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Proof of Concept Investigation for the Physical Emission Rate Estimator (PERE) to be Used in MOVES

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Assessment and Standards Division
Office of Transportation and Air Quality
U.S. Environmental Protection Agency

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Proof of Concept Investigation for the Physical Emission Rate Estimator (PERE) for MOVES

By Edward K. Nam
Ford Research and Advanced Engineering

ABSTRACT

The new EPA mobile source inventory model, Multi-scale mOtor Vehicle & equipment Emission System or MOVES, is an ambitious effort to model emissions from the micro to the macro level. To maintain consistency across the scales, a road load based quantity known as Vehicle Specific Power, or VSP, has been chosen as the primary causal variable in emissions formation for modeling purposes. This work attempts to take the physical link between driving activity and emissions one step further by introducing the Physical Emission Rate Estimator (PERE). PERE is meant to supplement the data driven portion of MOVES and fill in gaps where necessary. The model is essentially an effort to simplify, improve and implement the Comprehensive Modal Emissions Model (CMEM) developed at University of California, Riverside. PERE is based on the premise that for a given vehicle, (engine out) running emissions formation is dependent on the amount of fuel consumed. As such, it models fuel rate as well as CO_2 generation with some degree of accuracy, which is the first step in the MOVES development. Being a physically based model, it has the potential (with some modification) to model new technologies (vehicles meeting new emissions standards), deterioration, off-road sources, I/M programs, as well as being able to easily extrapolate to areas where data are sparse. It may even save in data taking costs in the long run. Before the concepts in PERE can be implemented however, it must be demonstrated to work in a limited case scenario. This paper is an attempt to demonstrate the feasibility of PERE on a sample of (hot running and non hi-emitting) Tier 1 vehicles. It is shown that the fuel consumption and CO_2 predictions were reasonably accurate for an independent driving sample, though uncertainty remains about a possible 'speed' effect. Fuel and CO_2 is the first installment of MOVES and is discussed in some detail in this paper.

The second part of this paper deals mainly with criteria pollutants. The engine out behavior is demonstrated to be relatively steady across engine families and for Tier 1 vehicles. This allows the model, which is calibrated to only a few samples of engine data, to be generalized to other data sets, where only tailpipe measurements are available. The engine out model is demonstrated to be reasonably accurate; both in estimating VSP based as well as total cumulative emissions. The catalyst (or tailpipe) portion of the model introduces some additional complexities, where it is demonstrated that VSP or fuel rate is not the only explanatory variable in emissions formation. A speed (or aggressivity) factor is encountered in the analysis, which needs to be investigated further. It is possible that the emissions will need to be further subdivided into modes of driving. This model is preliminary and will require more research, however, the initial validation looks promising.

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INTRODUCTION

The next generation emissions EPA inventory model: Multi-scale mOtor Vehicle & equipment Emission System or MOVES, is being designed with the recommendations of the National Research Council report in mind (2000). The report made many suggestions for the improvement of the MOBILE series of models. Subsequent EPA shootout projects proposed various alternatives to the MOBILE approach (Hart, et al., 2002). Based on these shootout projects, MOVES is tentatively designed so that emission rates would be derived from a road load based criterion known as Vehicle Specific Power (VSP). This is an effort to include more of a physical basis to the model, rather than relying on average driving cycle speeds, which may be too aggregate to correlate to finer scale emissions. The emission rates are determined from a look-up table of VSP bins, whose cells are occupied by various data sources (On-board emissions, dynamometer, I/M, Remote Sensing, etc) statistically combined. The model therefore is physically based but primarily data driven.

There are several approaches, which may be considered to supplement such a model. An alternative to a data driven statistical model is one that is guided more on physical principles. In contrast to binning data, a parameterized analytical function can be fitted to the data. Additionally, in lieu of aggregating the emissions from normal and hi-emitters from the real-world fleet into means or bins, the vehicle mix can be disaggregated and the emissions factors can be adjusted by this mix (this is what MOBILE does presently). The approaches are summarized in the table below: It is important to note that the approaches are not necessarily mutually independent, and that a spectrum of methodologies may exist between the extremes. By this nomenclature, the VSP approach is physical, binned, and fleet averaged. MOBILE, which is a macroscopic model is more statistical, parameterized, with disaggregated normal/hi emitters.

Table 1: The contrasting modeling approaches to calculating microscopic emissions factors for a fleet. The left side is generally more disaggregate or microscopic. The VSP approach is marked with a '√'.

Physical √	Statistical
Parameterized	Binned √
Normal/Hi Emitter Split	Normal/Hi Emitter aggregate √

There are two "modal" model systems, which enjoy some popular use. The first was developed mostly at Georgia Institute of Technology in a series of papers by Fomunung, Washington, Guensler, Bachman, and others. MEASURE is a model that predicts light duty vehicle emissions based on their operating conditions all within a GIS framework. The operating conditions are defined by their modes of operation, such as acceleration, cruise, deceleration and idle. The trip-

based emission rates are determined using a statistical approach of weighting the causal factors in a single equation for each criteria pollutant. These factors include average speed, proportion of driving within the modes of driving, transmission type, odometer, injector type, catalyst type, etc. The model is advantageous in many ways: it is capable of being calibrated with bag data, it is statistically robust, validation has been performed, and it is incorporated into a GIS framework. However, there are some disadvantages to this approach: it is limited in its ability to model control strategies as well as future fleet emissions; being a statistical model, there are no set physical limitations to the calibrated parameters. Physically, there are correlations between some of the variables, which may be more easily 'teased out' using a more physical model. However, there are many aspects of MEASURE, which influence the development of MOVES.

Another popular approach was developed mostly at the University of California, Riverside (CE-CERT) in a series of papers by Barth, An, Ross, Scora, Younglove, Levine (Malcolm), Wenzel, et al. The Comprehensive Modal Emissions Model, or CMEM, is based on physical principles, which derived a fuel rate from road-load and simple powertrain model. Emissions rates are then derived empirically from the fuel rate. The model has been validated in a number of studies for typical (or composite) vehicles and has the potential to model a wide variety of light as well as heavy-duty vehicles. CMEM will be described in greater detail in a later section.

This work is a proof of concept developing a physical parameterized model methodology from a subset of the data, namely "normally emitting" Tier 1 light duty vehicles. The first section describes the load-based emissions methodology, be it vehicle specific power, or fuel rate (both very similar). It also discusses and develops the fuel rate based methodology based on CMEM. This is the portion of the model that will output the fuel consumption as well as CO_2 emissions. Part II describes the model development process for the Physical Emission Rate Estimator (PERE), based on CMEM principles, potentially to be used in some similar form in MOVES. The section also describes the calibration of engine out (pre catalyst) and tailpipe (post catalyst) emissions to parametric functions. All of the analysis is for hot running operation. Cold start may have a significant impact on some of the trends and generalizations made in this paper, but will be a subject of a future study. Part III describes the validation that has been accomplished thusfar. A number of appendices supplement this paper, which explore tangential issues important to the development of the modeling methodology.

I - LOAD BASED APPROACH

Vehicle Specific Power

The current plan for MOVES is to use Vehicle Specific Power (VSP) as a variable on which their emission rates can be based (Koupal et al, 2002). The VSP approach to emissions characterization was developed by Jimenez-Palacios (1999). VSP is a measure of the road load on a vehicle; it is defined as the power per unit mass to overcome road grade, rolling & aerodynamic resistance, and inertial acceleration:

$$VSP = v * (a*(1+\varepsilon) + g*grade + g*C_R) + 0.5\rho*C_D*A*v^3/m \qquad (1)$$

where:

v: is vehicle speed (assuming no headwind) in m/s
a: is vehicle acceleration in m/s^2
ε: is mass factor accounting for the rotational masses (~0.1)
g: is acceleration due to gravity
grade: is road grade
C_R: is rolling resistance (~0.0135)
ρ: is air density (1.2)
C_D: is aerodynamic drag coefficient
A: is the frontal area
m: is vehicle mass in metric tonnes.

The equation can also have an added vehicle accessory loading term (air conditioner being the most significant) added to it. Moreover, higher order terms in rolling resistance can be added to increase accuracy of the model (Gillespie, 1992). Using typical value of coefficients, in SI units the equation becomes (C_DA/m ~ 0.0005):

$$VSP\ (kW/metric\ Ton) = v * (1.04*a + 9.81*grade(\%) + 0.132) + 0.00121*v^3 \qquad (2)$$

If future technologies such as low rolling resistance tires, and aerodynamic designs, vary these values significantly, that can be reflected with a change in the equation. It should be noted that the while it may be reasonable to assume typical values for rolling and aerodynamic resistance constants, it may pose a problem to assume a single mass for all cars (or vehicle types). There is approximately a factor of 2 difference in C_DA/m between an empty compact car and a full large passenger car (Jimenez, 1999). Using a single value for all LDVs (for example) can result in a significant error (in VSP) at high speeds when the aerodynamic resistance term dominates and when feedgas emissions are relatively high.

In this form, the VSP equation is physically based, but the emissions generated from it would be empirical. Looking at vehicle engine out emission trends as a function of this road load variable seems to give reasonably good correlation, even among different vehicles, as we shall demonstrate later.

This binning method easily lends itself to emissions factor generation. Data from Portable Emissions Measurement Systems (PEMS) and other sources can be used to populate each bin.

The main vehicle parameters required to obtain the emissions factor are (instantaneous) speed, and acceleration. If the more detailed equation 1 is used, then the vehicle mass and road grade are also required. As such, the model could also be used to quantify second-by-second emissions (g/sec). It could also be integrated with a microscopic traffic model to quantify emissions from a set of vehicles.

While it would be more accurate to fill these bins with engine out data, this is not often possible due to the scarcity of such data. The original approach, as described in Hart et al (2002) and Frey et al. (2002), fills these bins with tailpipe data. Throughout this paper, we will discuss both means of modeling, and will specify whether engine out or tailpipe data are being used.

This approach to emissions characterization has been widely accepted in the Remote Sensing Detection (RSD) community. This due to the fact that RSD measures road-side tailpipe emissions at a particular moment in time, and since the VSP method can be independent of vehicle mass, the calculations (and data taking) are simplified. Because of the static nature of RSD, the emissions values tend to be correlated to a particular road-load or VSP point, which can be directly measured. Quantifying the VSP allows for comparison between different measurement sites as well as with other types of modal data, such as those obtained from some dynamometer tests.

Figure 1 shows a sample NOx tailpipe emissions profile taken from a PEMS source. The curve is familiar to emissions modelers, where low load driving produces less emissions than higher load driving. One logical approach to modeling this effect would be to fit the emission curve to a smooth analytical function such as the following:

$$\mathrm{NOx} = a + b*\mathrm{VSP} + c*\mathrm{VSP}^2 + d*\mathrm{VSP}^3 + \ldots \qquad (3)$$

where *a, b, c, d*... are fitted parameters using perhaps least squares regression. With this parameterized function, data can be more easily interpolated and extrapolated to regions where data “holes” exist. This semi-empirical method of modeling emissions is approaching the physically based method used by UC Riverside.

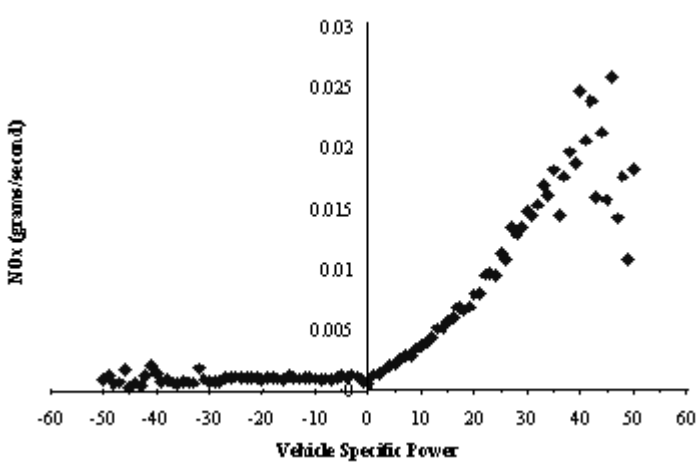

Figure 1 – A sample of NOx emissions as measured by PEMS.

Physical Parameterized (Fuel Rate) Approach

If the vehicle emissions system were modeled as a complete physical system, with as much physical detail as existing data permits, this would presumably result in the most "robust" prediction. Since tailpipe emissions formation is a physical process, one should be able to model this system in this fashion. Therefore, starting with a microscopic basis is likely to lead to a more robust model (though the results are not guaranteed to be more accurate in every case). It could be argued that a detailed microscopic model could be used as the building blocks for more aggregate macroscopic models, whereas one cannot easily derive a microscopic model based on a macroscopic one. Of course, the limiting factor in each of these models is the uncertainty in the activity input. The most microscopic modeling that occurs for vehicle emissions involves the characterization of the chemistry and physics of in-cylinder combustion combined with thermal, transport and catalytic chemistry aftertreatment processes. This level of modeling obviously requires knowledge of engine, catalyst, fuel parameters, etc, which are unknowable for the typical car in the fleet. It also assumes a level of knowledge of the manufacturer's engine calibration strategies, which are highly proprietary.

The most microscopic emissions model, which can be practically applied to a typical car in a technology class is exemplified by the Comprehensive Modal Emissions Model (CMEM) developed at the UC Riverside (there are others). This model has been tested and validated under a variety of conditions (Barth et al., 2000).

Quite simply CMEM takes the ubiquitous tractive road-load relation in equation 1 and combines it with a simple engine/transmission powertrain model to calculate a fuel rate. Fuel rate, or fuel consumption per unit time, forms the basis for CMEM, much as VSP forms the basis for the previous method. The basic independent variables are still speed and acceleration. The tractive (or brake) power (in kW) from equation 1 can be simplified to:

$$P_b(m,v,a) = A*v + B*v^2 + C*v^3 + m*v*(a* + g\sin\theta) \quad (4)$$

where

A, B, C, are rolling and aero resistive coefficients determined from dynamometer coast-down tests. The A and B coefficients are equivalent to the rolling resistance terms of equation 1 and the C coefficient represents the air drag coefficients.

If we assume a mass, and typical vehicle coefficients (as was done in eq 2), we would get nearly the identical results as equation 2. Hence these approaches are fundamentally similar. In fact a very simple conversion equation can be derived:

$$P_b(m,v,a) \fallingdotseq VSP * m \quad (5)$$

The mass independence of VSP is one of the strengths of the variable, as we mentioned earlier. However, vehicle mass (even among LDVs) may be a significant variable (Frey et al, 2002). CMEM goes on to further calculate fuel consumption rate, FR (g/s):

$$FR = \varphi * [K(N)*N(v)*V_d + P_b(m,v,a)/\eta + Pacc(T,N)/\eta] / LHV \quad (6)$$

where

φ: is the fuel air equivalence ratio (mostly =1)
K(N): is the power independent portion of engine friction, dependent on engine speed.
N(v): is the engine speed
V_d: is the engine displacement volume
η: is a measure of the engine indicated efficiency (~0.4).
Pacc(T,N): is the power draw of accessories such as air conditioning. This is a function of ambient temperature, T, and humidity (and engine speed for AC). Without AC, it is some nominal value ~ 1kW.
LHV: is the factor lower heating value of the fuel (~44kJ/g)

Fuel rate is relatively insensitive to K. The engine displacement, V_d can be classified by vehicle technology types; η is relatively constant from car to car and from model year to model year; and LHV is a known quantity, which can be adjusted (or assumed) based on the fuel type. Since this is a model for a typical vehicle, transmission effects and gear shift points tend to average out, so engine speed, N, can be very simply modeled as a function of speed and acceleration (Thomas and Ross, 1997). For MOVES, the engine speed model should be even further simplified. Future vehicles, (meeting new emissions standards) are not accounted for explicitly in this model, but can be developed in a future version if there is enough information in the literature. KNV_d is a friction term, which has less of an effect on emissions than the tractive, or brake power term (the inertial acceleration term dominates along with aero drag at higher speeds). As a result, it is not as crucial to model these terms with as much care. During enrichment, the parameter φ, is modified from Goodwin (1997):

$$\varphi = 1 + 0.036*(FR-FR_{th}) \tag{7}$$

The enrichment threshold, FR_{th} will be determined later. This is simply an approximation and the coefficient (0.036) should be recalibrated to incorporate new data. We will not explicitly model the enrichment fuel air equivalence ratio but it can be added later if necessary. A possible advantage of modeling φ explicitly lies in the ability to simulate certain types of failure modes such as when vehicles run rich, lean, or just have poor fuel control due to malfunctioning oxygen sensors, etc. The model could thus be linked with Inspection and Maintenance (IM) programs where the failure modes of On Board Diagnostic (OBD) parameters are tracked. A relatively simple model of φ for CMEM can also be found in Barth et al. (2000), however, the model relies on a simple model of the wide open throttle power curve, which may add unnecessary complication and detail.

We confirm that tractive power (or VSP) remains the primary driver of engine out emissions formation. This would show up as a first split in a hierarchical tree based regression (Frey et al, 2002). Finally, the fuel air equivalence ratio, φ, is almost always close to 1. Two notable operating exceptions will change this value enough to significantly affect overall emissions: cold start, and enrichment - both of which can and should probably be modeled explicitly due to their significant effects on the inventory.

