycle | Avg. speed (km/h) | Max speed (km/h) | Max acc. (km/h/s) | Duration (s) | Length (km) |
|---|---|---|---|---|---|
| Freeway, High Speed (FWYSP) | 101.12 | 119.52 | 4.32 | 610 | 17.15 |
| Freeway, LOS A–C (FWYA) | 95.52 | 116.96 | 5.44 | 516 | 13.68 |
| Freeway, LOS D (FWYD) | 84.64 | 112.96 | 3.68 | 406 | 9.54 |
| Freeway, LOS E (FWYE) | 48.8 | 100.8 | 8.48 | 456 | 6.18 |
| Freeway, LOS F (FWYF) | 29.76 | 79.84 | 11.04 | 442 | 3.66 |
| Freeway, LOS G (FWYG) | 20.96 | 57.12 | 6.08 | 390 | 2.27 |
| Freeway Ramps | 55.36 | 96.32 | 9.12 | 266 | 4.1 |
| Arterial/Collectors LOS A–B (ARTA) | 39.68 | 94.24 | 8 | 737 | 8.11 |
| Arterial/Collectors LOS C–D (ARTC) | 30.72 | 79.2 | 9.12 | 629 | 5.38 |
| Arterial/Collectors LOS E–F (ARTE) | 18.56 | 63.84 | 9.28 | 504 | 2.59 |
| Local Roadways | 20.64 | 61.28 | 5.92 | 525 | 2.99 |
| Non-Freeway-Area-Wide Urban Travel | 31.04 | 83.68 | 10.24 | 1348 | 11.6 |
| UDDS | 31.36 | 90.72 | 5.28 | 1368 | 11.92 |
| LA 92 | 39.36 | 107.52 | 11.04 | 1435 | 15.7 |
| ST01 | 32.32 | 65.6 | 8.16 | 248 | 2.224 |
| NYC | 11.36 | 44.32 | 9.6 | 600 | 1.888 |

## 5.4 METHODOLOGY

The main purpose of this study was to develop a simple and reliable emission model that can be easily implemented based on VT-CPFM to overcome previous shortcomings. Various models with polynomial functions were tested with assorted parameters to select the final model structure. Statistical tools were used to test the significance of the parameters and the validity of the model in estimating the emissions. Eventually, it was found that the square root model satisfied the criteria of simplicity and reliability, in addition to guaranteeing that the results would always be positive. The model combines the cubic function of instantaneous VT-CPFM fuel estimates and a linear speed term as expressed in Equation (5-7):

$$\sqrt{E(t)} = a + b.v(t) + c.F(t) + d.v(t).F(t) + e.F(t)^2 + f.F(t)^3 + g.v(t).F(t)^2 + h.v(t).F(t)^3 \quad (5\text{-}7)$$

where

$v(t)$ is the speed of the vehicle at time *t*;
$F(t)$ is the estimated fuel from VT-CPFM model at time *t*;
$E(t)$ is the CO or HC or $NO_x$ at time *t*; and
$a, b, c, d, e, f, g, h$ are regression model coefficients.

The fuel consumption was calculated based on each vehicle's characteristics, which were the inputs to a Matlab script that calibrated the model coefficients. For example, the Honda Accord's coefficients $\alpha_0$, $\alpha_1$, and $\alpha_2$ are 1.56E-03, 8.10E-05, and 1.00E-08, respectively. These coefficients were calibrated for each vehicle and thus could vary based on each vehicle's specific characteristics. Unsurprisingly, fuel was highly significant since vehicle emissions result from the combustion of fuel. Also, speed can be used as a reference for the driving condition of the car, whether it is at a high or low speed or even idling. The model preserves the same structure for all the emissions, which maintains the consistency and simplicity of the model, which has only eight coefficients and the two main variables, fuel and speed.

**Table 5-4**
MOVES mean base rate of CO based on the operating mode ID.

| Op Mode ID | Mean Base Rate |
|---|---|
| 0 | 1.97892 |
| 1 | 0.341669 |
| 11 | 6.80345 |
| 12 | 11.1072 |
| 13 | 10.2406 |
| 14 | 14.6935 |
| 15 | 21.3068 |
| 16 | 35.9513 |
| 21 | 8.86745 |
| 22 | 11.7489 |
| 23 | 15.1095 |
| 24 | 22.0873 |
| 25 | 25.0671 |
| 27 | 37.6451 |
| 28 | 126.328 |
| 29 | 267.543 |
| 30 | 939.666 |
| 33 | 6.65783 |
| 35 | 11.3684 |
| 37 | 16.7341 |
| 38 | 115.788 |
| 39 | 122.175 |
| 40 | 359.069 |

MOVES assigns the emission factors to the operating mode based on the vehicle dynamics data in each bin. Each bin has specific scenario combines VSP, speed and acceleration based on the operating mode. MOVES generates emission tables for CO, HC and NOx which consist of the mean base rate for the emission based on the operating mode bin (ID). Table 5-4 lists the operating mode ID and emission mean base rate for CO. For instance, if the vehicle speed is more than or equal to 1 mph and less than 25 mph and the VSP is more than or equal to 0 and less than 3 kW/tonne then, the operating mode ID will be 12, therefore the emission mean base rate will be 11.1072.

MOVES data were applied to the LA92 driving cycle to generate second-by-second emission profiles and VSP, which are connected with operating mode bins as previously discussed. LA92 was used since it covers a wide range of speeds, allowing the model to be tested under low-, average-, and high-speed values to ensure its applicability to different scenarios. The model underwent calibration and validation processes to estimate $R^2$ values, which indicate the goodness of fit of estimated emissions compared with MOVES data. Furthermore, the same calibrated coefficients were used to test the model on the 16 driving cycles to measure the trips' MAPE to further evaluate the model's validity. Table 5-5 shows a sample of calibrated coefficients that were used with each driving cycle.

**Table 5-5**
Sample model coefficients for Honda Accord.

| Emission | $a$ | $b$ | $c$ | $d$ | $e$ | $f$ | $g$ | $h$ |
|---|---|---|---|---|---|---|---|---|
| CO | −0.40332 | 0.009843 | 1150.500 | −16.196 | −613890 | 9845.700 | 109680000 | −1531600 |
| HC | −0.01302 | 0.000951 | 44.252 | −1.364 | −18956 | 783.120 | 3955400 | −109690 |
| $NO_x$ | −0.02749 | 0.000849 | 67.514 | −0.418 | −12241 | 441.820 | 1468800 | −53244 |

## 5.5 RESULTS AND DISCUSSION

The data were randomly split into training and testing sets to determine the goodness of fit of the emissions for each vehicle. The coefficients were calibrated from the training set and then applied to the testing set to analyze the performance of the model. Figure 5-1 illustrates the correlation between the estimated emissions from VT-CPFM and MOVES data. The emission estimates were plotted against measured data to fit a regression line to estimate $R^2$ values for each emission. All the emissions had a very good fit compared to measured data. However $NO_x$, had the best fit, followed by HC and CO, respectively. Figure 5-2 shows the correspondence of the estimated emission rates with MOVES data. The emission levels from MOVES and VT-CPFM were highly correlated and correspondent to each other.