Henceforth, when we refer to "modeled fuel rate", we are using equation 6. Using this approach, fuel rate has been modeled explicitly and accurately (including air conditioner usage) in the literature knowing only v, a and a few vehicle and ambient parameters: m, V_d, T, and humidity,

for generic vehicle types. An adaptation of this model for air conditioner was established by Nam (2000). Estimating parameters, this can be modified to be consistent with RSD VSP reporting schemes.

CO_2 can also be estimated based on the fuel rate. Assuming that the hydrogen to carbon ratio in fuels will also vary based on the fuel type, blend and cetane number. For typical gasoline, the ratio is roughly 1.85. This gives the following calculation for CO_2 based on a carbon balance:

$$CO_2 = 44[(FR-HC)/(12.0+1.85) - CO/28] \quad (8)$$

Where each of the values are in mass units. This equation implies that a knowledge of CO and HC emissions as well as fuel rate are necessary to calculate CO_2. As we shall see later, HC and CO are small correction terms. CO_2 results obtained using this equation, are 'modeled' or 'calculated' values to be compared with direct measurements.

Another advantage to this approach of modeling engine load is that it allows for the modeling of off-road engines. This is described in some detail in Appendix A. The proof of concept is reserved for a future study.

A further advantage of this fuel approach is that it can potentially be used to model fuel effects explicitly. Some details for this are described in Appendix B, but a proof of concept should be conducted in the future.

A Comparison of VSP and Fuel Rate

There are several advantages to fuel rate over VSP:

- Fuel rate as a load surrogate is physically more causal to emissions production due to its powertrain derivation (rather than road-load, which is a step removed)
- Fuel consumption (and effects) can be modeled explicitly (with no fitted parameters) as opposed to empirically
- CO_2 emissions can be approximated from the fuel calculations (carbon balance), so may not require an empirical fit.
- Some future powertrain improvements can be modeled: improved engine efficiency, engine downsizing, enrichment strategy, weight increase/reduction, catalyst improvement etc.
- Fuel based models can estimate area-wide fuel consumption, which can be compared with fuel sales on a macroscopic level. CO_2 estimated from this "fuel sales" based methodology can be compared with that obtained from a more microscopic approach.
- The methodology is more microscopic, thus it can be used to build up more aggregate models
- The methodology is older and more developed than VSP
- Since the load surrogate is related to engine load rather than road load only, non-road modal emissions may also be modeled using the same approach
- This fuel based methodology also aligns with the specific fuel based reporting of emissions such as grams emissions per gram of fuel (or CO_2)

- Different fuel types can be modeled explicitly with physical parameters.

Both the fuel rate and the VSP approaches require a further empirical step of measuring emissions and either binning or analytical function fitting. Dividing fuel rate by mass (similar to VSP) has been shown to help some of the correlations (Nam, 1999). Thus we see that the approaches are quite similar in some ways, yet CMEM is more physically rigorous, whereas VSP is simpler. In fact, a CMEM-like model could be used to populate VSP bins, though the reverse may not necessarily be true.

Figure 2 compares Fuel Rate and VSP more directly. The VSP was calculated using equation 2. Fuel rate was calculated from a carbon balance (equation 8), rather than a direct measurement from the fuel delivery system. Henceforth, this is what we refer to as "measured fuel rate" since it is the closest value we have to a direct measurement. Note that weight splits the trends, such that all other things being equal, heavier cars consume more fuel for a given VSP value. This is not too surprising, and hints that in order to predict fuel consumption (and CO_2) using only VSP values, the weight distributions must be known. Even if using the general form of the equation (1), engine displacement is not a term in the equation, as it is for fuel rate. Frey et al., (2002) showed that engine displacement was one of the factors that affected emissions. Note that VSP values can be negative during higher decelerations.

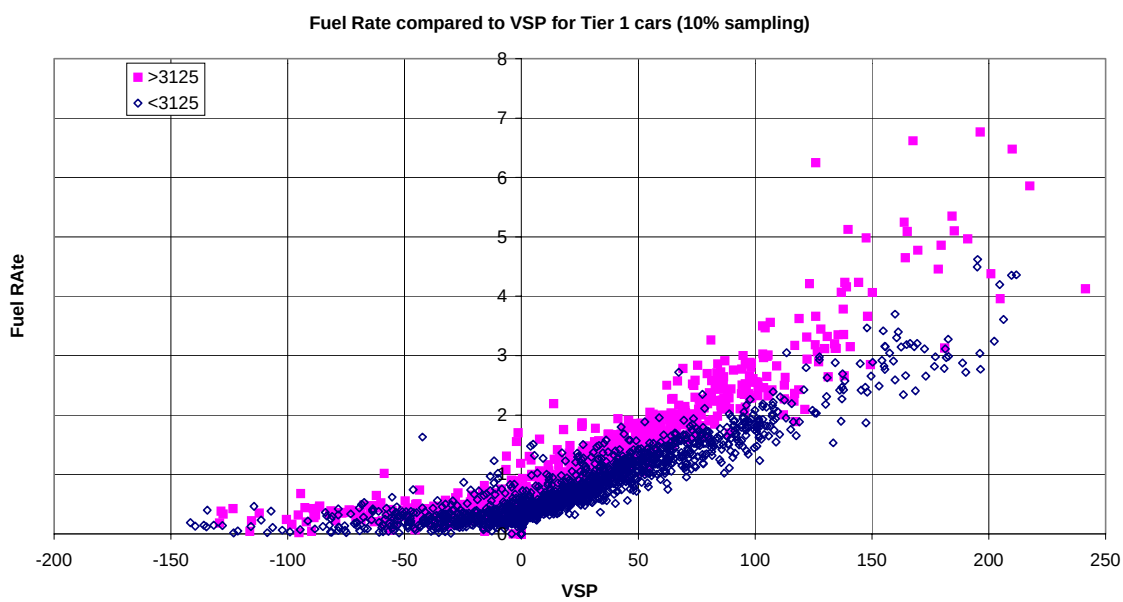

Figure 2. Fuel Rate (measured) compared to VSP for a variety of normal emitting Tier 1 cars. Each point is 1 second of data.

In conclusion, it has been demonstrated that basing hot-stabilized emissions (engine out or tailpipe) on VSP alone can introduce a fair amount of variability due to an assumed vehicle mass. Any estimate of fuel consumption or CO_2 in particular will merely be an estimate based on the initial values chosen for the VSP equation (2). In fact, there is a range of values one can choose for this equation, each giving a different result. If some of the parameters in equation 1 were used, this would lead to more accurate value of VSP, and such a variable would be very

similar to fuel rate, as we shall see later. Henceforth in this report, any calculation of VSP will be based on equation 1, using assumed values from Thomas and Ross (1997). CMEM employs dynamometer A, B, C coefficients to complete equation 1, but those coefficients are not always easy to obtain. A fuel rate approach decreases some of the variability at the cost of adding parameters, such as vehicle weight, engine size, powertrain efficiency etc., which are currently available or estimated from the database.

The major disadvantage that CMEM is cited to have, is that it includes a catalyst model (since fuel rate mainly gives empirical engine out emission trends), whereas VSP models tailpipe directly. However, as we shall see later, this may not really be a disadvantage at all, but rather a strength of the model. Since both are roughly based on road-load, and both ultimately predict tailpipe emissions, the only difference is in essentially how many parameters, or what level of complexity is used to obtain the final result. CMEM can be significantly simplified to nearly the complexity of the VSP approach. However, by its nature, the physical approach is more complex, and may require additional training for some users. Ultimately though, both are calibrated to the same data, so the final tailpipe model should be similar. Before this is discussed in more detail, we will first compare the binning to the analytical fit approach to modeling, which is a separate (but related) topic.

Binning vs Parameterized Approach

We have briefly mentioned the relationship between binning data and fitting a parametric equation. Here, we compare the two methods in more detail, both assume a physical basis for the model (VSP or fuel rate). Both are useful depending on the circumstance. Throughout this paper, we will use both, where appropriate.

Binning

Advantages

1. Simple
2. Data driven: each bin relates real data
3. Bins can be sized to optimize fit
4. Can fit analytical form to bin heights
5. Does not require constant recalibration
6. Easy to implement
7. Easy to update
8. Consistent across scales
9. Uncertainty can be quantified

Disadvantages

1. A LOT of data must be taken
2. Difficult to interpolate gaps accurately
3. Nearly impossible to extrapolate gaps beyond scope of data
4. Difficult to incorporate data from many sources (true for all approaches)
5. Can end up being a “black box” of statistics
6. Difficult to disaggregate to analytical approach if needed

Parameterized

Advantages	Disadvantages
1. Fits interpolate excellently	1. Value is fitted thus may not necessarily reflect measurement at any given value
2. Fits can extrapolate outside the bounds of data to some extent	2. Difficult to incorporate data from many sources
3. Data needs are fewer, due to above two cases (cost is less)	3. Requires recalibration with each data set
4. Comprehensible/explainable mathematical trends	4. More calculation intensive (may reduce software efficiency)
5. Can populate data bins or cells- can aggregate to bin approach if needed	5. The model may be more complicated, and require additional training for users.
6. Easy to implement	
7. Easy to update	
8. Consistent across scales	
9. Uncertainty can be quantified	

Comprehensive Modal Emissions Model (CMEM)

CMEM is designed to model emissions on a second by second basis using parameterized functions. Since MOVES does not require predictions on this scale, or for specific vehicles, CMEM can be simplified to be applicable to macro-level inventory analysis based on speed and acceleration profiles or distributions. We have already presented some ways that the complexity in CMEM can be reduced. There are quite a number of parameters used in the model that can take on an assumed fixed value. If at some later time, technology forces a change or variation in these parameters, then that can be reflected in the model (unlike in MOBILE, where new correction factors must be introduced). This is a great strength of the combined physical-based model and the parametric approach.

A list of the CMEM parameters, their applicability to MOVES and the model sensitivity to the parameters is presented in Appendix C.

Cold Start/Soak
Cold start and Soak can be modeled with a correction factor approach. The first 100-200 minutes of a car operation can be a separate mode of cold start. This can be modeled with an algebraic HC, CO, NO “correction” factor. It is not necessary to have an integrated modal (or second by second) cold start model at this time, since it is really its own separate mode of operation. This improvement can be undertaken in a future study.

A Simpler Catalyst Model
Since MOVES does not need to accurately model second by second emissions, the goal is to reduce the number of fitted parameters in a catalyst model. Engine (with fuel injection) technology improvements leading to emission reduction (with the exception of EGR) have had a relatively minor effect on (engine-out) emissions in the past few decades in comparison to catalyst (and air fuel control) improvements. So an aftertreatment system modeled separately would be able to model these technological improvements in isolation. However, as we will see

later, a suitable aftertreatment model is difficult to design. The details are described in greater detail in the next section.

Aggregate Engine Out Trends

In order to prove that a model like CMEM can be used to estimate emissions from a fleet of vehicles, it may be necessary to split engine out from tailpipe emissions. The difficulty with this approach is that in most cases, engine out data is not available. We hypothesize that engine out emissions have not changed significantly since the introduction of fuel injection and oxygen sensor feedback to maintain stoichiometric combustion conditions. These include vehicles starting from the early 1990s. This section attempts to prove out this hypothesis.

Figure 3 shows the (modeled) engine-out CO trends as a function of fuel rate for the 11 UC Riverside normal emitting composite (or average) cars. The slopes are determined from the calibration parameters used in the Riverside model, which are made for the composite car (second by second average of several vehicles). The categories are in the title of the figure. Category 1 (no catalyst) has significantly higher emissions in the engine. It is likely that cars without catalysts ran richer. The trend appears that the slope is dropping as new technologies and standards are introduced. The Tier 0 to Tier 1 drop is significant (~50%). Within emissions standards though, the emissions trends (sloped) are similar. Note that the tier 1 composite vehicles are close to the average. The Tier 0 emissions are more spread out. This may be due to deterioration effects or engine variation (carbureted vs fuel injected). Further investigation of this may be required.

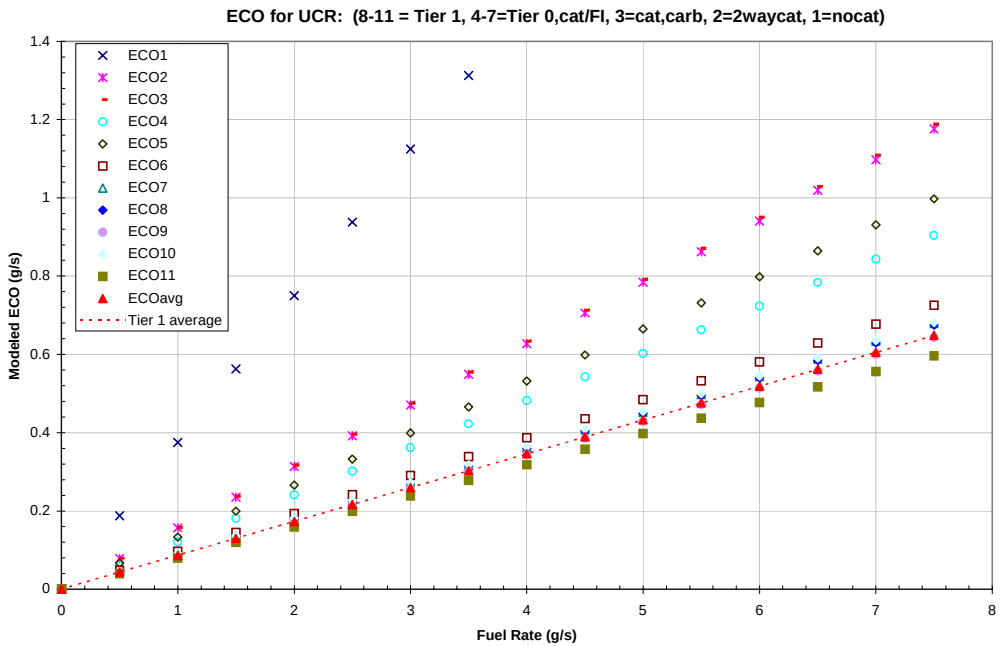

Figure 3. Modeled Engine out CO in CMEM

Figure 4 indicates that Tier 1 trends are also tight with HC. From this, we might conclude that for CO and HC, we can aggregate Tier 1 vehicles together from an engine out standpoint. We have

yet to prove this for tailpipe results. There is somewhat more scatter for the Tier 0 composite cars. Category 5 composite car (3way cat, fuel inject) emits the most, then the non-cat cars.

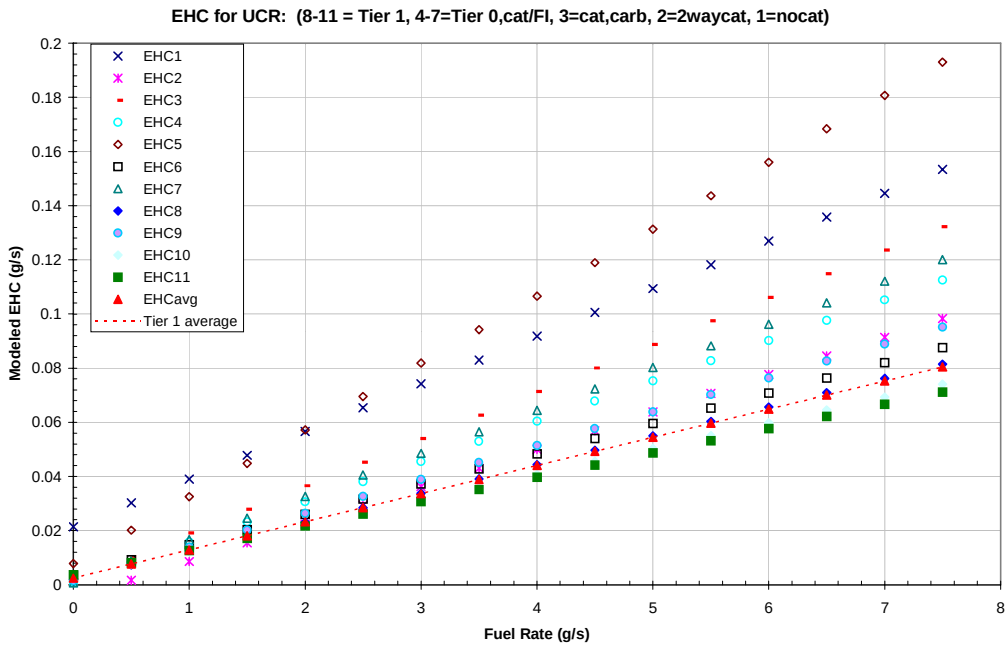

Figure 4. Modeled Engine out HC in CMEM

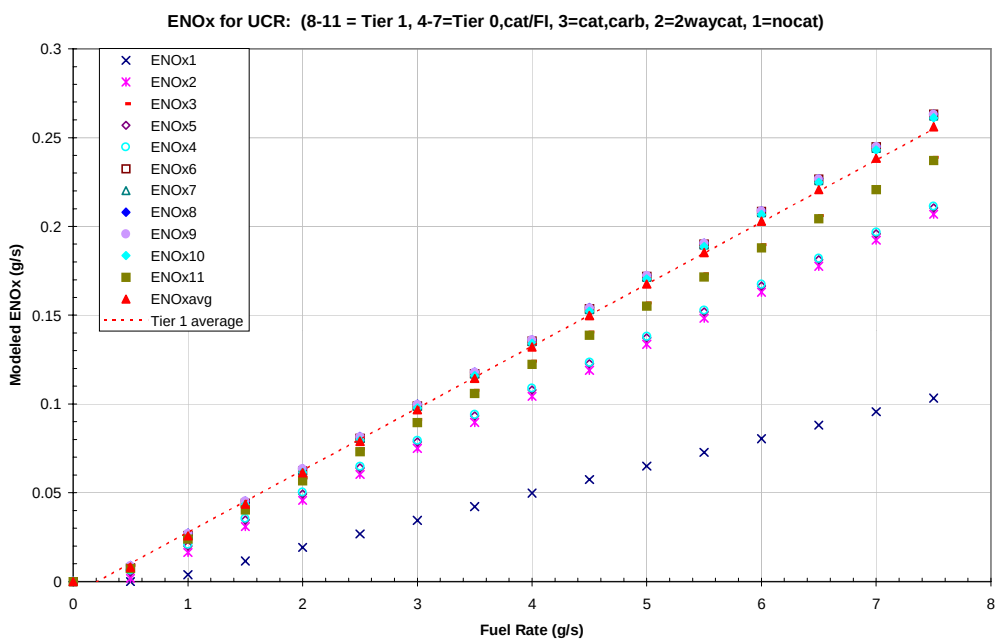

Figure 5. Modeled Engine out NOx in CMEM

Figure 5 also shows that the Tier 1 composite cars are tight for NOx. However, the engine out NOx emission trends are higher in Tier 1 than in older cars. This supports the belief that the

older cars may have run more rich. Except for the non-catalyst composite car, the Tier 0 composite cars are also very tight (and able to be aggregated).

The results above hint that, engine emissions (for properly functioning cars) are relatively constant within an emissions standard, even when isolated by power to weight ratio and odometer. However, these results were obtained by using modeled coefficients from composite vehicles. To fully justify this, the variation in the individual vehicles (of different weights, engine sizes, etc), should be examined. This is revisited in part 2.

Vehicle Data

The dataset for this study was taken from the set of normal emitting Tier 1 vehicles from the NCHRP data set taken at UC Riverside. The data was isolated from the rest of the EPA dataset. due to the second-by-second engine out emissions measured. Hi-emitters will be analyzed in a separate document. The FTP bag emissions include bag 2, and the latter 475 seconds of bag 3 (after catalyst light-off). The data includes 41 vehicles, most having FTP as well as US06 tests. The MEC (modal emissions cycle) tests were left out for validation purposes. The vehicles are listed on table 2. Due to the limited number of vehicles, the sample is not representative of the mix of (Tier 1) vehicles in the fleet.

The FTP and US06 bag emissions, used in the correlations in this section, are combined without any weighting. The bag emissions are calculated by summing the second-by-second values and then dividing by the distance traveled in the driving trace (g/mile). Due to this summation approach, even though there are almost three times as many FTP points as US06 points, the US06 cycle has a stronger influence on the aggregate emissions due to the much higher emissions values. Due to the difficulty of working with large time trace data, this aggregation is a first pass attempt at looking for obvious trends. Naturally, a modal or second by second analysis is required once a hint of correlation is seen in the aggregate data. This is done in later sections. It is important to note that the emissions figure include a US06 cycle, which can sometimes exhibit emission spikes, so "high emissions" do not necessarily imply a necessity for a "hi-emitter" classification. The known parameters for the vehicles include the following:

- Vehicle Make/Model
- Model Year
- Engine Size
- Number of Cylinders
- List Weight
- Odometer
- Rated Power
- VIN

Table 2. The table of normal emitting Tier 1 vehicles in the NCHRP study.

Vehicle	Make	Model	Model Yr	Eng Sz	N Cyli	List Wt	Wt ton	Odomete	Rated Pwr	Category
133	Honda	CIVIC	1995	1.5	4	2375	1.1875	52111	70	8
163	Honda	CIVIC	1994	1.5	4	2625	1.3125	78056	102	8
250	Oldsmobi	98	1994	3.8	6	3875	1.9375	54825	149.94	8
263	Honda	CivicEX	1995	1.6	4	2750	1.375	54843	102	8
266	Plymouth	Acclaim	1994	2.5	4	3125	1.5625	56936	104.99	8
284	Honda	Accord	1993	2.2	4	3500	1.75	97869	140	8
302	Ford	Taurus	1995	3	6	3625	1.8125	63558	140	8
187	Toyota	Paseo	1995	1.5	4	2375	1.1875	56213	100	9
191	Saturn	SL2	1993	1.9	4	2625	1.3125	63125	124	9
192	Honda	CivicDX	1994	1.5	4	2375	1.1875	57742	102	9
199	Dodge	Spirit	1994	2.5	6	3000	1.5	57407	141	9
201	Dodge	Spirit	1994	2.5	6	3000	1.5	56338	141	9
229	Honda	CivicLX	1993	1.6	4	2625	1.3125	61032	125	9
242	Saturn	SL2	1994	1.9	4	2625	1.3125	64967	124	9
260	Toyota	CamryLE	1995	3	6	4000	2	51286	188	9
281	Honda	AccordEX	1993	2.2	4	3250	1.625	72804	140	9
17	Toyota	Tercel	1995	1.5	4	2250	1.125	23249	93	10
75	Ford	Mustange	1995	3.8	6	3500	1.75	28905	145	10
80	Ford	Taurus	1997	3	6	3625	1.8125	3415	140.19	10
92	Saturn	Saturn	1996	1.9	4	2625	1.3125	18000	100	10
105	Saturn	Saturn	1996	1.9	4	2625	1.3125	7107	100	10
129	Honda	Accord	1995	2.2	4	3250	1.625	37194	130	10
253	Toyota	Corolla	1996	1.8	4	2875	1.4375	29480	100.11	10
282	Geo	Metro	1996	**1**	3	2000	1	32034	60.58	10
324	Chevy	Malibu	1997	3.1	6	3375	1.6875	3015	130.44	10
329	Plymouth	Breeze	1997	2	4	3250	1.625	23099	114.74	10
32	Cadillac	NS	1996	4.6	8	4000	2	13287	275	11
33	Buick	Lesabr	1996	3.8	6	3500	1.75	22607	205	11
37	Honda	Civic	1995	1.6	4	2250	1.125	49814	102	11
48	Infinity	G20	1995	2	4	3000	1.5	21468	140	11
53	Plymth	Breeze	1996	2	4	3000	1.5	15096	132	11
54	Chevy	Capri	1994	4.3	8	4250	2.125	43625	200	11
67	Ford	T-Bird	1996	4.6	8	4000	2	16390	205	11
74	Dodge	Neon	1996	2	4	2500	1.25	5312	132	11
102	Dodge	Spirit	1994	3	6	3000	1.5	49492	141	11
104	Nissan	Sentra	1995	1.6	4	2750	1.375	35291	115	11
108	Toyota	Camry	1994	3	6	3625	1.8125	22258	188	11
116	Chevy	Cavalr	1996	2.2	4	2875	1.4375	5690	120	11
120	Chevy	Camaro	1996	3.8	6	3625	1.8125	25877	200	11
123	Chry	Lebaron	1995	3	6	3375	1.6875	22197	141	11
286	Honda	AccordLX	1995	2.2	4	3000	1.5	20606	130	11

Weight, Engine Size and Power

Figure 6 shows the relationship between engine size, weight and rated power. Clearly all of these quantities are correlated. A relationship based on one should be assumed to apply to the other. It might be possible to use these relationships to fill in data holes when engine size or rated power are needed, but are lacking in the data set.

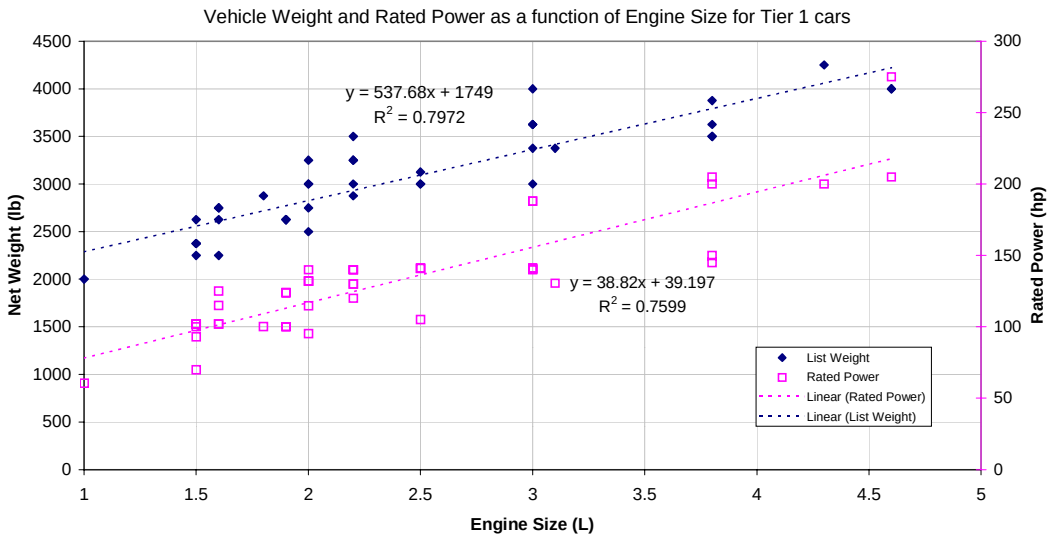

Figure 6. The relationship between vehicle weight, rated power, and engine size.

Odometer

Figure 7 shows the relationships between model year and odometer reading for the vehicles. The (California) vehicles appear to be driven at a rate of approximately 18,000 miles per year.

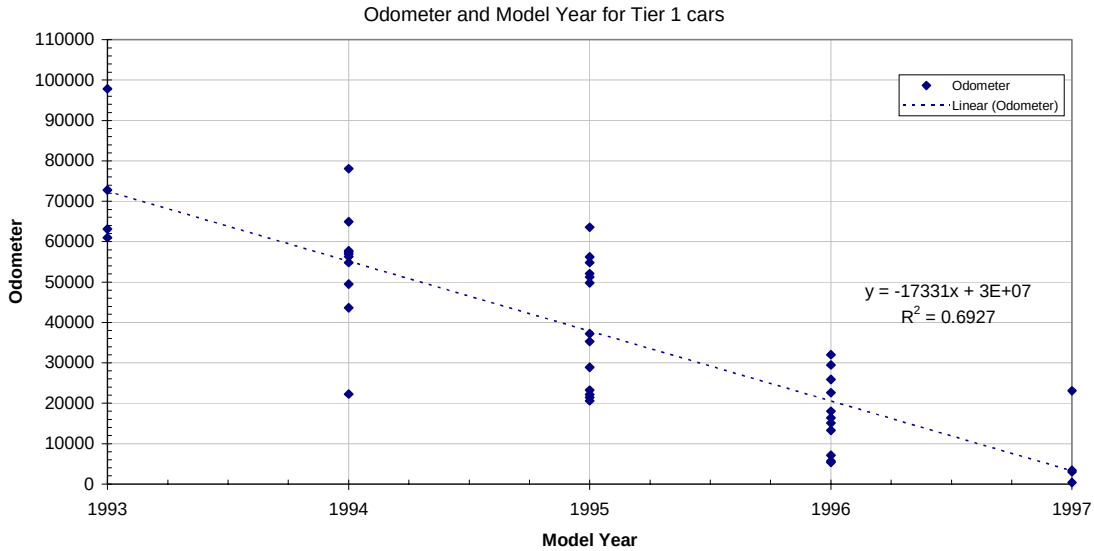

Figure 7. Odometer as a function of model year.

Table 3 shows the emissions index trends as a function of odometer (for normal emitting tier 1 cars). Emissions index is the grams emissions per gram of fuel, and isolates the effect to emissions only, without necessarily confounding deterioration with other factors in the fuel system. The hypothesis is that engine out emissions will remain relatively robust with age (based on figures 3-5), but the catalyst will deteriorate more. This will be born out by a low correlation with engine-out, and a slightly better correlation with tailpipe emissions.

The results indicate that there is a correlation with odometer in engine out as well as tailpipe emissions although the first is smaller.

Table 3. Correlation coefficients for emissions index and odometer.

ECO/FR	EHC/FR	ENOx/FR	TCO/FR	THC/FR	TNOx/FR
0.153	0.208	0.233	0.326	0.392	0.428

To ensure that there isn't a relationship between odometer and fuel rate emissions, the correlation coefficient for fuel rate with odometer is found to be: $\rho_{Odo,FR}$ = -0.0336, which is negligible.

These deterioration rates do not necessarily apply for the entire fleet. Before these rates are used, it would be important to obtain more data. We do NOT separate out odometer in the following sections. We leave that to the next stage of model development. This will undoubtedly be a source of variability in our model.

Emission Rate Chooser Flow Chart for MOVES (excludes cold start)

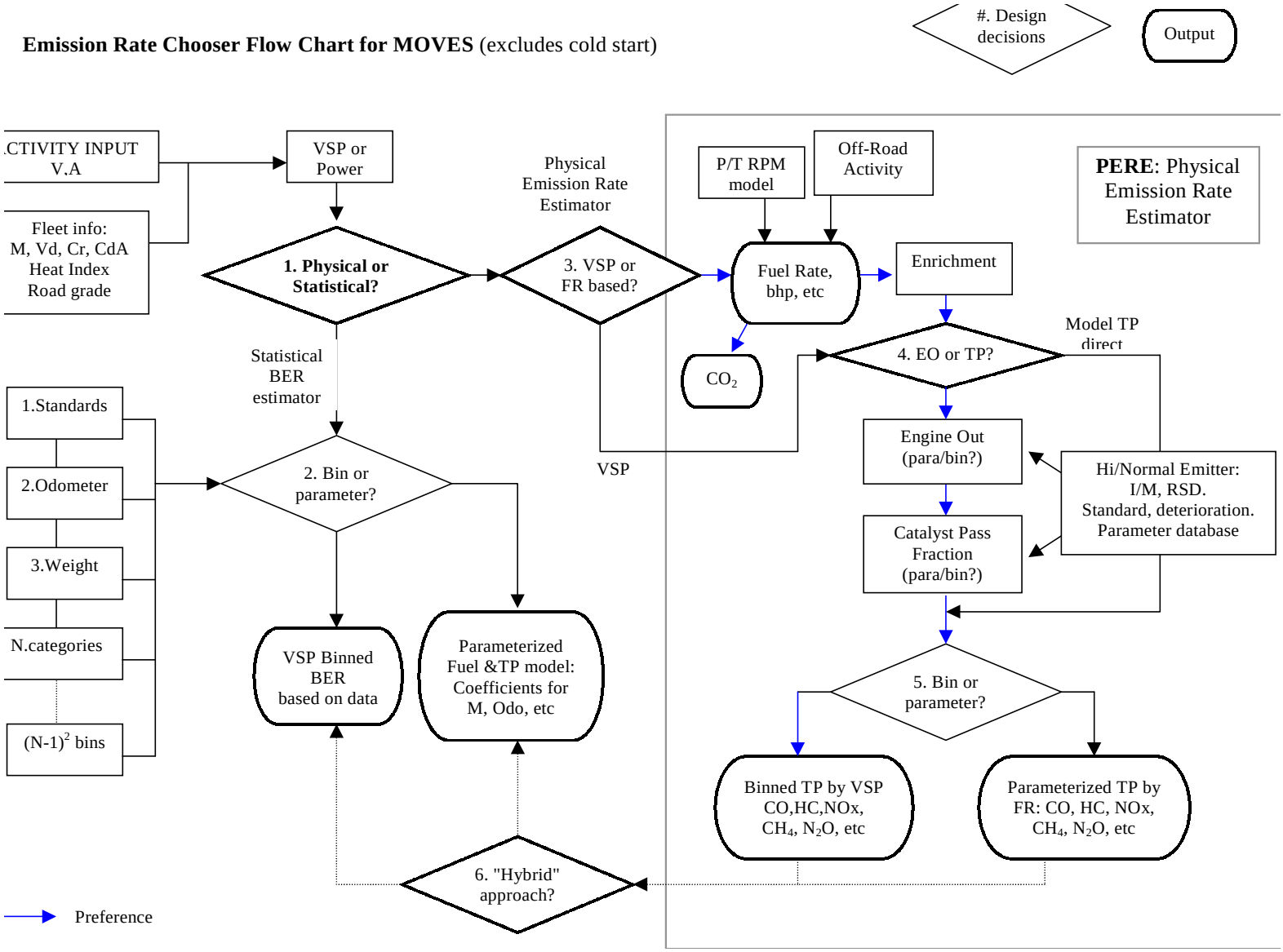

Figure 8. Decision trees for the integration of a Physical Emissions Rate Estimator.

II- THE PHYSICAL EMISSION RATE ESTIMATOR (PERE)

We have already outlined the advantages and uses for a physical model as a basis to fill (extrapolate as well as interpolate) bins with few real data. The flow chart on the previous page (figure 8) demonstrates some means by which this may be accomplished. The following sections describe some of the decision-making processes. The data used in this section is from the NCHRP data set (table 2) collected at UC Riverside.

Fuel Rate and CO_2

Using equation 1 and 6, fuel rate is modeled with some degree of accuracy. The only addition necessary was an engine speed model. This was obtained from Thomas and Ross (1997). The results are not tremendously sensitive to shift points, so this simple model is sufficient. Stationary off-road vehicles should have a more complex engine speed model. Figure 9 compares the model to measurement. $R^2 = 0.89$ and the slope is 1.