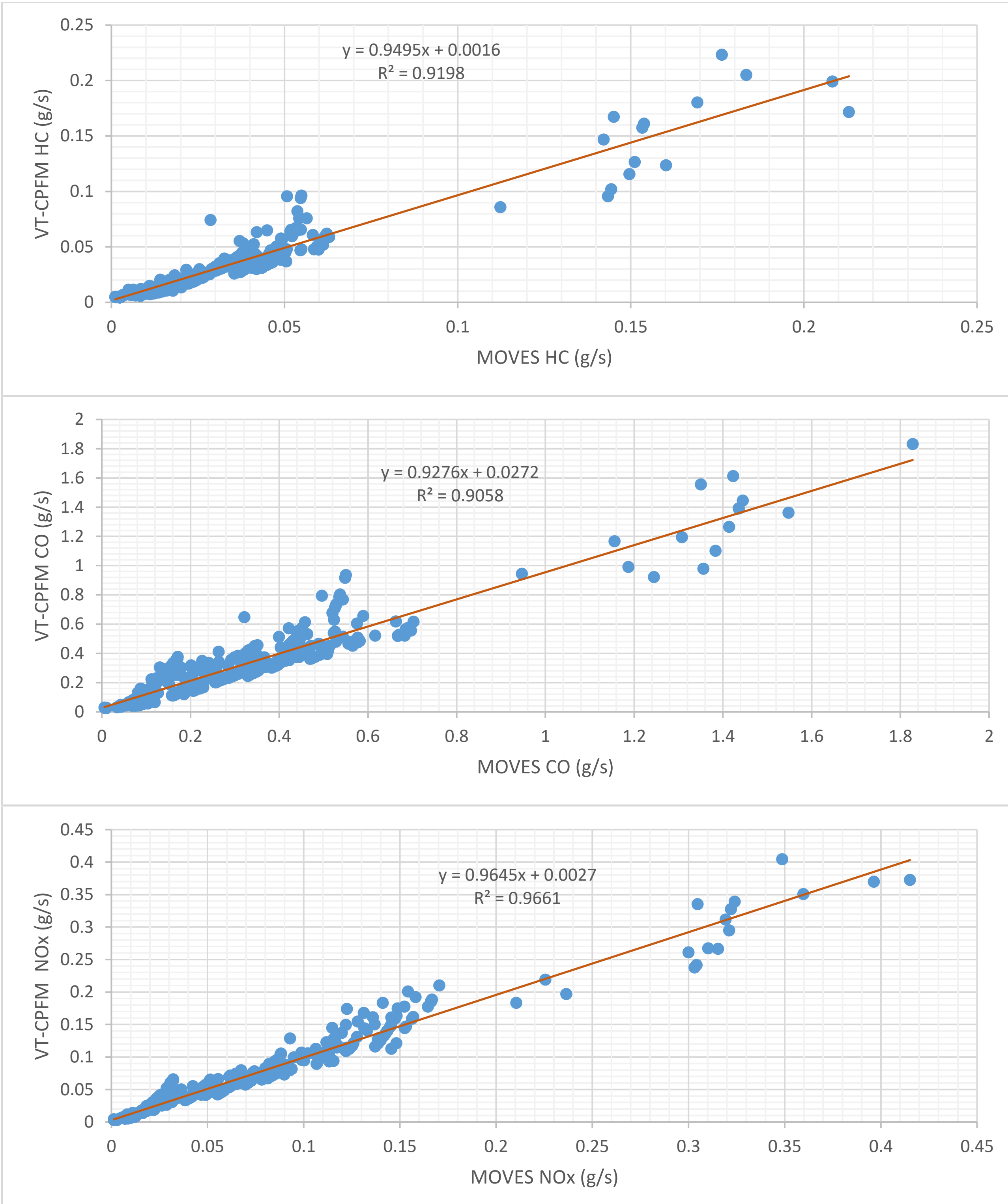



**Figure 5-1 Correlation of estimated emissions with MOVES data.**

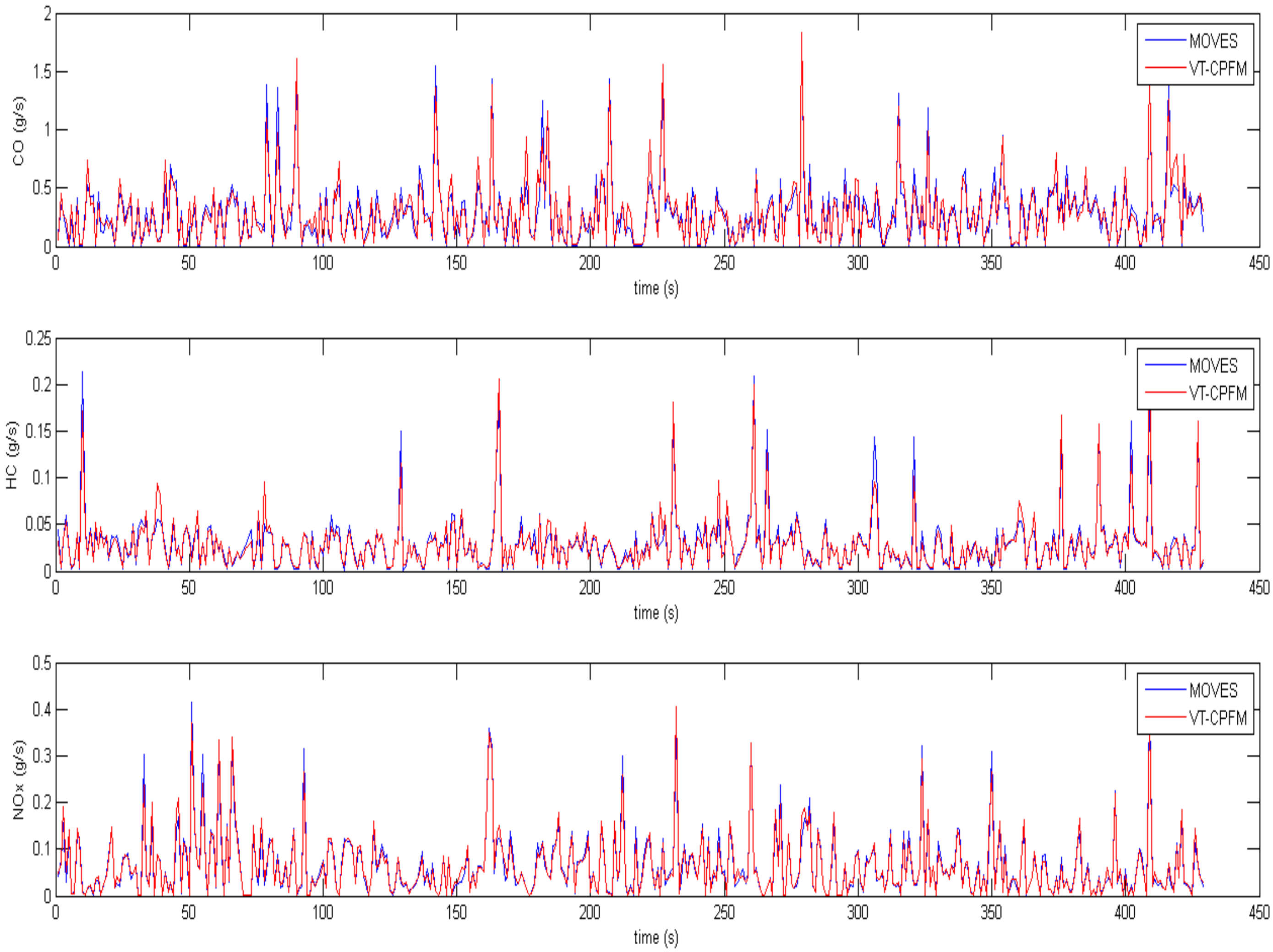



**Figure 5-2 Correspondence of VT-CPFM emissions with MOVES.**

Table 5-6 lists all the $R^2$ values of the emissions for each vehicle. The coefficients of determination for CO, HC, and $NO_x$ were higher than 0.9, which implies the robustness of the model in estimating the emission rates. $NO_x$ had the highest average $R^2$ of 0.9595, followed by HC then CO (0.9118 and 0.9002, respectively).