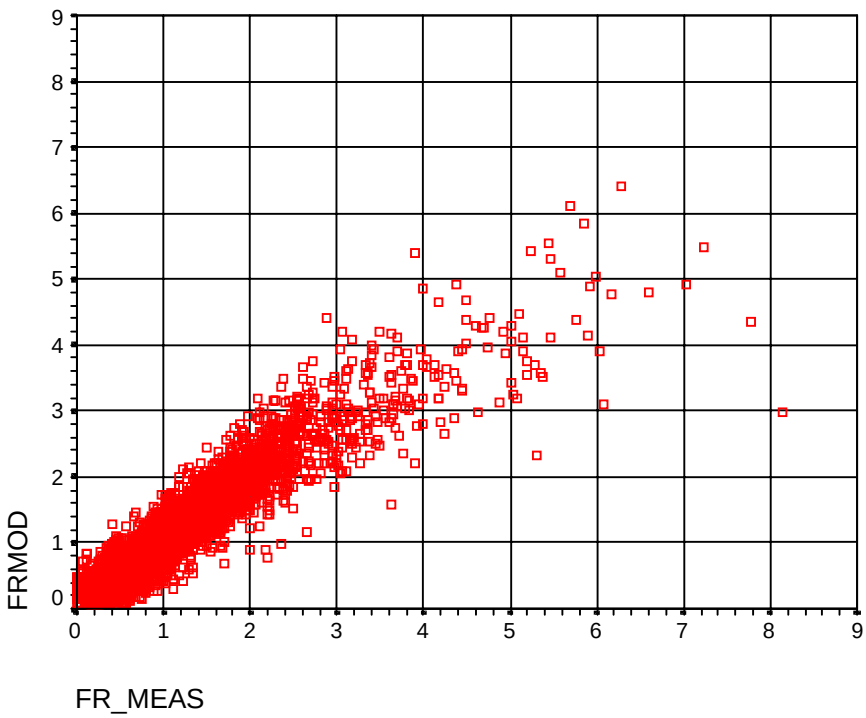

Figure 9. Fuel Rate measured and modeled (10% sampling of data). Each point is a second of sampled data.

Using equation 8 and assuming that the fraction of CO and HC are miniscule compared to fuel and CO_2, the latter quantity can be calculated to fair degree of accuracy. Figure 9 shows the comparison. $R^2 = 0.90$ and the slope is 1. CO_2 was calculated from basic physics, rather than from an empirical relationship.

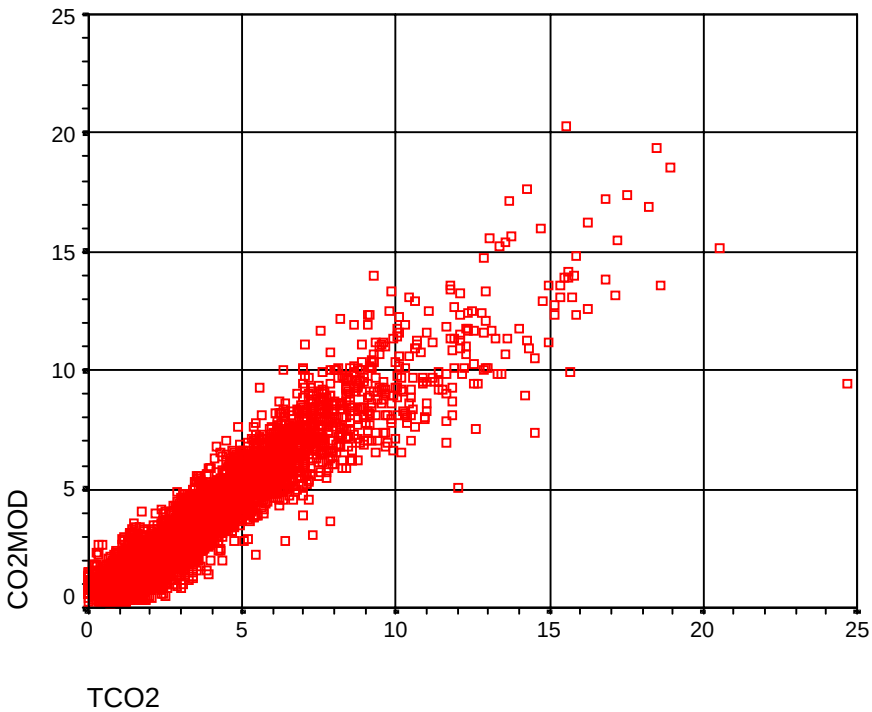

Figure 10. CO2 modeled and measured (x-axis).

We move on to the analysis of criteria pollutants: CO, HC, and NOx.

Second by Second Engine-Out Emissions

Direct modeling of tailpipe emissions from VSP or fuel rate is possible (decision node 4 in figure 8), but it is not recommended. An example of this type of analysis is provided in Appendix D. We have already established the engine out emissions can be aggregated for all of the Tier 1 vehicles, we will now determine the significance of the differences between the vehicles from observing the second by second data. The scatter or variability in this data should be isolated first. This will help us to determine if different relationships or vehicle bins are required on this scale. Since we are trying to minimize error, we will study emissions trends with VSP and with measured FR, rather than with modeled FR. As we mentioned earlier, measured FR is calculated from a carbon balance of the mass emissions (based on equation 8):

$$FR = (CO_2/44 + CO/28)*(13.85) + HC \qquad (9)$$

assuming a molar hydrogen to carbon ratio in the fuel of 1.85 for gasoline. Using this value of FR rather than the one modeled from speed, accel, etc. leads to a better understanding of trends. Later, we will use the modeled fuel rate to do the calibration and validation.

In the following study, we compare trends with both FR and with VSP to determine the better independent (activity) variable. This is decision node 3 on the flow chart.

Engine Out CO

Figures 11 and 12 show 10% of the second by second points of the Tier 1 cars on the US06 cycle (~7000 points). The FTP points were omitted since they would likely cluster at the low values of CO and FR. The fuel rate relationship indicates that for some portion of the dataset, ECO is linear with FR. This is consistent with CMEM and the literature. The relationship is linear with VSP as well, but the scatter is somewhat less well defined with VSP. The correlation coefficient is 0.65 for fuel rate and 0.46 with VSP:

$$\rho_{ECO/FR} = 0.65$$
$$\rho_{ECO/VSP} = 0.46$$

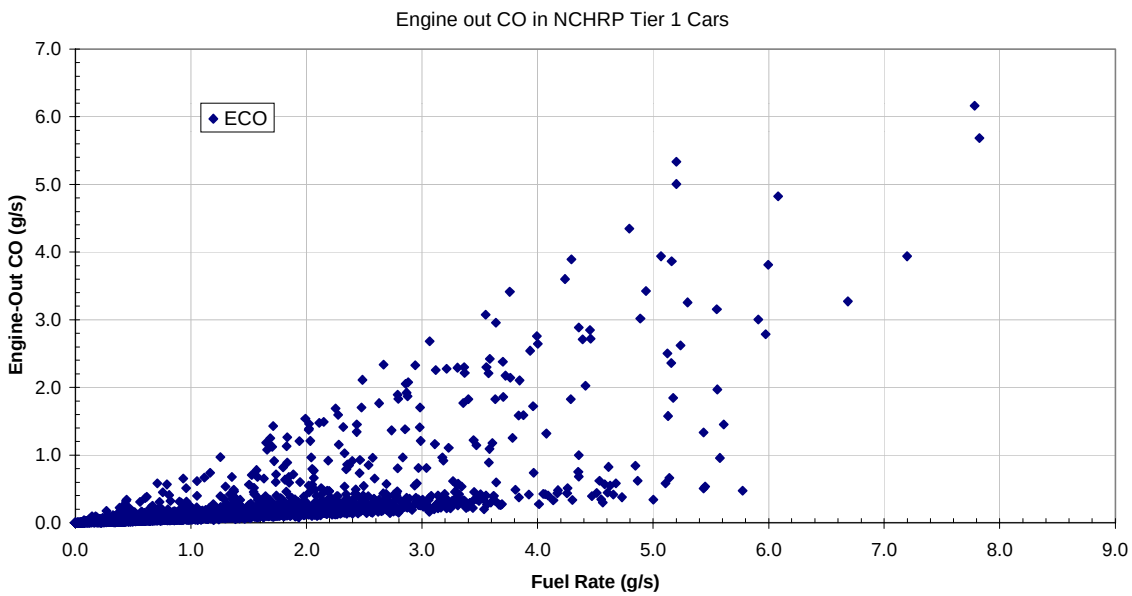

Figure 11. Engine out CO vs Fuel Rate for the NCHRP Tier 1 cars run on the US06 cycle (10% sampled)

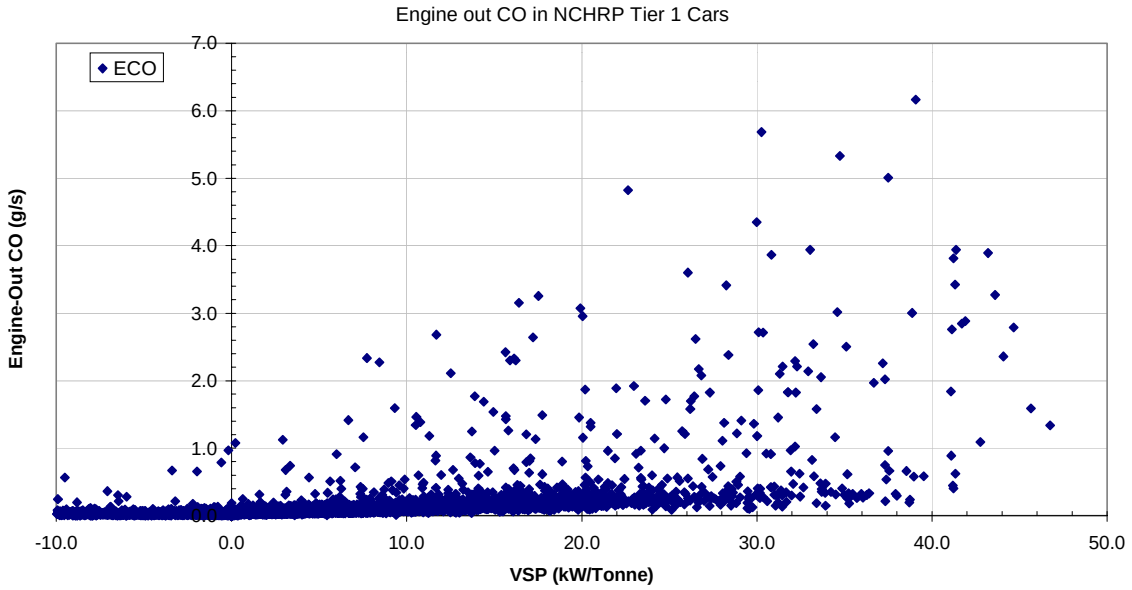

Figure 12. Engine Out CO vs VSP for the NCHRP Tier 1 cars run on the US06 cycle (10% sampled).

Enrichment

Since CO emissions are extremely sensitive to enrichment, the scatter from the fuel rate plot is assumed to come from enrichment. The ECO deviates from the simple linear relationship upon enrichment, when the trend sharply increases (many references). The point at which the enrichment occurs is referred to as the enrichment threshold. An example of this threshold can be seen in the figure 13. Notice the sharp "knee" where the linear relationship starts to increase. This can be modeled with a piecewise linear function.

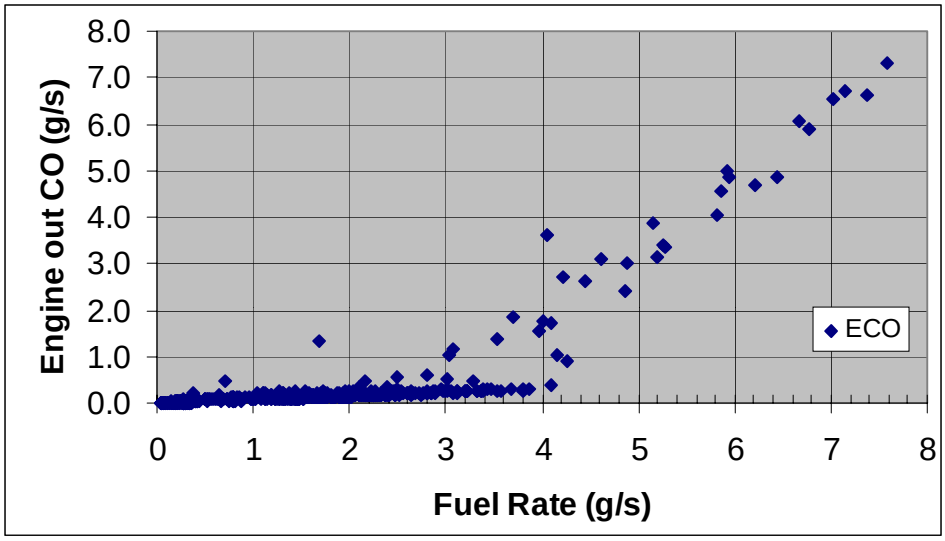

Figure 13. An example of ECO trends as a function of fuel rate for the Honda Accord (vehicle 284 on the NCHRP dataset). The "knee" that separates the two linear regions is the enrichment threshold.

While all the Tier 1 vehicles follow the same low FR trend, the location of the knee might change, thus a family of enrichment curves would be visible (thus causing the scatter when viewed all on a single plot). Nam (2000) determined that the enrichment threshold is dependent on the product of weight and engine displacement. Using a larger data set, we investigate this further. Table 4 shows the correlation of fuel rate threshold with various vehicle parameters. Vehicle weight apparently has the best correlation, though they are all good. However, this table does not include other light trucks, whereas the former study included some. Future analysis should be conducted to include light trucks to see which of the variables gives the strongest correlation.

Table 4: Correlations of enrichment threshold with vehicle parameters.

Parameter	Correlation
Weight	0.875
Weight*Vd	0.863
Vd	0.861
Rated Power	0.756

Figure 14 demonstrates this trend with weight and displacement. The trend is less pronounced when enrichment threshold is plotted as a function Power/weight. *Truck thresholds are expected to follow the trend, but this requires additional study*.

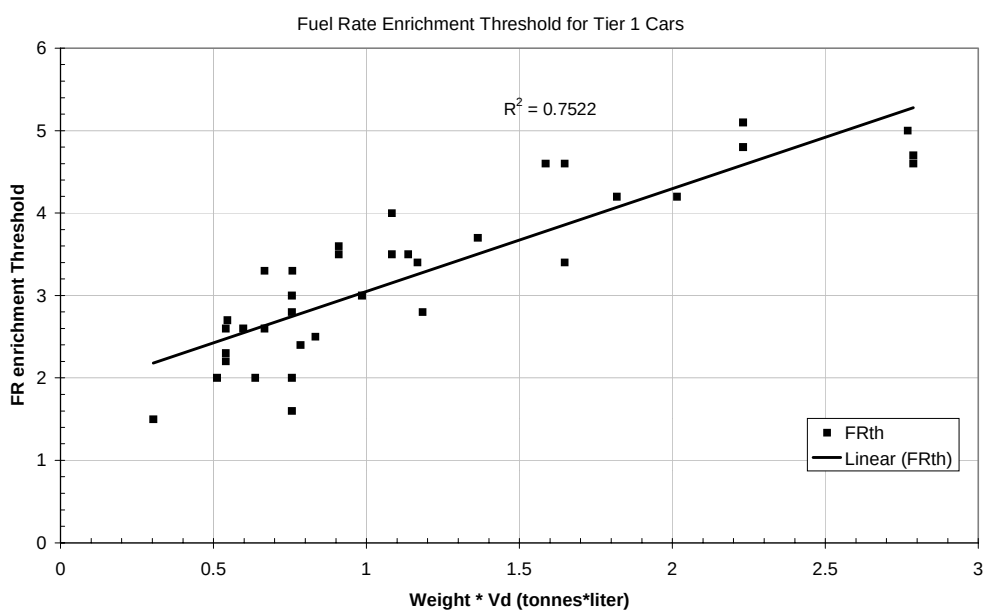

Figure 14. Enrichment threshold as a function of weight * engine displacement.

CMEM models ECO in the following manner:

$$ECO = [c_0 * (1-\varphi^{-1}) + a_{CO}] * FR \quad (10)$$

where

c and a are fitted parameters
φ is the normalized fuel to air ratio.

This equation is satisfactory as it stands and can be used for MOVES. However, the enrichment threshold relationship can be used to simplify the model and remove the dependence on φ altogether.

If FR < FRth

$$ECO = a_{1CO} * FR. \quad (11)$$

If FR ≥ FRth

$$ECO = a_{2CO} * (FR-FRth) + a_{1CO} * FRth, \quad (12)$$

where

a's are fitted parameters, whose ratio may be defined by a simple constant. The latter part of the equation is needed to ensure continuity. Also,

$$FRth = A*Wt*Vd + B \quad (13)$$

is determined from the analysis above. The weight and engine displacement can either be assumed or a distribution can be input into the model based on fleet information. A and B are fitted coefficients using linear regression.

$$A = 1.26 \pm 0.12, \qquad B = 1.82 \pm 0.16$$

This enrichment relationship will be used in other portions of the model where enrichment plays a role.

Engine Out HC

The engine out relationships with fuel rate and VSP are shown in the following two figures. Both for Fuel rate and VSP, the trends are reasonable. The correlation coefficients are:

$\rho_{EHC/FR} = 0.44$
$\rho_{EHC/VSP} = 0.34$

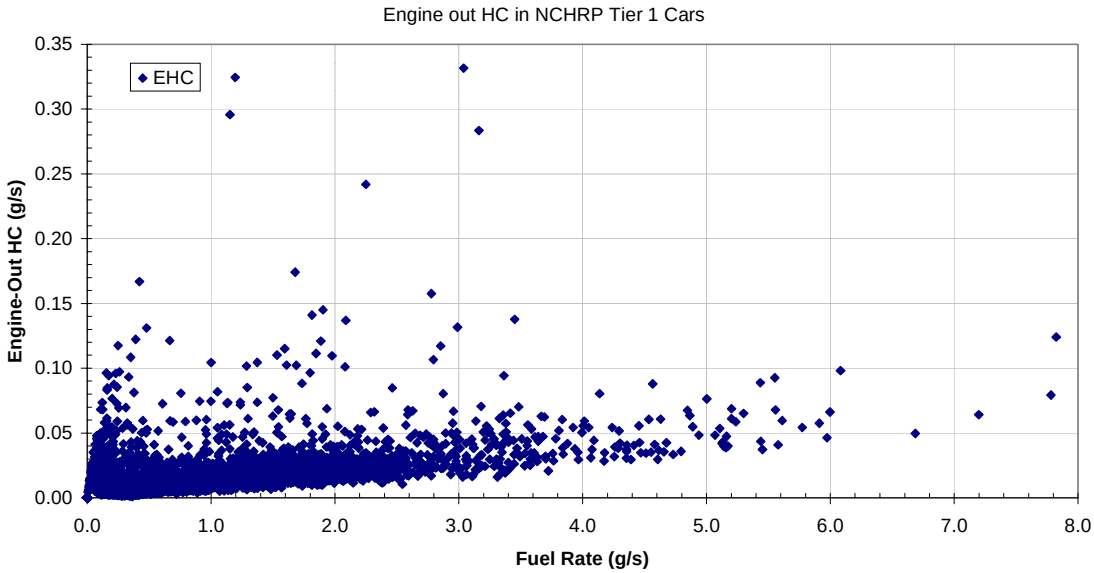

Figure 15. Engine Out HC as a function of Fuel Rate for Tier 1 cars on the US06 cycle.

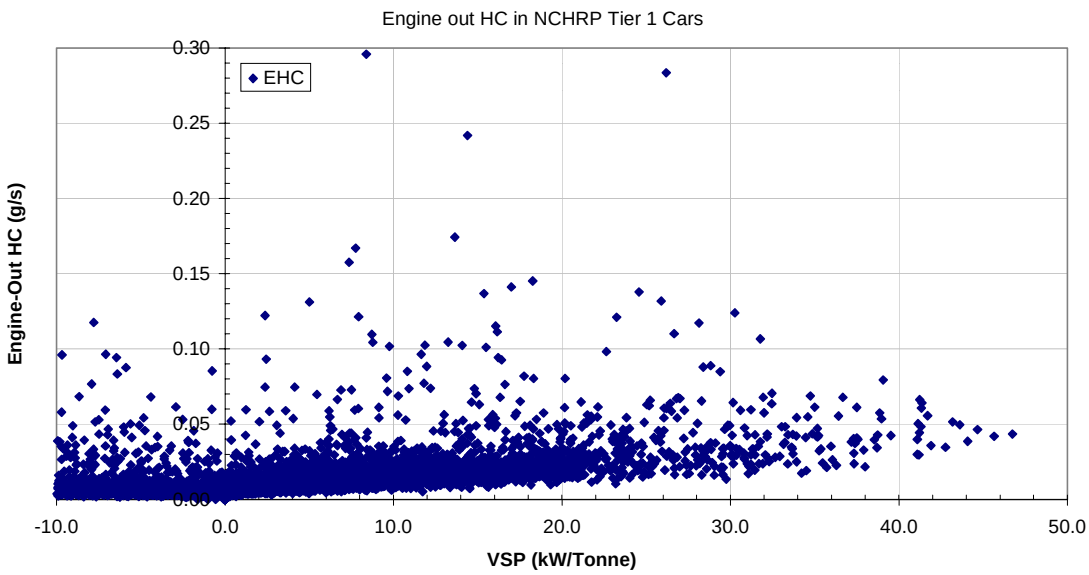

Figure 16. Engine Out HC emissions as a function of VSP for Tier 1 cars on the US06 cycle.

CMEM models EHC in the following manner:

$$EHC = a_{HC} * FR + r_{HC} \tag{14}$$

where

a and r are fitted parameters.

This is a simple linear equation with an offset. The offset is typically quite small, but not insignificant. The analysis above supports the use of the above parameterized equation to predict engine out HC emissions. CMEM also adds modules for enleanment events, which complicate the model. The enleanment HC puffs should only significantly affect emissions from vehicles with malfunctioning catalysts, and should only add a small error to the model.

Engine Out NOx

The following figures show the ENOx trends with fuel rate and VSP. The plots are both quite scattered, though the fuel rate relationship is better. The correlation coefficients are:

$\rho_{ENOx/FR} = 0.81$

$\rho_{ENOx/VSP} = 0.73$

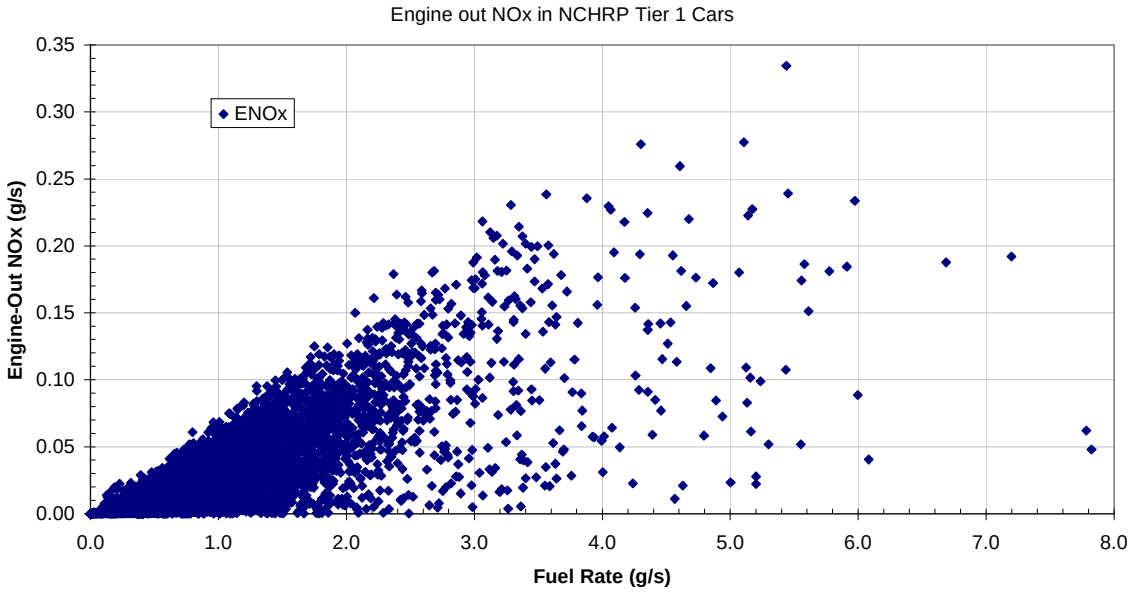

Figure 17. Engine Out NOx emissions as a function of Fuel Rate for Tier 1 cars on the US06 cycle.

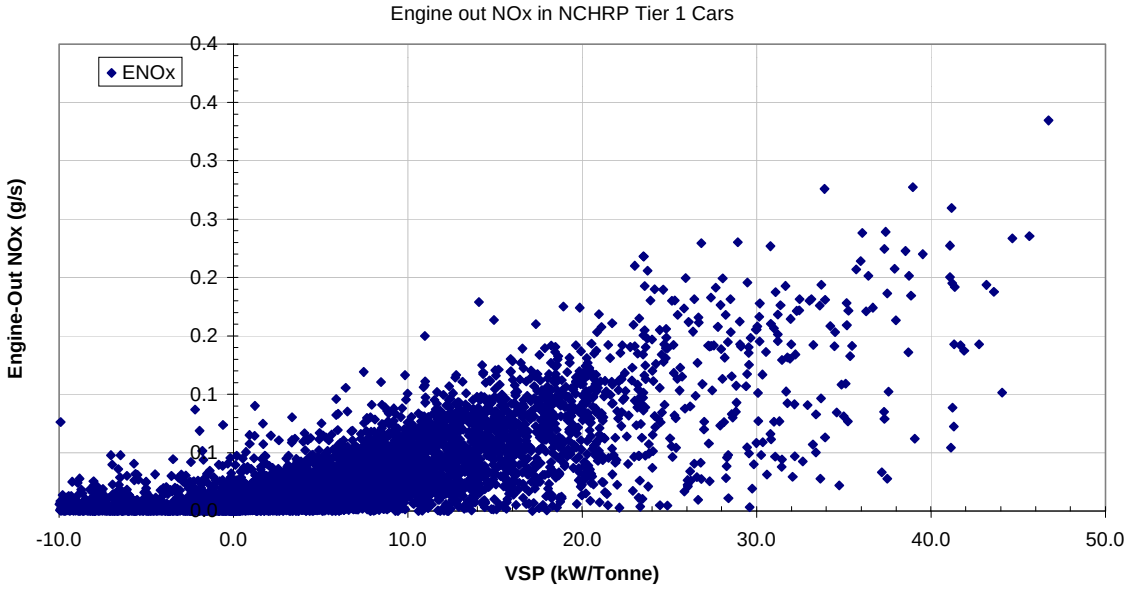

Figure 18. Engine Out NOx emissions as a function of VSP for Tier 1 cars on the US06 cycle.

We need to study this scatter in more detail. The hypothesis is that, the effect is due to differing levels of exhaust gas recirculation (EGR) strategy among the manufacturers (Nam, 2000). In this study it was observed that NOx emissions was simply linear with fuel rate with vehicles that used little to no EGR, but was non-linear (2nd order term) with engines that incorporated strong EGR. The hypothesis indicates that the family of curves should look like the following figure.

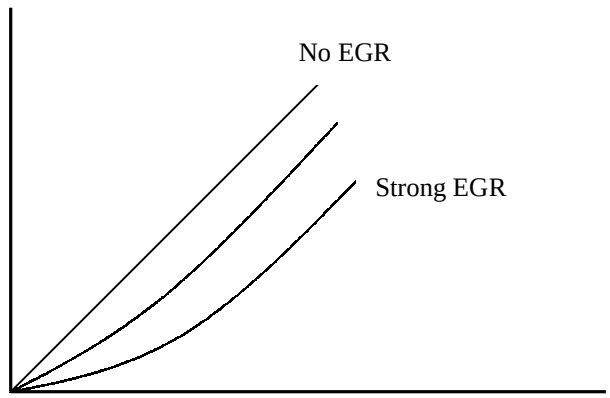

Figure 19. Expected family of NOx curves for varying levels of EGR.

The following series of figures support this hypothesis.

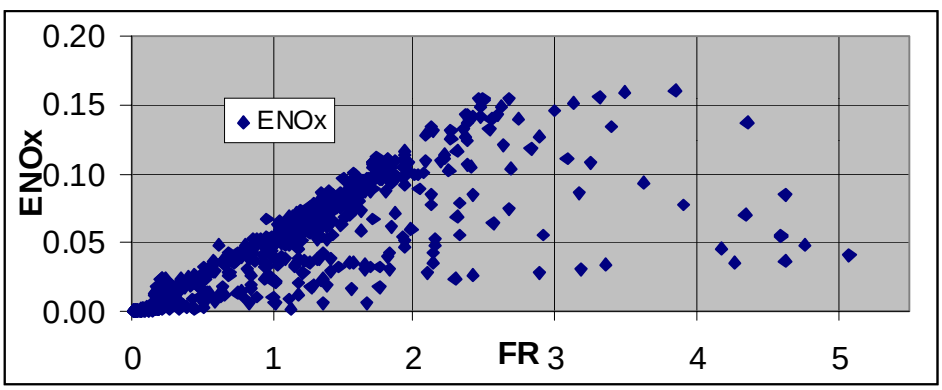

Figure 20. NOx trends without EGR (vehicle 213 category 8- 95 Civic)

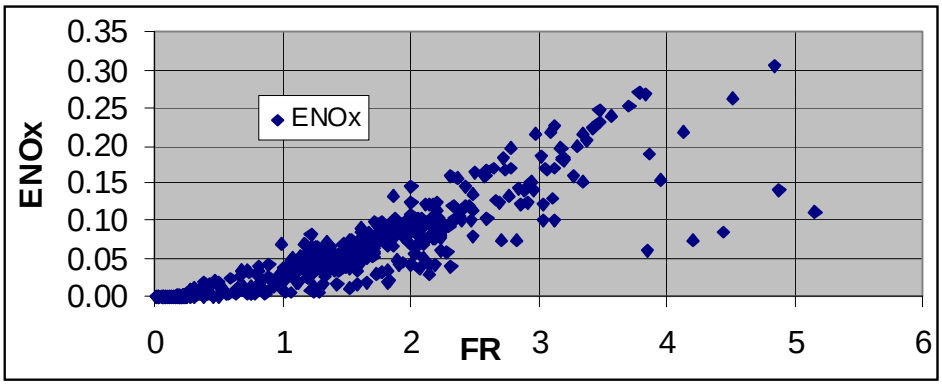

Figure 21. NOx trends with light EGR (vehicle 281, category 9- 93 Accord)

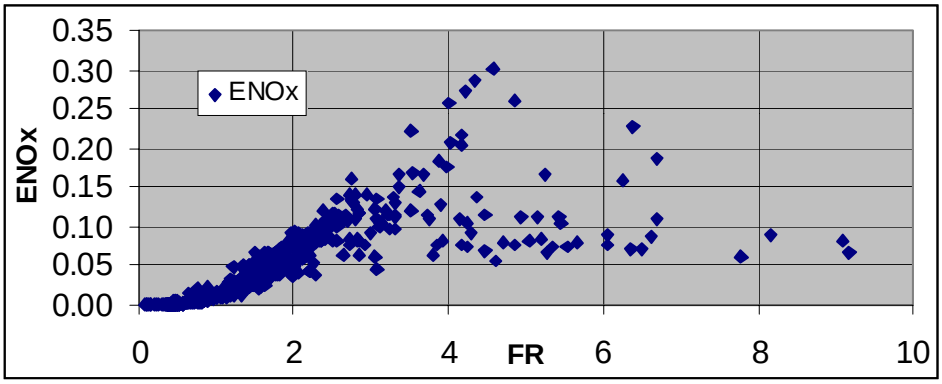

Figure 22. NOx trends with heavy EGR (vehicle 302, category 8- 95 Taurus)

Much of the high fuel rate scatter in the plots are due to enrichment events.

However, there are some vehicles that don't follow this trend of increasing non-linearity with increasing EGR. One such example is presented in the following figure. Notice that the slope is low compared to the previous plots. It is conceivable that the EGR ramps up even at high loads in this vehicle.

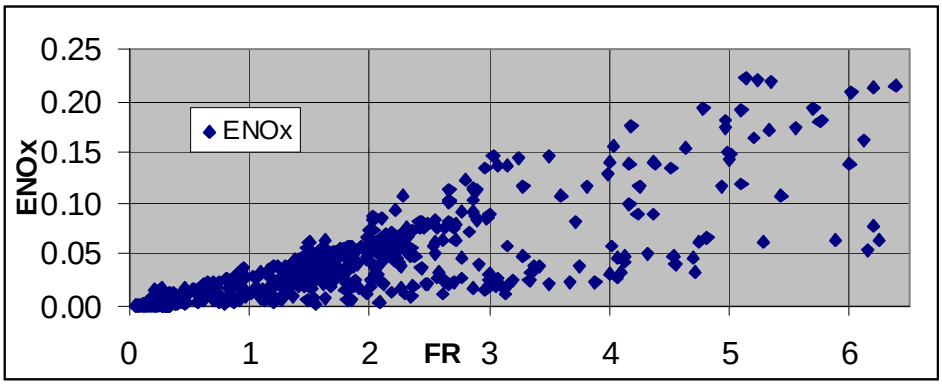

Figure 23. NOx trend with Heavy EGR. (Vehicle 260, category 9, '95 Camry). It does not follow the trends above.

Engine out NOx has been modeled separately as a linear function in CMEM such that

$$ENOx = a_{NOx} * FR \tag{15}$$

where

a is a fitted parameter.

Due to EGR effects and the significance of low load emissions when the air conditioner is on, Nam (2000) added a second order term, but we will simplify this further:

If $FR \leq FR_{th}$

$$ENOx = a_{1NOx} * FR + a_{2NOx} * FR^2 \tag{16}$$

where

FR_{th} is the enrichment threshold (equation 17)

If $FR > FR_{th}$

$$ENOx = a_{3NOx} * (FR- FR_{th}) + [a_{1NOx} * FR_{th} + a_{2NOx} * FR_{th}^2] \tag{17}$$

The added terms are to ensure continuity. This is the form of the NOx model used for the rest of this paper. While it is disadvantageous to complicate, or add parameters, to CMEM, this factor may be necessary to improve the long-term predictability of the MOVES.