**Table 5-6**
Coefficient of determination of the emissions for each vehicle.

| Make/Model | $R^2$ (CO) | $R^2$ (HC) | $R^2$ ($NO_x$) |
|---|---|---|---|
| Honda Accord | 0.9000 | 0.9135 | 0.9590 |
| Nissan Altima | 0.9004 | 0.9117 | 0.9601 |
| Toyota Camry | 0.9002 | 0.9097 | 0.9603 |
| Chrysler 300 | 0.9000 | 0.9143 | 0.9616 |
| Honda Civic | 0.9006 | 0.9104 | 0.9589 |
| Ford Focus | 0.9009 | 0.9101 | 0.9571 |
| Ford Fusion | 0.8995 | 0.9133 | 0.9608 |
| Chevrolet Malibu | 0.9005 | 0.9145 | 0.9605 |
| Mazda 3 | 0.9001 | 0.9097 | 0.9580 |
| Hyundai Sonata | 0.9014 | 0.9101 | 0.9588 |
| Chevrolet Cruze | 0.8990 | 0.9123 | 0.9591 |
| Toyota Corolla | 0.9007 | 0.9089 | 0.9587 |
| Average | 0.9003 | 0.9115 | 0.9594 |

**Table 5-7**
MAPE of driving cycles.

| Driving Cycle | MAPE (CO) | MAPE (HC) | MAPE ($NO_x$) |
|---|---|---|---|
| LA04 | 9.50% | 9.12% | 8.49% |
| ARTA | 15.56% | 16.54% | 10.15% |
| ARTC | 15.56% | 14.31% | 6.15% |
| ARTE | 5.91% | 6.11% | 0.77% |
| FWYSP | 11.96% | 10.51% | 0.74% |
| FWYA | 18.02% | 14.22% | 5.53% |
| FWYD | 0.86% | 0.33% | 2.04% |
| FWYE | 8.53% | 3.25% | 3.16% |
| FWYF | 15.86% | 9.16% | 2.48% |
| FWYG | 16.97% | 3.80% | 3.67% |
| LOCL | 10.58% | 10.45% | 8.20% |
| RAMP | 18.05% | 24.4% | 16.14% |
| ST01 | 15.91% | 15.23% | 10.05% |
| AREA | 15.36% | 10.45% | 4.37% |
| LA92 | 4.05% | 7.31% | 5.09% |
| NYC | 5.28% | 12.12% | 6.99% |

The model's performance was further investigated by applying it to the 16 driving cycles listed in Table 5-3 and calculating the MAPE of the trips for each vehicle. MAPE was used to forecast the error in estimating the emissions as a measure of performance. Table 5-7 presents the average MAPE of the vehicles for CO, HC, and $NO_x$ for each driving cycle. The MAPE did not exceed approximately 18% for any of the emissions on any of the driving cycles except for HC on RAMP. These cycles provide a good test of the model since they represent different combinations of speed and acceleration values, including aggressive driving behavior, similar to real-world driving conditions. The tests indicate that the model can be applied to different scenarios and capture different ranges and driving conditions.

Figure 5-3 illustrates the capability of VT-CPFM to capture the transient behavior of the emissions in the NYC driving cycle. Figure 5-3 demonstrates the correspondence of the emission estimates with MOVES data. The model had the best fit and highly correlated with $NO_x$, which was expected from the goodness of fit and MAPE values. However, all the emissions were consistent with the measured data and nearly within the same range, which reflects the reliability of the model. Although, VT-CPFM overestimated the emissions over MOVES, this could be because MOVES averages the emission rates over LDVs, whereas VT-CPFM focuses on each vehicle's parameters individually to estimate the emissions based on the each vehicle's specific characteristics. Overall, the estimates and measured data behave similarly based on the resulting engine load from driving conditions.

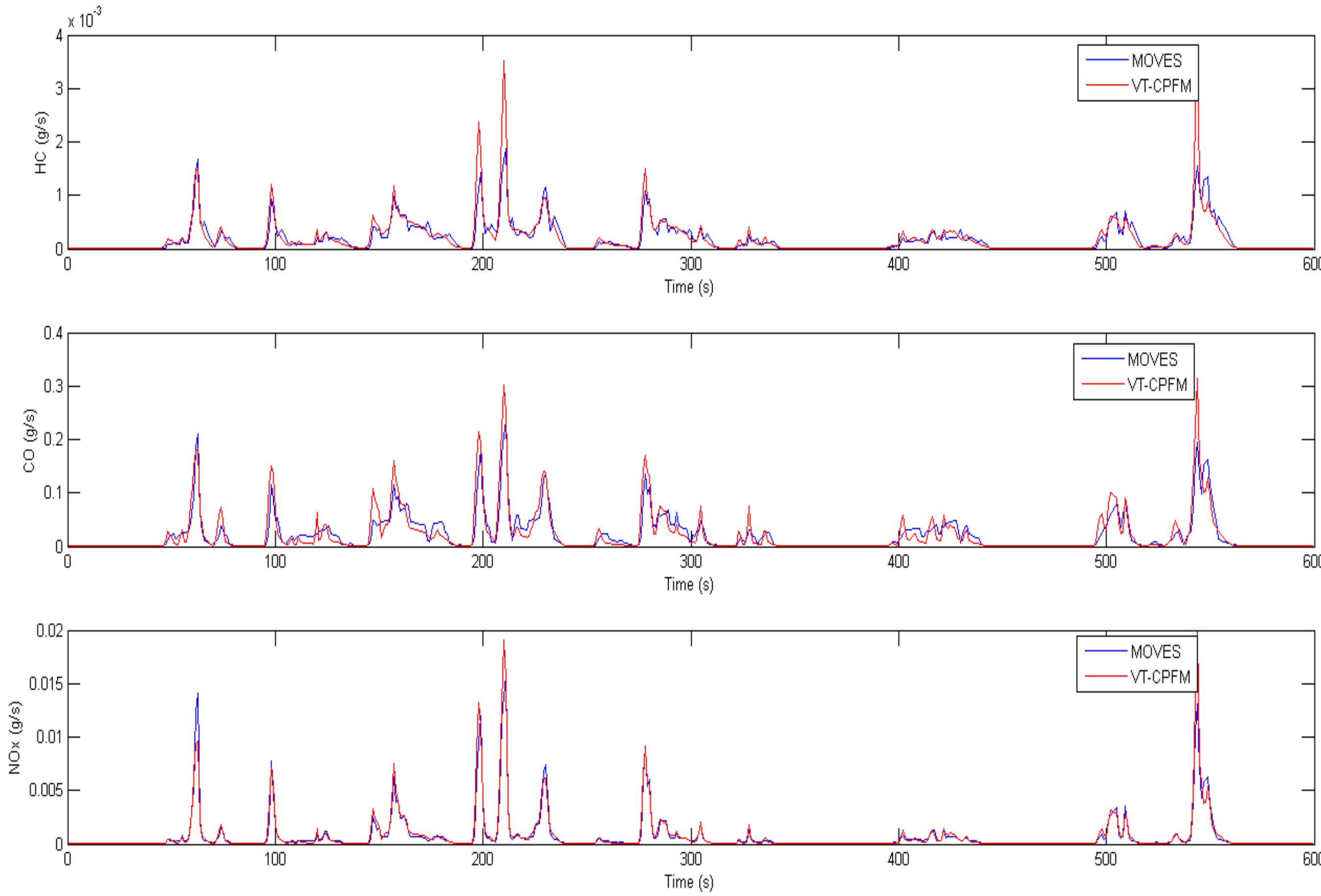



**Figure 5-3 Honda Accord estimated emissions on NYC cycle.**

A general LDV model was also developed to capture the emissions of any LDV without the need to calibrate its coefficients. The general LDV model summarizes the tested LDVs' parameters based on model year to generalize the model for any LDV in the same year, thus requiring less time for the calibration process. Table 5-8 presents the LDV average model's MAPE for CO, HC, and $NO_x$ for the 16 driving cycles. This model provides an approximate estimate of the emissions of each tested vehicle, which can be used as a reference or to sketch out the emission profile of a vehicle. It can also be used to interpret the relationship between driving conditions and emissions rates, but for more-accurate estimates the model should be calibrated for each vehicle individually. Figure 5-4 shows the correspondence of the average model and MOVES data, where they were consistent.

**Table 5-8**
MAPE of driving cycles for LDV average model.

| Driving Cycle | MAPE (CO) | MAPE (HC) | MAPE ($NO_x$) |
|---|---|---|---|
| LA04 | 7.85% | 7.73% | 6.38% |
| ARTA | 13.28% | 14.45% | 7.87% |
| ARTC | 12.67% | 12.11% | 3.82% |
| ARTE | 3.29% | 3.74% | 1.73% |
| FWYSP | 15.92% | 15.38% | 2.45% |
| FWYA | 21.97% | 16.74% | 8.29% |
| FWYD | 2.31% | 2.51% | 0.52% |
| FWYE | 6.39% | 1.85% | 0.87% |
| FWYF | 13.64% | 6.90% | 0.01% |
| FWYG | 16.28% | 3.22% | 1.66% |
| LOCL | 9.37% | 9.27% | 6.12% |
| RAMP | 14.15% | 22.11% | 13.89% |
| ST01 | 13.48% | 13.29% | 7.87% |
| AREA | 12.94% | 8.23% | 2.00% |
| LA92 | 0.45% | 4.81% | 2.63% |
| NYC | 6.44% | 13.57% | 9.45% |

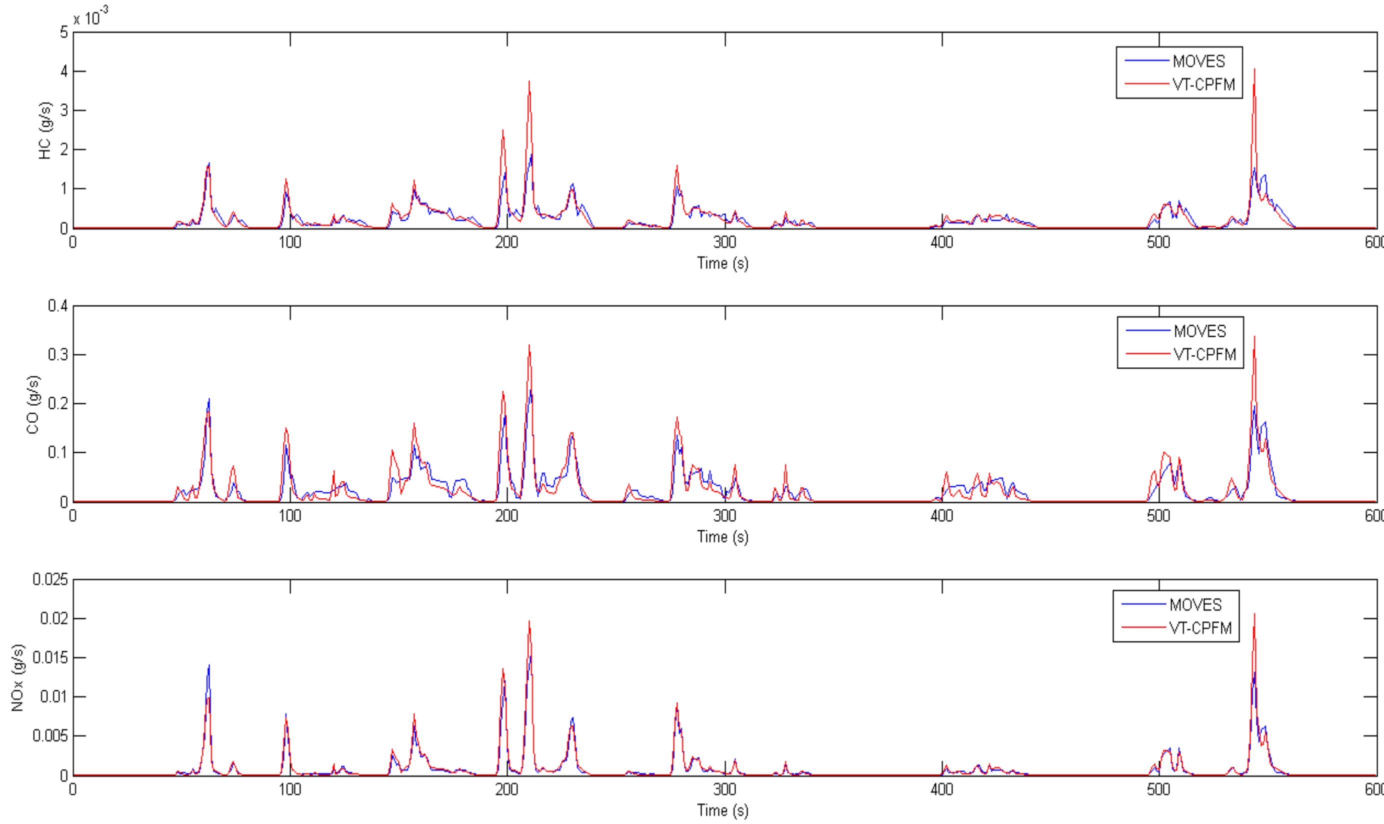



**Figure 5-4 Average LDV estimated emissions on NYC cycle.**

The emission model was tested on the vehicles to develop a generalized model. The purpose of the generalized model is to allow for the calibration of the model coefficients using publicly available vehicle parameters as input to acquire the coefficients automatically through a Matlab script similar to the concept of the VT-CPFM. The vehicle parameters were tested to examine their significance on the model to select the most significant parameters among them. The city and highway fuel economy ratings were the most significant parameters in estimating the model coefficients. Figure 5-5 illustrates the correlation between the calculated coefficients from fuel economy ratings and the coefficients calibrated from each vehicle individually. Table 5-9 lists the fuel economy ratings used in developing the generalized model. Each coefficient from the listed vehicles was the dependent variable, where the fuel economy ratings were the explanatory variables.