Air Conditioner

Excess emissions from air conditioner usage can also be modeled using a physical approach. Nam (2000) modeled emissions employing the fuel rate approach. Basically, the air conditioner seems to affect emissions linearly with the added load for CO and HC. By adding the excess load into equation (6), the added emissions can be directly calculated using the same (engine out and tailpipe) emissions parameters. Thus an increase in fuel rate results in a proportionate increase in CO and HC emissions. The emissions from NOx, however was seen to be non-linear at low load because of reduced exhaust gas recirculation effects. The details of the model can be found in the reference. The activity portion of AC usage was determined from Koupal (1998).

Engine Out Calibration

Using the relations above, the parameters shown in table 5 were calibrated along with their uncertainties. The fits were determined using a simple least squares fitting routine on the SPSS software program. The uncertainties are 95% confidence intervals determined from the output of the fit. The uncertainty in the parameter due to test variability is assumed to be follow a normal distribution. However, from observations of the emissions scatter, it is likely that the estimation of the uncertainties can be improved using lognormal, or some other asymmetric distribution transformation. This task will be left to the next step of model development. The following table shows the R^2 fit to all of the second by second data in the Tier 1 NCHRP data set and the % error to the total measured emissions (proportional to bag). This is the simplest level validation since it is validating to the same data set used to calibrate the model. The bag comparisons and the fits are quite good as well, with the exception of HC. This is due to the extremely low values of HC in the data set as well as the omission of an enleanment (or "hydrocarbon puff") model. However, we hypothesize, that the catalyst will eliminate most of the puffs.

Table 5. Engine out emissions fitted parameters with high and low 95% confidence values.

Parameter	Value	St Dev	95% CI LO	95% CI HI
C0	0.4074	0.0072	0.3929	0.4219
aCO	0.1174	0.0004	0.1167	0.1182
aHC	0.0100	0.0001	0.0099	0.0101
rHC	0.0049	0.0001	0.0047	0.0050
a1NO	0.0043	0.0001	0.0041	0.0044
a2NO	0.0219	0.0001	0.0216	0.0222
a3NO	-0.0026	0.0017	-0.0060	0.0008

	R^2	% error
ECO	0.61	4.6
EHC	0.25	-0.6
ENOx	0.66	-9.3

One of the most stringent validation criteria for emissions modeling is to ensure that it matches both the total (or bag) as well as the second by second emissions. A tool that is often used to verify this is the cumulative emissions plot. Figures 24 and 25 show the cumulative emissions for each of the species during the FTP and US06 driving respectively. Since this is a cumulative plot over all (or most of) the vehicles in the data set, the model will undoubtedly overpredict on some vehicles and underpredict on others. It should be reiterated that this model is not meant to be used to predict emissions for a particular car, therefore a second by second validation may be too stringent a criteria.

Comparison of this engine model calibration to the measurements indicate that HC is relatively well across FTP and US06 type of driving. The model also indicates that the calibration for all species is good for the US06 cycle, however CO and NOx overpredict at lower loads (FTP type driving). It is possible that the catalyst model can compensate for this, but the discrepancy should be investigated further. It is interesting to note that the US06 data is ‘driving the calibration’ due to its relatively high emissions levels (compared to the FTP). It raises the question of whether these are the appropriate driving cycles to calibrate the model. More will be discussed on this later.

Using these parameters, we can calibrate a tailpipe emissions model, even if engine out data is lacking. The variability with these coefficients is small enough to justify the use of these same parameters for all similar engines. The majority of uncertainty and variability in emissions comes from the catalyst, which we will discuss in the next section. However, with improved technology changes expected for the future, it will be necessary to occasionally collect engine out emissions data to keep the model well calibrated.

In conclusion, we have demonstrated that engine out emissions have a correlation with measured fuel rate. It is even slightly better than the correlation with VSP. This is natural since fuel rate, as an engine load, is more causal to engine emissions than a road load variable such as VSP. However, the correlations are still good with VSP, and can be used also. The scatter that is evident for CO and NOx is apparently due to vehicle variations of enrichment thresholds and EGR rates respectively. The enrichment thresholds can be explicitly modeled as a function of vehicle weight and engine size. The EGR scatter is somewhat more complicated to model, due to lack of data. It is likely that the model may have to resort to a simple average for NOx, as we have done above.

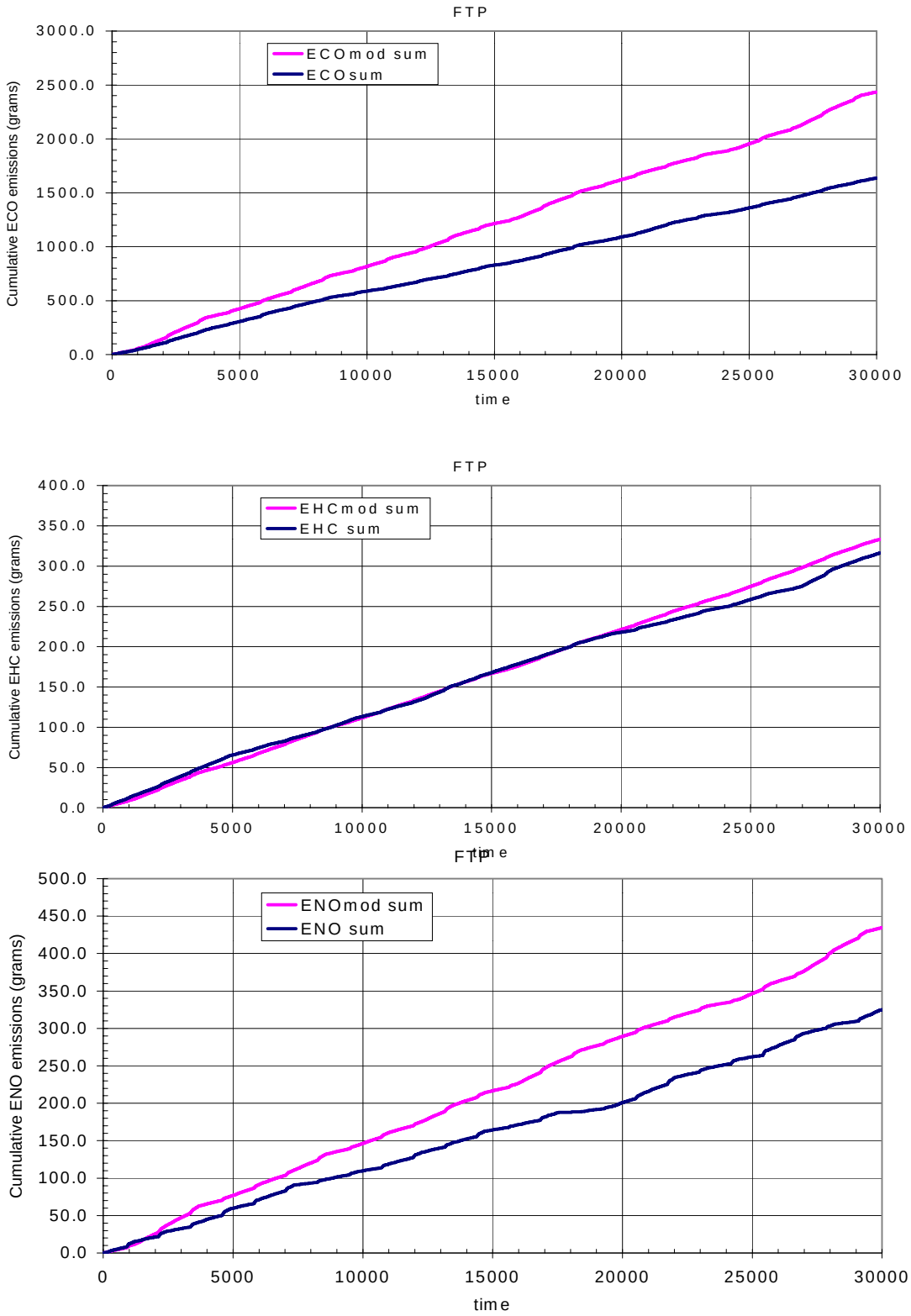

Figure 24. Measured and modeled cumulative engine out FTP emissions for CO, HC and NOx

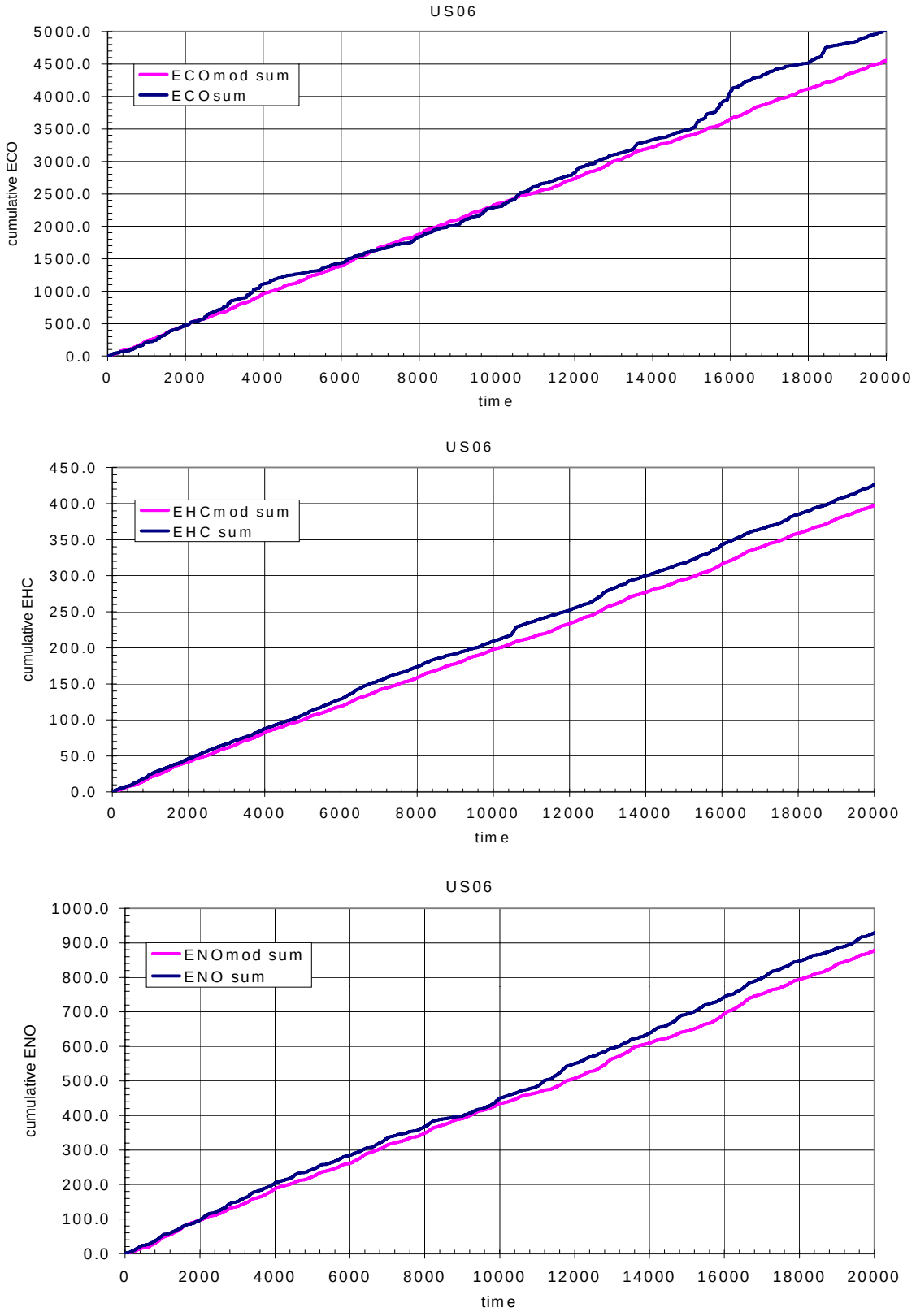

Figure 25. Cumulative engine out measured and modeled CO, HC, and NOx emissions from the US06 cycle.

Second by Second Catalyst Pass Fractions

The aftertreatment system in an automobile (including catalyst and air to fuel ratio) is one of the most complicated vehicle systems to capture in a model. This is because the conversion of pollutants on the catalyst is highly sensitive to the air to fuel ratio of the combustion and the flow rate of exhaust. The stoichiometric mass ratio of air to fuel ratio (A/F) required for complete combustion in the engine is approximately 14.6. As little as a half of a percent lean of this value could lead to significant NOx spikes (Nam, 1999). This is caused by an excess of oxygen in the exhaust stream, which in turn prevents the reduction of NOx into its elemental parts: O_2 and N_2. Alternately, rich excursions produce CO (and to a lesser extent HC) spikes, since a lack of oxygen in the exhaust stream prevents the oxidation of CO into CO_2.

Without accurate measurements of the A/F, catalysts can, at best, only be roughly approximated. The data is not available, and the modeling of A/F is beyond the scope and use cases for MOVES. However, we demonstrated that we can predict when vehicles will go into enrichment, so CO and HC emissions should be somewhat easier to model than NOx.

The catalyst pass fraction is defined as the ratio of tailpipe to engine out emissions:

$$CPF = TP/EO \tag{18}$$

or

$$TP = CPF * EO$$

When CPF = 0, the catalyst converts all (or 100%) of the pollutants. In more familiar terms, it is related to the catalyst efficiency (%) by the following equation:

$$\text{Cat Eff} = 100\% * (1 - CPF) \tag{19}$$

It is easier to deal with CPF since we are searching for trends that increase with tailpipe emissions. During extreme breakthrough events, it is sometimes possible for TP > EO (or for CPF > 1) at any given second. Theoretically this is unphysical, but it is possible to measure this as an artifact of timing mismatches between the second by second engine out and tailpipe measurements.

The following sections describe a model for the catalyst pass fraction during hot running operation. Cold start is substantially different and calls for a different approach. Since cold start only occurs during an early portion of a trip, it will be modeled in a future report.

CPF CO and HC

Previous studies have found loose correlations between CPF and FR or with Engine out emissions. CMEM, for example, employs the following equation for both CO and HC:

$$CPF = 1 - \Gamma * exp[(-b-c*(1-\varphi^{-1}))*FR] \tag{20}$$

where

Γ is the maximum CO (or HC) catalyst efficiency
b is the stoichiometric fitted parameter

c is the enrichment fitted parameter
φ is the normalized fuel to air ratio.

At its asymptotes, this equation approaches 0 when FR=0, and 1 when FR=∞, which roughly says that as the exhaust volume flow increases, the catalyst ability to oxidize the pollutants decreases due to the decreased exposure time. This is also known as "catalyst breakthrough". Generally, this may be true, but the catalyst correlation (ρ) with fuel rate is quite poor, and it is even worse with VSP:

$\rho_{CPFCO/FR} = 0.42$
$\rho_{CPFCO/VSP} = 0.27$

The hydrocarbon trends are not as clear as those of CO. The CPFHC correlation coefficients are listed below:

$\rho_{CPFHC/FR} = 0.34$
$\rho_{CPFHC/VSP} = 0.23$

Figure 26 shows the relationship between CPFCO and FR. The points have been separated by stoichiometric/enrichment and light/heavy categories. While the scatter is excessive, there is still a general increasing trend with FR, but there is no obvious weight trend discerned.

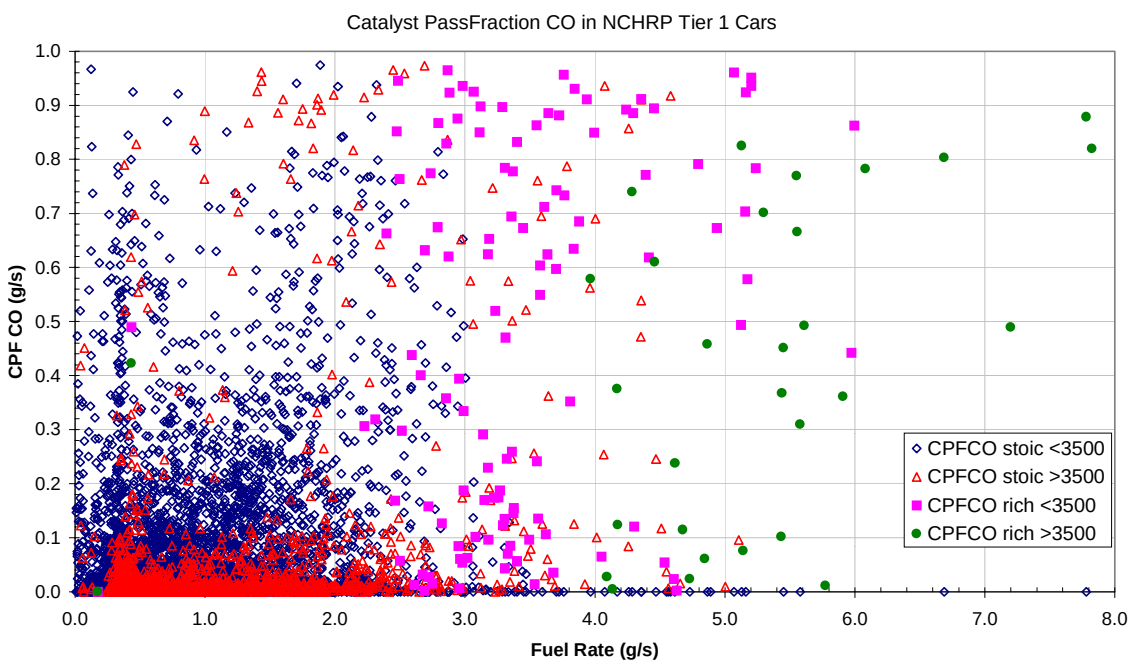

Figure 26. CPFCO as a function of FR for Tier 1 cars.