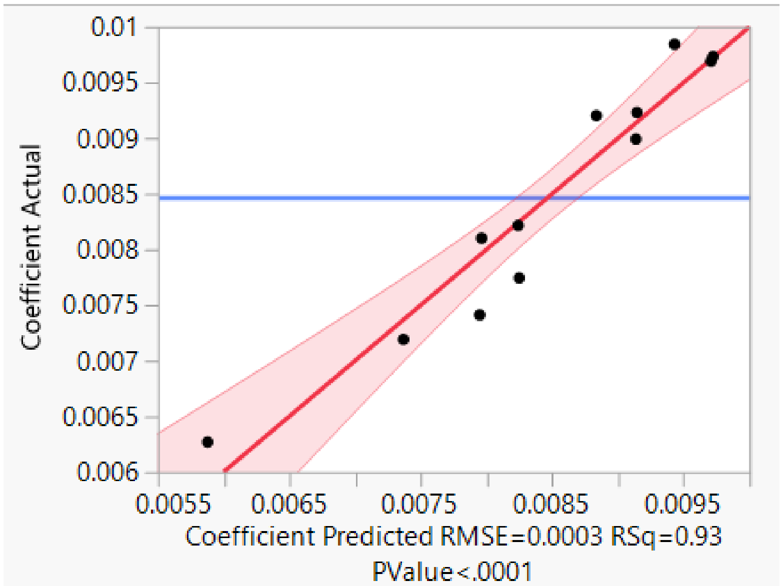
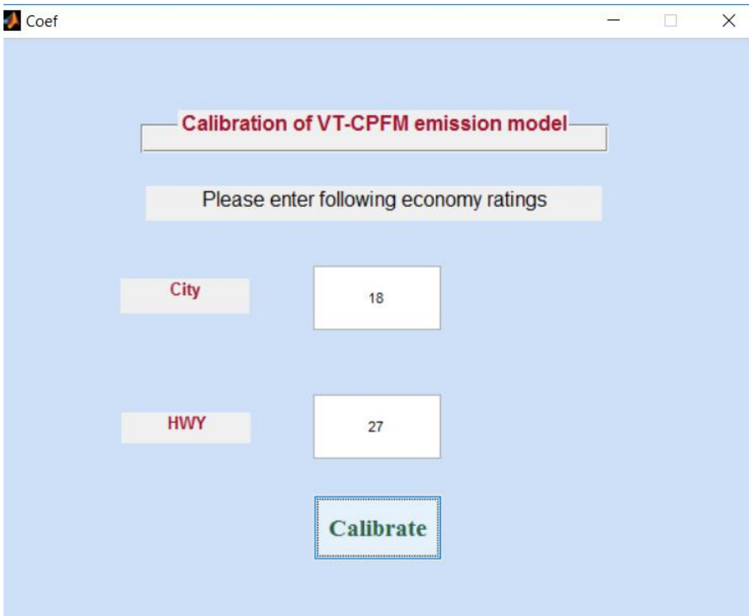



**Figure 5-5 Significance of the fuel economy ratings on model coefficients**

**Table 5-9**
Fuel economy ratings of the tested LDVs

| Vehicle | City | Hwy |
|---|---|---|
| Honda Accord | 23 | 34 |
| Honda Civic | 28 | 39 |
| Ford Focus | 28 | 38 |
| Mazda 3 | 24 | 33 |
| Toyota Camry | 25 | 35 |
| Nissan Altima | 23 | 32 |
| Ford Fusion | 23 | 33 |
| Chevrolet Cruze | 26 | 38 |
| Chevrolet Malibu | 22 | 33 |
| Hyundai Sonata | 24 | 35 |
| Chrysler 300 | 18 | 27 |
| Toyota Corolla | 27 | 34 |

The model will use the fuel economy ratings to generate the confidents for each emission automatically through Matlab graphical user interface (GUI). Figure 5-6 demonstrates the dodge charger fuel economy ratings input to generate the table of the 8 coefficients for each emission.




| | CO | HC | NOx |
|---|---|---|---|
| 1 | -0.3973 | -0.0281 | -0.0132 |
| 2 | 0.0097 | 8.4348e-04 | 9.3882e-04 |
| 3 | 875.4379 | 53.9458 | 34.7269 |
| 4 | -12.2648 | -0.3246 | -1.0265 |
| 5 | -3.4105e+05 | -8.5930e+03 | -1.1110e+04 |
| 6 | 5.4775e+03 | 253.5469 | 436.6130 |
| 7 | 4.0113e+07 | 8.5824e+05 | 1.5679e+06 |
| 8 | -5.7471e+05 | -2.2876e+04 | -4.2323e+04 |

**Figure 5-6 Generalized model emissions calibration tool**

The generated coefficents from the generalized model were applied on the emission model to compute the estimated emissions. These estimates were plotted with the second-by-second MOVES data on NYC cycle to genrate the to illustrate the correspondence between the estimates and the measured MOVES data. Figure 5-7 demonstartes the vehicle emission behavior of the MOVES data was similar the estimated emissions. Overall, the etsimates followed the same trend of the measured data.

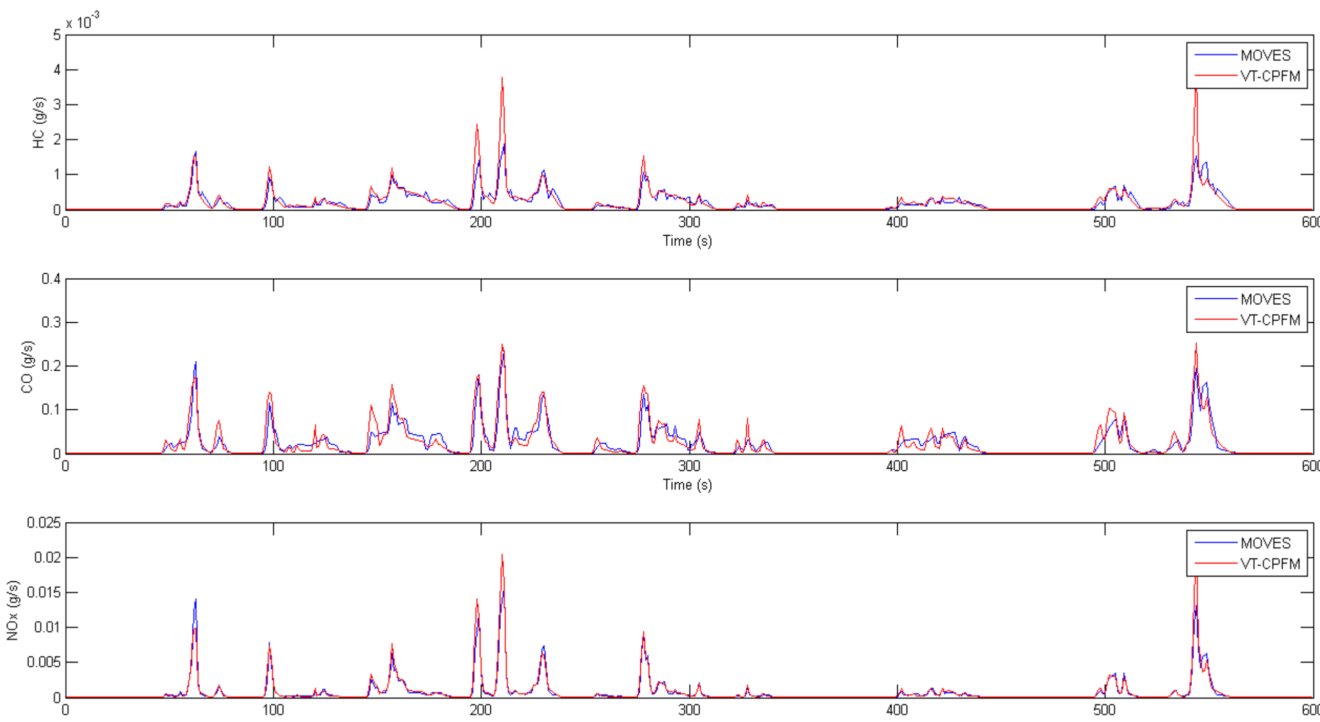



**Figure 5-7 Instantaneous generalized model emissions validation (Dodge Charger)**

## 5.6 CONCLUSIONS AND FUTURE RESEARCH

This study extended the VT-CPFM model to capture LDV emissions (CO, HC, and $NO_x$) to overcome the shortcomings of the majority of existing models. The research focused on developing a reliable emission model that is simple in its structure, which in this case consists of eight coefficients and two main variables, the instantaneous fuel estimate and speed.

The model's estimates were compared against MOVES to assess its validity. Also, the model was implemented on 16 driving cycles representing real-world driving conditions. The average coefficient of determination ($R^2$) for the emissions exceeded 0.9 for all the vehicles, and the maximum MAPE was approximately 18%. In addition, an LDV average model was developed for the same model year of the tested vehicles to provide approximate estimates for any other tested vehicle to save calibration time. The LDV average model provides an emission profile of a trip, but the prediction accuracy may be affected compared to calibrating each vehicle individually.

For future research, testing the model against real-world data from vehicles would provide an additional measure of performance to assess validity. Although the model was tested in a previous study against real-world data from ORNL gathered by the EPA and had satisfying results, the vehicles were older models manufactured from 1988 to 1997 (Abdelmegeed et al., 2015). Also, the generalized model generated promising results, however the model should include other vehicle categories as SUVs and minivans.

## ACKNOWLEDGMENTS

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# Chapter 6: Conclusions and Future Research

## 6.1 CONCLUSIONS

This research presented an effort to enhance the VT-CPFM model, which can be used to enhance the current state-of-practice vehicle emissions estimation. The research focused on constructing a simple and reliable model that could be easily calibrated and applied to estimate CO, HC and $NO_x$ emissions. Although, the model depends on fuel as the sole explanatory variable for light-duty vehicles, it can estimate the emissions more accurately by adding the speed parameter. The model maintains its consistency by utilizing instantaneous fuel estimates and speed to predict heavy-duty diesel truck emissions. The model overcomes two major shortcomings that most existing models suffer from, namely; it does not produce a bang-bang control system and uses publicly available data to calibrate model parameters. The model for the two classifications of vehicles was calibrated and validated using cross validation methods. Furthermore, the performance of the model was further investigated and validated against other current state-of-the-practice models. Although the model does not use extensive data to calibrate the model parameters and does not require special devices to measure required data, it resulted in approximately better estimates than current state-of-the-art models. The applicability of the model was tested on various vehicles to show consistency in results. The same model can be used to estimate the three types of emissions. In addition, the simplicity of the model will save time and money.

### 6.1.1 Developing VT-CPFM to estimate LDVs emissions

- The model includes instantaneous fuel estimates and speed to simplify the model utilization.
- The estimated emission rates were highly correlated to in-field data. In addition, the model performance was evaluated by comparing the model against VT-Micro estimates, which had a good fit for CO, HC and $NO_x$.
- The model was tested and compared with MOVES data developed by EPA, which revealed the model robustness.
- The recent data were used to demonstrate the applicability of the proposed model on newer vehicle technologies.
- The model was tested on older and recent vehicle models to reveal the consistency in results.
- The model was implemented on 16 driving cycles to ensure the validity of the model.
- The developed average model provides emission profiles for the trip to save calibration time. However to improve the accuracy of the estimates, the model should be calibrated individually on each vehicle.

### 6.1.2 Heavy-duty diesel trucks emission model based on VT-CPFM

- The same model structure of LDVs was used to ensure its reliability and applicability on different vehicles classifications and characteristics.
- The model was calibrated and validated based from data provided by the University of California, Riverside. The eight HDDTs had accurate estimates based on $NO_x$ good fit which is the key target emission.
- The performance of the model was further investigated by comparing the estimates against CMEM model structure. The average $R^2$ values of CO, HC and $NO_x$ were higher than

CMEM revealing the robustness of the model. Also, the SMAPE and MAPE of the model were lower than CMEM.

### 6.2 FURTHER RESEARCH

The following recommendations can be pursued to expand and enhance the current research work:

- With regards to future work, recent HDDT data should be utilized to demonstrate the applicability of the proposed model on newer vehicle technologies such as such as selective catalytic reduction (SCR) on vehicle emissions. Given that the VT-CPFM focuses on developing tailpipe emissions directly, where the specifics of the engine and the exhaust system is not needed to develop the model, it is anticipated that this should not be challenging.

- It would be better if EPA recommends that truck manufacturers provide the fuel economy ratings of trucks to save time in calibrating the VT-CPFM model coefficients.

- Also, real-world data for later LDVs should be used to capture the impact of emerging technologies since MOVES data were only used for recent models. Although, it was not easy to acquire these data by contacting different organizations, the data were either not complete or there were errors in collecting them which resulted in inconsistency in their estimation. Moreover, there were attempts to collect the emission data over 8 months with AxionGO which is a portable emissions measurement system (PEMS). However, the device could not estimate the mass of the emissions due to errors in the sensors.

- Further research may be conducted to generalize the model on any light-duty vehicle model where the parameters do not have to be calibrated manually for each dataset. Other vehicle categories such as: minivans and light-duty trucks (LDTs) should be tested and included in the modeling procedure. However, preliminary analysis revealed that the model coefficients can be estimated directly from EPA city and highway fuel economy ratings only.