The scatter in CPF plots is tremendous. HC, and NOx are no better in this regard. After a significant effort to attempt to parameterize CPF behavior for all of the data points in this study, it was deemed best to either complicate the model beyond the level of CMEM (by including an air to fuel ratio algorithm, temperature model, and perhaps even "engine stress"), or greatly

simplify it (sacrificing some accuracy). We chose the latter route. The approach selected is to bin the CPF by VSP. In the flow chart (figure 8), this is just above decision 5. Figure 27 shows the CPF binned by VSP. It is advantageous to bin data since it has an averaging effect over time, smoothes out some very stochastic and “spiky” time series data.

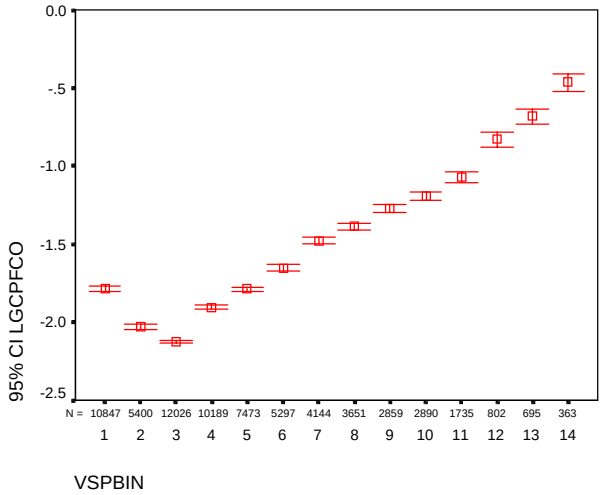

Figure 27. CPFCO binned by VSP and plotted logarithmically.

The plot appears well behaved but upon further investigation we encounter the following difficulty. When the measured CPF is separated for the FTP and US06 cycles (figure 28), we unexpectedly see a bifurcation in the data. An effect is also visible on HC, though it isn’t as significant. The effect is not as pronounced when plotted on a linear scale.

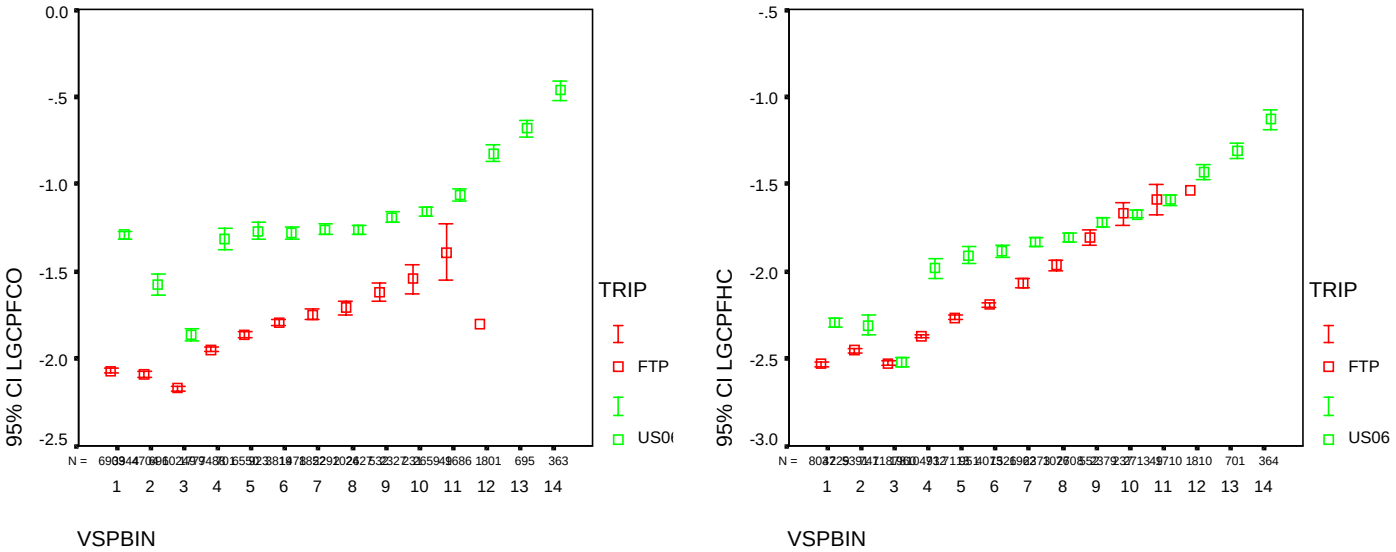

Figure 28. Measured CPF CO and HC binned by VSP but separated by driving cycle.

This separation in the data does not appear to be an engine out phenomena, but rather that of the aftertreatment system. Figure 29 and 30 show engine out and tailpipe CO respectively confirming this. There is a slight engine out discrepancy in bins 4 and 5, but it is much more

pronounced in the tailpipe plot. Similar relationships occur when plotted as a function of fuel rate instead of VSP.

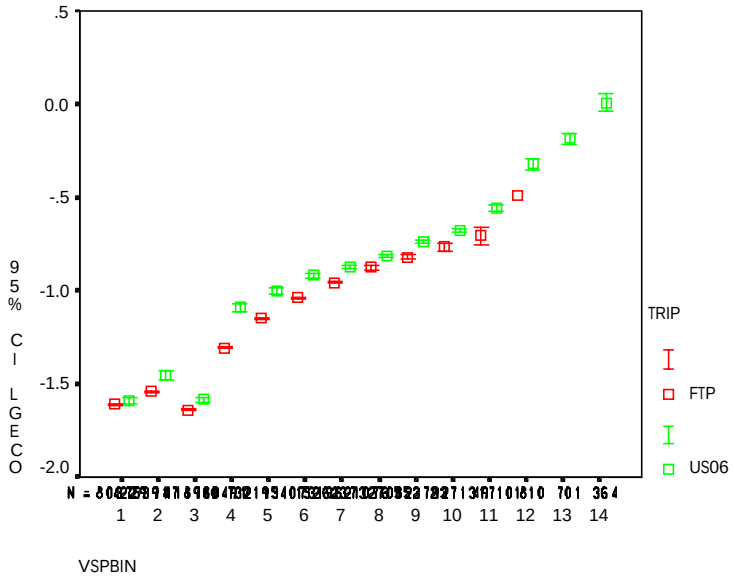

Figure 29. Measured ECO binned by VSP and separated by driving cycle.

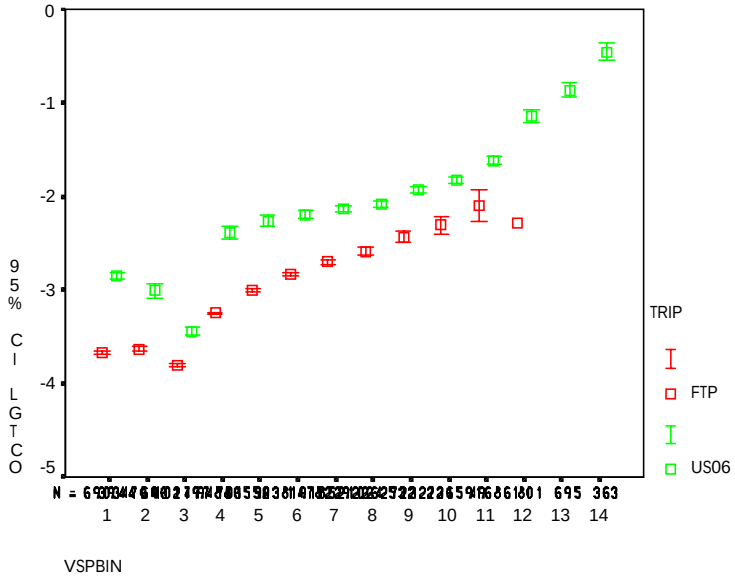

Figure 30. Measured TPCO binned by VSP and separated by driving cycle.

The plots indicate that for the same road load conditions, tailpipe emissions are higher in the more aggressive high–speed driving cycle. Younglove et al (1999) and Frey et al. (2002, Appendix A-7) noticed this “speed effect” in their studies as well. The latter study observed it in the RSD data. Their conclusion was that speed was the differentiating factor. Some driving has higher speed activity at lower VSP. It is still possible to be driving at high speed yet have nearly zero VSP if the vehicle is not accelerating. Figure 31 shows the speed distribution of the two cycles as a function of VSP.

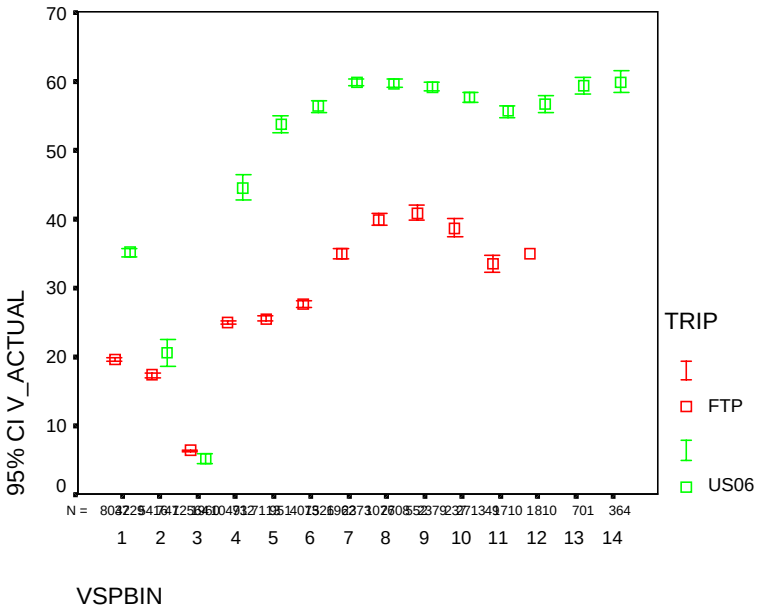

Figure 31. Speed on the FTP and US06 cycles within each VSP bin.

However, this alone is not likely sufficient to cause a significant increase in emissions since the engine does not need to work hard during coasting and braking, thus it is not expected to have higher emissions during these periods. There are many reasons why this may occur: throttle dither, catalyst breakthrough, enrichment, other engine strategy differences, or something else unforeseen. Further investigation is required to find the cause and then capture the phenomena in PERE.

Separating out by modes, figure 32 shows CPFCO by VSP bin where only the accelerating data points are employed. Note that the bifurcation is significantly reduced when compared to figure 31. Figure 33 shows the points where the vehicle is coasting or decelerating, verifying that these modes are the major cause of the split. There is little difference in the coasting and the deceleration profiles, so they are combined for this study. The definitions of the modes of driving for this report are outlined in table 6. The enrichment mode is not included on this table.

Table 6. Modes of driving.

Mode	**Condition**
Deceleration	accel < -0.2 mph/s
Idle	v < 2 mph
Cruise	-0.2 < accel < 1 mph/s
Acceleration	accel > 1 mph/s

It is likely that the definition of cruise (based only on acceleration) will change depending on the speed. In a future study, it may be advantageous to better define these modes of driving. Cruise driving implies that the driver is not driving at exactly the same speed or throttle. Every driver dithers the throttle some amount. Even when using cruise control, road grade keeps the throttle changing in order to maintain constant speed. Moreover, the added (minor) decelerations that

occur during cruise driving, tend to reduce the instantaneous value VSP (as well as fuel rate).It is this low acceleration type of driving we are defining as the “cruise” mode.

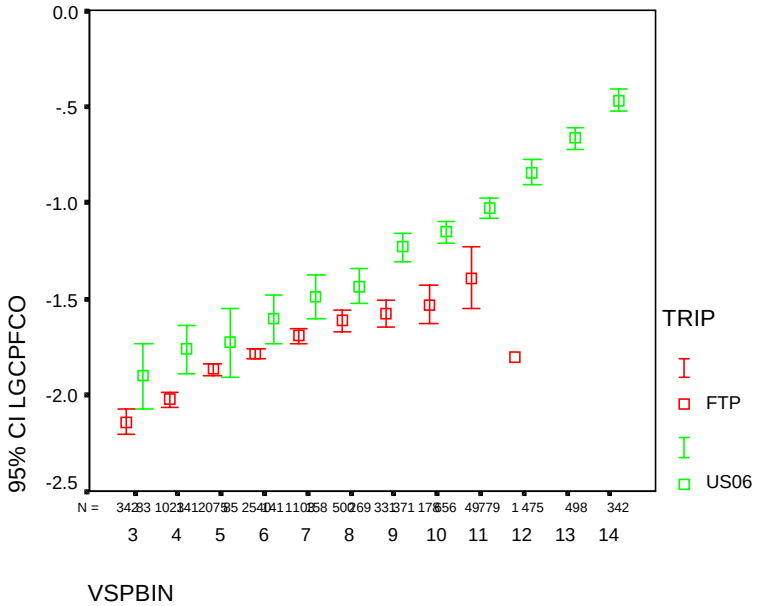

Figure 32. CPFCO by VSP bin. Only the points where accel > 1.0 mph/s are included.

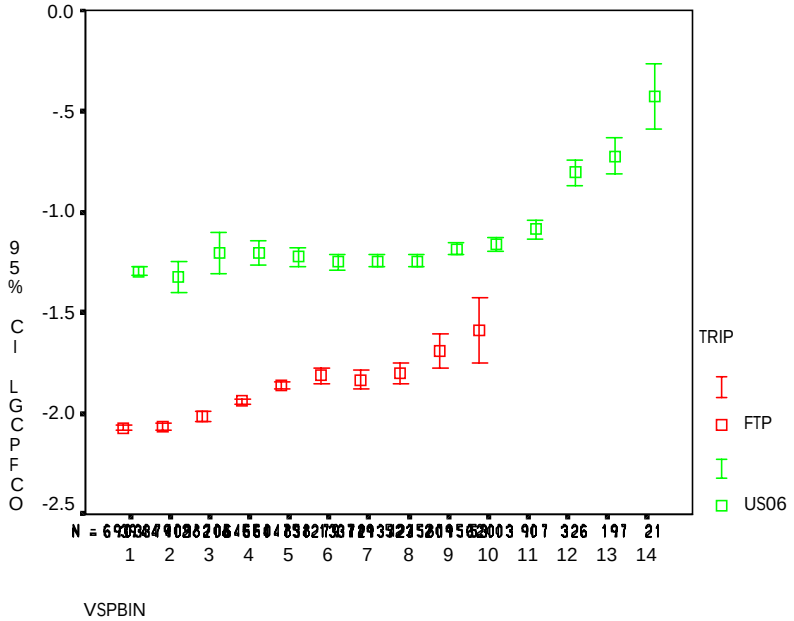

Figure 33. Cruise and decel CPF CO data as a function of VSP bin. Idle is omitted.

According to the above modal definitions, we can devise the following ‘preliminary’ model for CPFCO.
During acceleration and enrichment (low accel) events:

$$CPF = (1 - \Gamma)*exp(b_1*FR) \tag{21}$$

For higher emitter vehicles, it may be necessary to modify these algorithms so that they maximize around 1.

During cruise and decelerations, the quantification is not as straightforward. The difference between these two driving cycles is the aggressiveness of their cruise sections. Second by second aggressiveness is very difficult to quantify without knowing the history. We will leave it up to a future study to better quantify this. For this study, we will correct merely by speed as was recommended by Frey et al. (2002). In Figure 34, the CPFCO is plotted by (instantaneous) speed bin, where the bins are in 5 mph increments as defined in table 7.

Table 7. Speed bins

Bin	Speed Range (mph)
1	0-5
2	5-10
3	10-15
…	
10	45-50
…	
15	70-75
16	75+

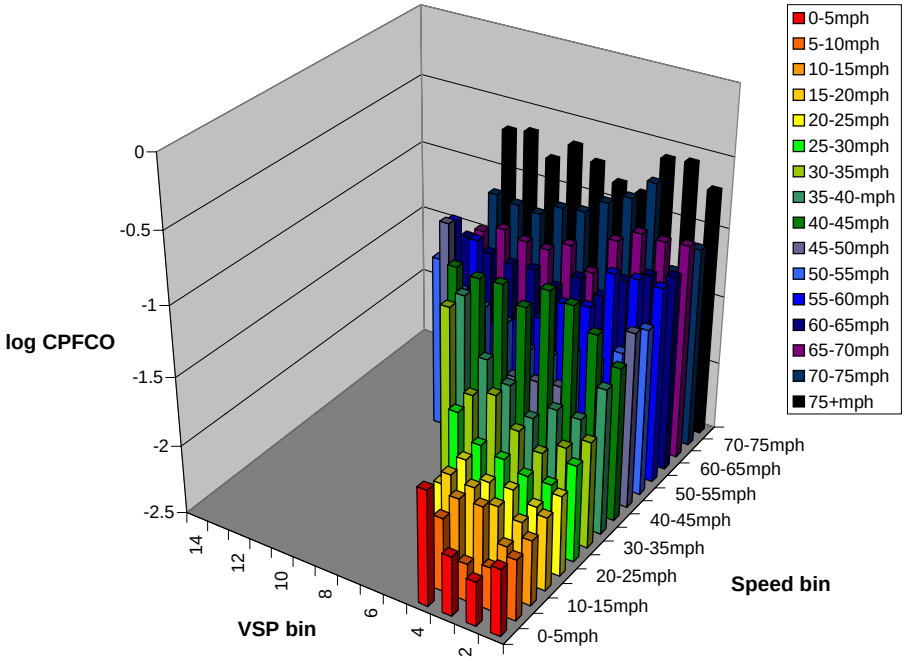

Figure 34. CPFCO during cruise and deceleration plotted by VSP and speed bins.