# Appendix A

**Matlab code to calibrate the model**

Simplified code to generate the model coefficients with or without another dataset to validate the model

```
%% Subaru Data
Subaru_Data=xlsread('ORNL_Data.xlsx','Subaru','H2:M1478');
Subaru_speed=Subaru_Data(:,1);
Subaru_acc=Subaru_Data(:,2);
Subaru_fuel=Subaru_Data(:,3);
Subaru_CO=Subaru_Data(:,4);
Subaru_HC=Subaru_Data(:,5);
Subaru_NOx=Subaru_Data(:,6);
% Power and Resistance calculation
H=0;
rho=1.2256;
Cd=0.35;
Ch=1-0.085.*H;
Af=1.8362;
m=1350;
Cr=1.75;
c1=0.0328;
c2=4.575;
% resistance formula
R_Subaru=(rho/25.92)*Cd*Ch*Af.*((Subaru_speed).^2)+9.8066*m*(Cr/1000)*
(c1.*(Subaru_speed)+c2)+9.8066*m*0;
% Power on  formula
P_Subaru=(((R_Subaru+m.*(1.04.*Subaru_acc))./(3600.*0.92))).*(Subaru_s
peed);

%fuel consumption rate from VT-CPFM
F_Subaru=zeros(length(P_Subaru),1);
for i=1:length(P_Subaru)
    if(P_Subaru(i)>=0)
F_Subaru(i)=0.00033831+(0.00013049)*P_Subaru(i)+(1e-6)*P_Subaru(i)^2;
    else

F_Subaru(i)=0.00033831;
    end
end

% Calibration and validation of the model
HCE=[]
for i=1:100 % number of simulation (cross validation)
    t_fuel=F_Subaru; % save your orginal data (predictrors)
    t_velocity=Subaru_speed;
    t_HC=(sqrt(Subaru_HC)); %save our orignal response
   t_ones=ones(length(Civic_emission),1);
ind=randsample(length(Civic_emission),floor(length(Civic_emission)*0.3
)); % choose the raws randomly into 70/30
    Fuel_test=t_fuel(ind); % get the test (predictor)
   V_test=t_velocity(ind);
```

```
    t_fuel(ind)=[];% get the training data (predictor)
    t_velocity(ind)=[];
    HC_test=t_HC(ind);% get the test (response)
    t_HC(ind)=[];% get the training (response)
    test=t_ones(ind);
    t_ones(ind)=[];

   % x=[t_ones t_fuel t_fuel.^2 t_fuel.^3]; % Construct your x matrix
without speed
       x=[t_ones t_velocity t_fuel t_velocity.*t_fuel t_fuel.^2
t_velocity.*t_fuel.^2 t_fuel.^3 t_velocity.*t_fuel.^3]; % Construct
your x matrix with speed paramter
   % BETA=inv(x'*x)*x'*t_HC;% Estimae the model Coeficients
   BETA=inv(x'*x)*x'*t_HC;
    HCE=[HCE BETA]; % save the HCeficients
    estimates=mean(HCE');  %get the mean of Coeficients
   % pred=[test Fuel_test Fuel_test.^2 Fuel_test.^3]*BETA;
    pred=[test V_test Fuel_test V_test.*Fuel_test Fuel_test.^2
V_test.*Fuel_test.^2 Fuel_test.^3  V_test.*Fuel_test.^3]*BETA;

    SST=sum((HC_test-mean(HC_test)).^2);
    SSE=sum(((HC_test-pred).^2));
    R2(i)=1-(SSE/SST); %

    estimates=mean(HCE');             %resulted coefficients
    SMAPE(i)=mean((abs(HC_test-pred))./((HC_test+pred)./2));
    MAPE_HC(i)=(abs(sum(HC_test)-sum(pred)))./sum(HC_test);
end
R2=mean(R2)
```

**Calibration of the model without dividing the data, if there is another dataset**

```
Subaru_emission=sqrt(Subaru_HC);
tbl=table(Subaru_emission,Subaru_speed,F_Subaru,'VariableNames',{'Suba
ru_emission','Subaru_speed','F_Subaru'});
 modelspec='Subaru_emission~Subaru_speed*F_Subaru^3';
 md1=fitlm(tbl,modelspec)
```

# Appendix B

The environmental Protection Agency and the National Highway Traffic Safety Administration (NHTSA), DOT have developed greenhouse gas (GHG) emissions and fuel efficiency standards for heavy and medium-duty vehicles (DieselNet, 2017).

The GHG emissions and fuel efficiency standards were developed based on two phases:

1. Phase 1 regulation: it covers model years (MY) 2014-2018.
2. Phase 2 regulation: it applies to MY 2021-2027 vehicles and was published on August 16, 2016.

The combination tractors standards were adopted based on three categories: weight class, cab height and roof height as represented in table B-1 (DieselNet, 2017).

Table B-1 Final Phase 1 (2017) and Phase 2 (2027) combination tractor standards

| Category | EPA $CO_2$ Emissions g/ton-mile | | | NHTSA Fuel Consumption gal/1,000 ton-mile | | |
|---|---|---|---|---|---|---|
| | Low Roof | Mid Roof | High Roof | Low Roof | Mid Roof | High Roof |
| Final Phase 1 Standards (2017) | | | | | | |
| Day Cab Class 7 | 104 | 115 | 120 | 10.2 | 11.3 | 11.8 |
| Day Cab Class 8 | 80 | 86 | 89 | 7.8 | 8.4 | 8.7 |
| Sleeper Cab Class 8 | 66 | 73 | 72 | 6.5 | 7.2 | 7.1 |
| Final Phase 2 Standards (2027) | | | | | | |
| Day Cab Class 7 | 96.2 | 103.4 | 100.0 | 9.44990 | 10.15717 | 9.82318 |
| Day Cab Class 8 | 73.4 | 78.0 | 75.7 | 7.21022 | 7.66208 | 7.43615 |
| Sleeper Cab Class 8 | 64.1 | 69.6 | 64.3 | 6.29666 | 6.83694 | 6.31631 |
| Heavy-haul Class 8 | 48.3 | | | 4.74460 | | |

Table B-2 lists the engine-based standards must be met by heavy-heavy-duty (HHD) and medium-heavy-duty (MHD) diesel engines used in tractors (DieselNet, 2017).

Table B-2 Engine standards for engines installed in tractors (SET cycle)

| Category | Year | $CO_2$ Emissions | Fuel Consumption* |
|---|---|---|---|
| | | *g/bhp-hr* | *gallon/100 bhp-hr* |
| MHD Engines | 2014 | 502 | 4.93[a] |
| | 2017 | 487 | 4.78 |
| | 2021 | 473 | 4.6464 |
| | 2024 | 461 | 4.5285 |
| | 2027 | 457 | 4.4892 |
| HHD Engines | 2014 | 475 | 4.67[a] |
| | 2017 | 460 | 4.52 |
| | 2021 | 447 | 4.3910 |
| | 2024 | 436 | 4.2829 |
| | 2027 | 432 | 4.2436 |

* Equivalent NHTSA standards based on 10,180 g $CO_2$ per gallon of diesel
[a] Voluntary in MY 2014 and MY 2015.

Table B-3 demonstrates the emission standards of commercial trailers based on phase 2 (DieselNet, 2017).

Table B-3 Final (MY 2027) standards for full-aero box vans

| Category | | EPA $CO_2$ Emissions | NHTSA Fuel Consumption |
|---|---|---|---|
| | | *g/ton-mile* | *gal/1,000 ton-mile* |
| Dry Van | Long | 75.7 | 7.43615 |
| | Short | 119.4 | 11.7288 |
| Refrigerated Van | Long | 77.4 | 7.60314 |
| | Short | 123.2 | 12.10216 |

Table B-4 Phase 1 final (MY 2017) vocational vehicle standards

| Category | EPA $CO_2$ Emissions | NHTSA Fuel Consumption |
|---|---|---|
| | *g/ton-mile* | *gal/1,000 ton-mile* |
| Light Heavy Class 2b-5 | 373 | 36.7 |
| Medium Heavy Class 6-7 | 225 | 22.1 |
| Heavy Heavy Class 8 | 222 | 21.8 |

Table B-5 Phase 2 final (MY 2027) vocational vehicle standards

| Category | EPA $CO_2$ Emissions g/ton-mile | | | NHTSA Fuel Consumption gal/1,000 ton-mile | | |
|---|---|---|---|---|---|---|
| | Urban | Multi-purpose | Regional | Urban | Multi-purpose | Regional |
| Vehicles with CI engines | | | | | | |
| Light Heavy Class 2b-5 | 367 | 330 | 291 | 36.0511 | 32.4165 | 28.5855 |
| Medium Heavy Class 6-7 | 258 | 235 | 218 | 25.3438 | 23.0845 | 21.4145 |
| Heavy Heavy Class 8 | 269 | 230 | 189 | 26.4244 | 22.5933 | 18.5658 |
| Vehicles with SI engines | | | | | | |
| Light Heavy Class 2b-5 | 413 | 372 | 319 | 46.4724 | 41.8589 | 35.8951 |
| Medium Heavy Class 6-7 | 297 | 268 | 247 | 33.4196 | 30.1564 | 27.7934 |

Table B-6 represents the Engine standards for light heavy-duty (LHD), medium heavy-duty (MHD), heavy heavy-duty (HHD) diesel engines and for heavy-duty gasoline engines (DieselNet, 2017).

Table B-6 Engine standards for engines installed in vocational vehicles (FTP cycle)

| Category | Year | $CO_2$ Emissions | Fuel Consumption* |
|---|---|---|---|
| | | *g/bhp-hr* | *gallon/100 bhp-hr* |
| LHD Engines | 2014 | 600 | 5.89[a] |
| | 2017 | 576 | 5.66 |
| | 2021 | 563 | 5.5305 |
| | 2024 | 555 | 5.4519 |
| | 2027 | 552 | 5.4224 |
| MHD Engines | 2014 | 600 | 5.89[a] |
| | 2017 | 576 | 5.66 |
| | 2021 | 545 | 5.3536 |
| | 2024 | 538 | 5.2849 |
| | 2027 | 535 | 5.2554 |
| HHD Engines | 2014 | 567 | 5.57[a] |
| | 2017 | 555 | 5.45 |
| | 2021 | 513 | 5.0393 |
| | 2024 | 506 | 4.9705 |
| | 2027 | 503 | 4.9411 |
| HD Gasoline Engines | 2016 | 627 | 7.06 |

* Equivalent NHTSA standards based on 10,180 g $CO_2$ per gallon of diesel
[a] Voluntary in MY 2014 and MY 2015.

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# Appendix C

**The coefficents of the developed model based on MOVES data listed in the following tables:**

**Table C-1 HC Model Coefficients**

| Vehicle | *a* | *b* | *c* | *d* | *e* | *f* | *g* | *h* |
|---|---|---|---|---|---|---|---|---|
| Honda Accord | -0.01302 | 0.000951 | 44.252 | -1.364 | -18956 | 783.120 | 3955400 | -109690 |
| Honda Civic | -0.00673 | 0.000808 | 38.527 | -1.288 | -17800 | 860.610 | 4605900 | -134070 |
| Ford Focus | -0.00474 | 0.000730 | 34.848 | -1.091 | -15170 | 715.120 | 3721600 | -106840 |
| Mazda 3 | -0.00478 | 0.000750 | 28.035 | -0.937 | -10035 | 504.250 | 2114900 | -61927 |
| Toyota Camry | -0.00641 | 0.000776 | 33.039 | -1.035 | -12918 | 590.910 | 2742300 | -78216 |
| Nissan Altima | -0.00754 | 0.000817 | 32.830 | -1.054 | -12417 | 569.990 | 2525200 | -72352 |
| Ford Fusion | -0.01098 | 0.000897 | 40.174 | -1.245 | -16563 | 702.750 | 3417500 | -95527 |
| Chevrolet Cruze | -0.01139 | 0.000899 | 46.507 | -1.412 | -21773 | 903.430 | 5033400 | -139350 |
| Chevrolet Malibu | -0.01289 | 0.000941 | 41.495 | -1.263 | -16646 | 681.370 | 3242500 | -89492 |
| Hyundai Sonata | -0.01019 | 0.000880 | 39.853 | -1.247 | -16734 | 723.050 | 3569800 | -100420 |
| Chrysler 300 | -0.01343 | 0.000935 | 34.251 | -1.003 | -11018 | 434.420 | 1688500 | -45783 |
| Toyota Corolla | -0.00761 | 0.000769 | 38.755 | -0.174 | -1052 | 254.050 | -89464 | -21917 |

**Table C-2 $NO_x$ Model Coefficients**

| Vehicle | *a* | *b* | *c* | *d* | *e* | *f* | *g* | *h* |
|---|---|---|---|---|---|---|---|---|
| Honda Accord | -0.02749 | 0.000849 | 67.514 | -0.418 | -12241 | 441.820 | 1468800 | -53244 |
| Honda Civic | -0.01578 | 0.000807 | 56.197 | -0.347 | -5189 | 467.370 | 432040 | -55373 |
| Ford Focus | -0.01330 | 0.000787 | 55.028 | -0.266 | -6679 | 397.690 | 725250 | -47150 |
| Mazda 3 | -0.01263 | 0.000792 | 41.541 | -0.235 | -2209 | 272.480 | 77200 | -24513 |
| Toyota Camry | -0.01612 | 0.000799 | 51.532 | -0.269 | -6278 | 329.410 | 641430 | -35323 |
| Nissan Altima | -0.01769 | 0.000810 | 49.676 | -0.288 | -5513 | 315.470 | 523320 | -32168 |
| Ford Fusion | -0.02399 | 0.000833 | 61.636 | -0.366 | -10042 | 395.240 | 1150000 | -45582 |
| Chevrolet Cruze | -0.02505 | 0.000833 | 72.556 | -0.416 | -14416 | 511.450 | 1905000 | -67872 |
| Chevrolet Malibu | -0.02754 | 0.000846 | 64.087 | -0.384 | -11214 | 385.820 | 1269200 | -43854 |
| Hyundai Sonata | -0.02250 | 0.000828 | 60.827 | -0.362 | -9514 | 405.070 | 1094200 | -47189 |
| Chrysler 300 | -0.02924 | 0.000844 | 54.600 | -0.304 | -8439 | 248.760 | 777100 | -23142 |
| Toyota Corolla | -0.00165 | 0.000654 | 24.984 | -0.819 | -8804 | 471.550 | 2011200 | -59242 |

**Table C-3 CO Model Coefficients**

| Vehicle | *a* | *b* | *c* | *d* | *e* | *f* | *g* | *h* |
|---|---|---|---|---|---|---|---|---|
| Honda Accord | -0.40332 | 0.009843 | 1150.500 | -16.196 | -613890 | 9845.700 | 109680000 | -1531600 |
| Honda Civic | -0.27270 | 0.008100 | 1090.500 | -15.248 | -694070 | 11048.000 | 149260000 | -1995600 |
| Ford Focus | -0.20828 | 0.007191 | 928.000 | -12.785 | -560190 | 9046.400 | 114050000 | -1552000 |
| Mazda 3 | -0.22990 | 0.007411 | 796.760 | -11.046 | -407830 | 6488.700 | 70695000 | -935110 |
| Toyota Camry | -0.24885 | 0.007743 | 878.260 | -12.179 | -463120 | 7467.700 | 82224000 | -1125900 |
| Nissan Altima | -0.28227 | 0.008215 | 891.000 | -12.447 | -450910 | 7236.800 | 76858000 | -1048000 |
| Ford Fusion | -0.35610 | 0.009201 | 1051.100 | -14.744 | -550520 | 8846.000 | 96674000 | -1343900 |
| Chevrolet Cruze | -0.35997 | 0.009230 | 1195.300 | -16.714 | -704420 | 11330.000 | 139000000 | -1942800 |
| Chevrolet Malibu | -0.39652 | 0.009733 | 1067.700 | -14.988 | -532520 | 8548.300 | 88877000 | -1244200 |
| Hyundai Sonata | -0.34013 | 0.008991 | 1052.900 | -14.765 | -567650 | 9120.400 | 102730000 | -1422100 |
| Chrysler 300 | -0.39745 | 0.009691 | 853.790 | -11.894 | -337310 | 5417.800 | 44483000 | -627540 |
| Toyota Corolla | -0.13990 | 0.006269 | 703.210 | -9.565 | -380980 | 6073.300 | 70187000 | -913590 |