From figure 34, it appears that cruise and decel CPFCO is relatively independent of VSP. Thus, we can model it the following way:

$$CPF = (1 - \Gamma)*exp(b_2*v) \quad (24)$$

Completing figure 34, the next figure shows what it would look like if all the VSP, speed bins were filled. Notice also that high speed, emissions seem to be relatively independent of VSP. These cells tend to be highly populated by the high speed cruise portions of the US06 cycle.

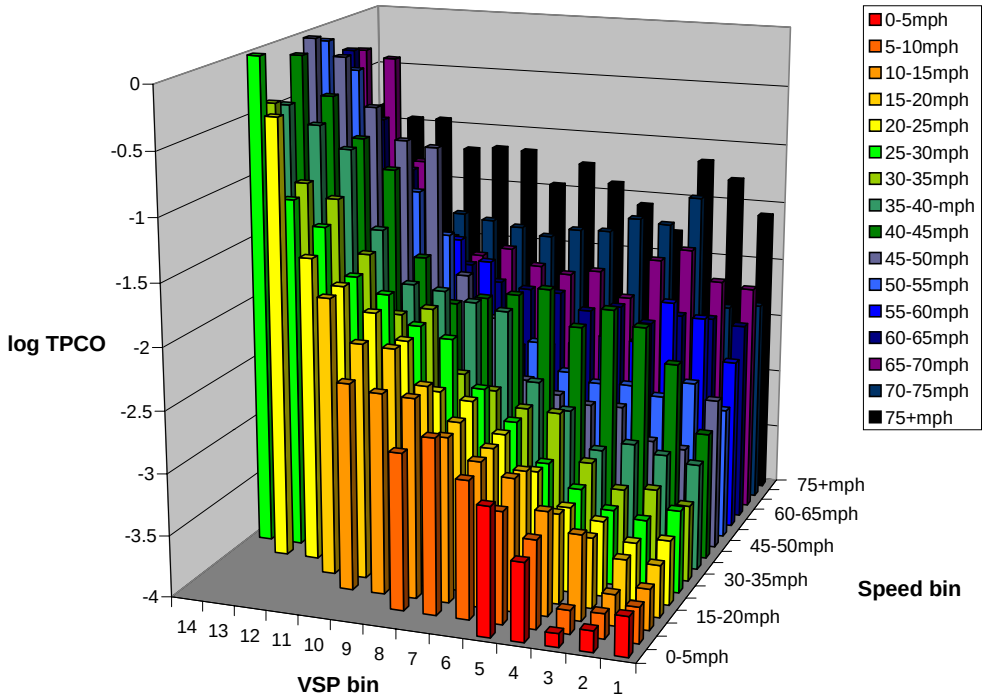

Figure 35. Measured TP CO for the FTP and US06 driving cycles as a function of VSP and speed.

Due to the specific nature of the two driving cycles used to calibrate, speed may only be an incidental causal variable. It is unknown at this time, whether less aggressive high speed cruises (e.g. using cruise control) would give lower emission rates. Looking more closely at the MEC01 cycle (the driving cycle used to validate this model) should shed more light on this since it has a number of cruise events at varying speeds. Complicating matters, figure 36 indicates that speed alone will not explain the cruise/decel difference between the two cycles.

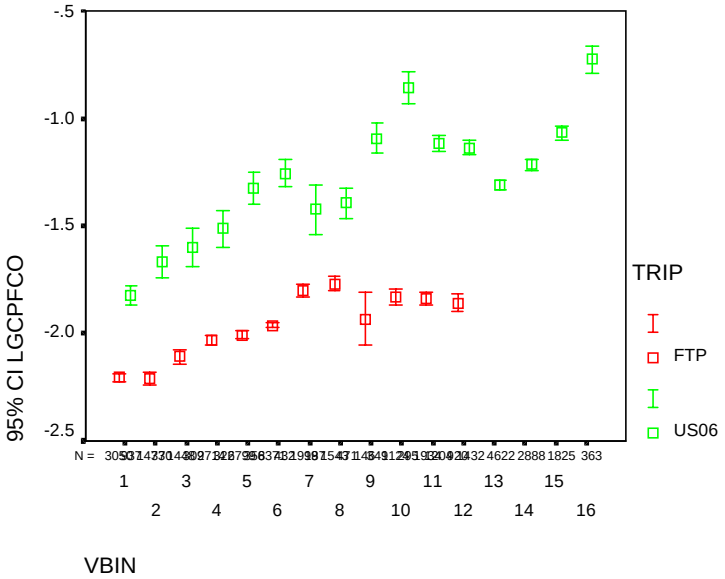

Figure 36. CPF CO during cruise and decels vs speed and separated by driving cycle.

Another limitation of this methodology is that equations 22 and 23 are not necessarily continuous (temporally). However, this may not pose a serious problem as long as second by second emissions are not being modeled.

It is clearly necessary to calibrate this model based on a more varied sample set. To get a sense for the limitations of these two driving cycles, Figure 37 shows the relative activity of the FTP and US06 driving cycles on a VSP and speed grid. Figure 38, shows the activity in a sample of on-road driving (taken from the EPA PEMS data set) conducted in southeast Michigan. Note the lack of driving within speed range 30 to 50 mph for the driving cycles. This indicates that the driving cycles accelerate through this region, rather than cruising in it (hence the lack of activity). This could potentially bias the CO model more toward a straight VSP approach due to the lack of cruise driving.

However, it is clear that within the cruise mode, there is a speed or aggressivity affect on emission, even within a VSP bin. The same effect is not evident for HC during cruise.

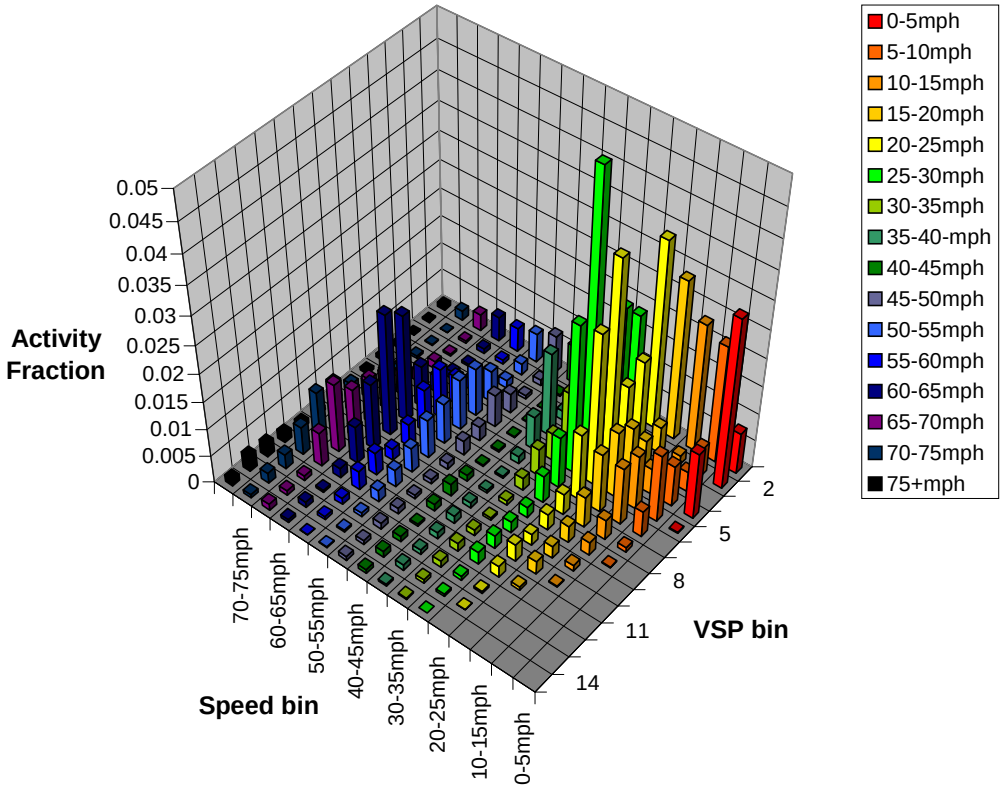

Figure 37. Activity fraction of VSP and speed bins for the FTP and US06 cycles. Idle is omitted.

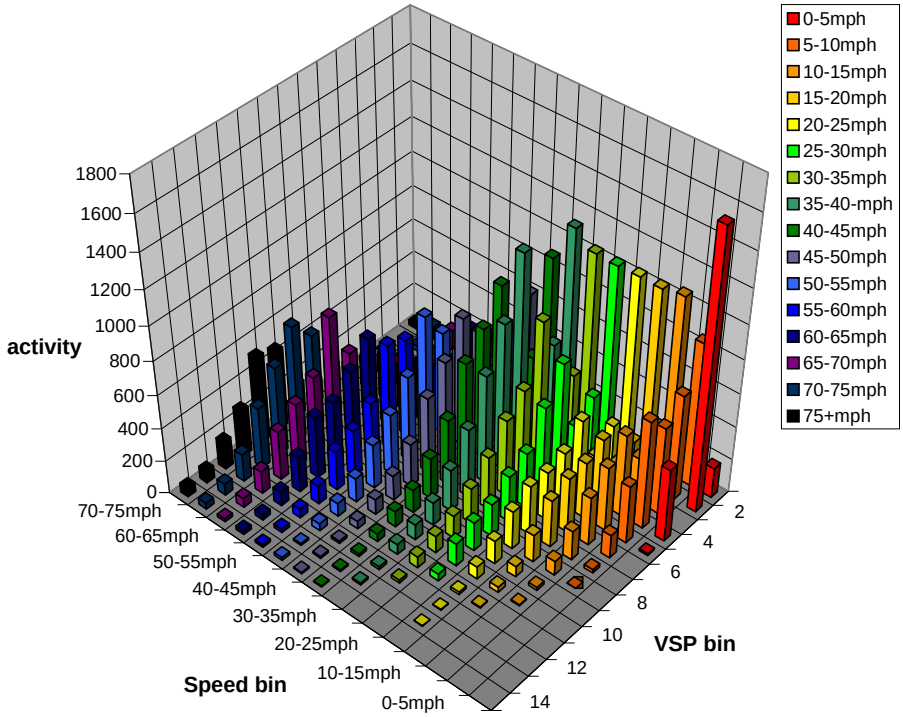

Figure 38. Activity of On-board emissions data. This is a sample of driving in southeast Michigan from 18 drivers.

For CPF HC, the discrepancy originates from decelerations. Figure 39 shows the CPF HC points so that only the cruise and acceleration points are plotted. Figure 40 shows only the deceleration points. The discrepancy in deceleration is undoubtedly due to enleanment arising from deceleration fuel shut off (An et al., 1998). Due to the positive terms in equation 1, it is possible to be decelerating, yet have a positive VSP.

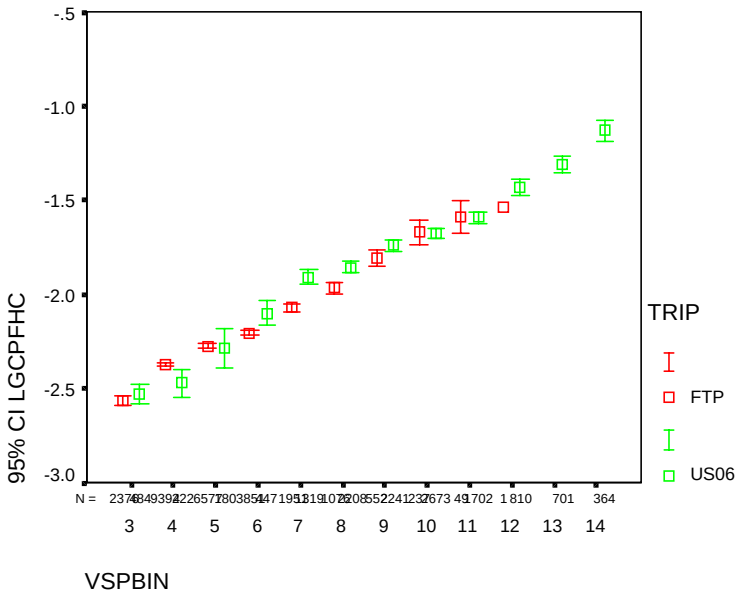

Figure 39. Cruise and acceleration CPF HC as a function of VSP bin. Idle is omitted.

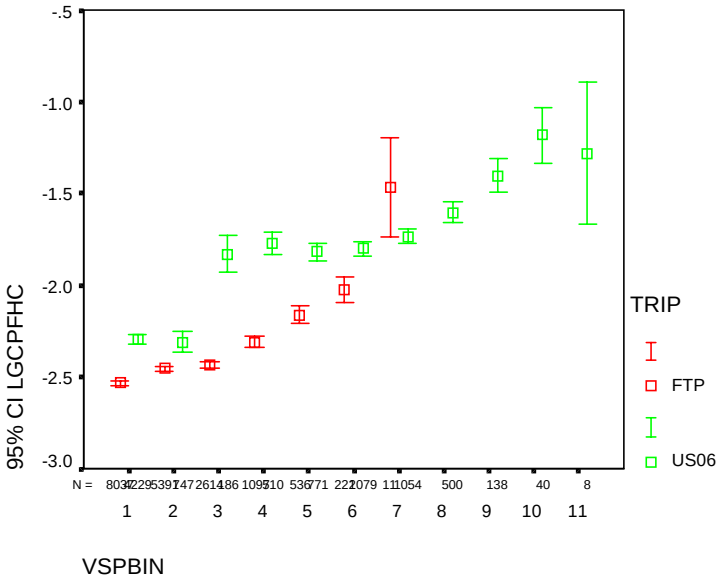

Figure 40. Deceleration CPF HC as a function of VSP bin.

To better isolate this effect, we create deceleration bins:

Table 8. Deceleration bins

Accel Bin	Range (mph/s)
1	< -3
2	[-3,-2)
3	[-2,-1)
4	[-1,0)

Figure 41 shows that the hydrocarbon puffs are breaking through the catalyst in the positive VSP values but moderate decelerations (accel bin 3, VSP bins 3-6). The large error bars indicate that there are few data points with high decelerations in positive VSP bins (VSP bin >3).

A simple relationship that might work for HC during cruise, accelerations, and slow decelerations, is as follows (same as for CO):

$$CPF = (1 - \Gamma_{HC})*exp[b_{1HC}*FR] \tag{23}$$

During decelerations, it is similar to CO:

$$CPF = (1 - \Gamma_{HC})*exp[b_{2HC}*v] \tag{24}$$

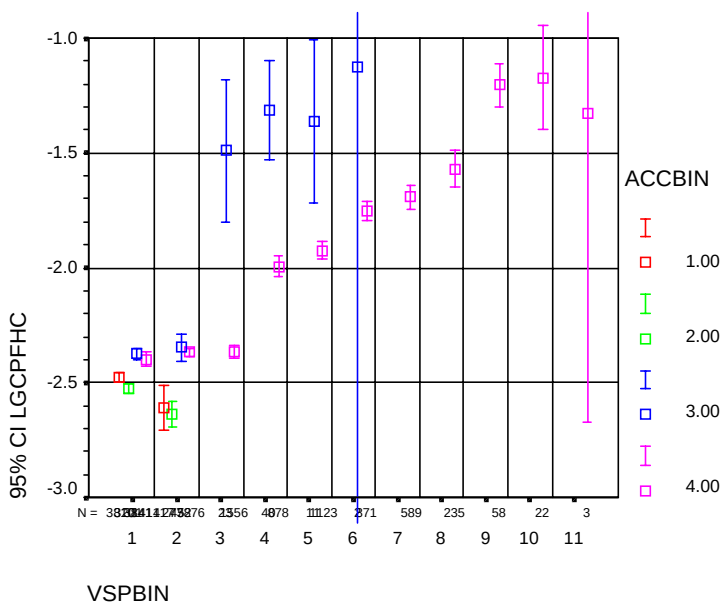

Figure 41. Deceleration CPF HC as a function of VSP bin split by binned acceleration.

Many previous publications employ the use of speed, acceleration, emissions (or even v*a, v and emissions) "maps" to model emissions (Pischinger, 1998). The approach presented here maps road load and speed with emissions for the some of the modes of driving.

CPF NOx

Historically, the catalyst behavior of NOx has always been extremely difficult to model. This is due to many of the factors mentioned above. Just a simple study of the correlations gives the following:

$\rho_{CPFNOx/FR}$ = -0.01
$\rho_{CPFNOx/VSP}$ = -0.02
$\rho_{CPFNOx/EINOx}$ = -0.07

The CPF NOx trends as a function of FR are extremely scattered (not shown). The VSP, speed CPF plot is shown on Figure 42. There is no simple monotonically increasing function that would describe this relationship. The NOx curves have a local maxima or “islands” of emissions. There appears to be two minima at VSP bin 5 at roughly 25 and 55 mph. There may also be one at 65 (the cruise sections of the US06). Oddly, these roughly correspond to the activity peaks in figure 38.

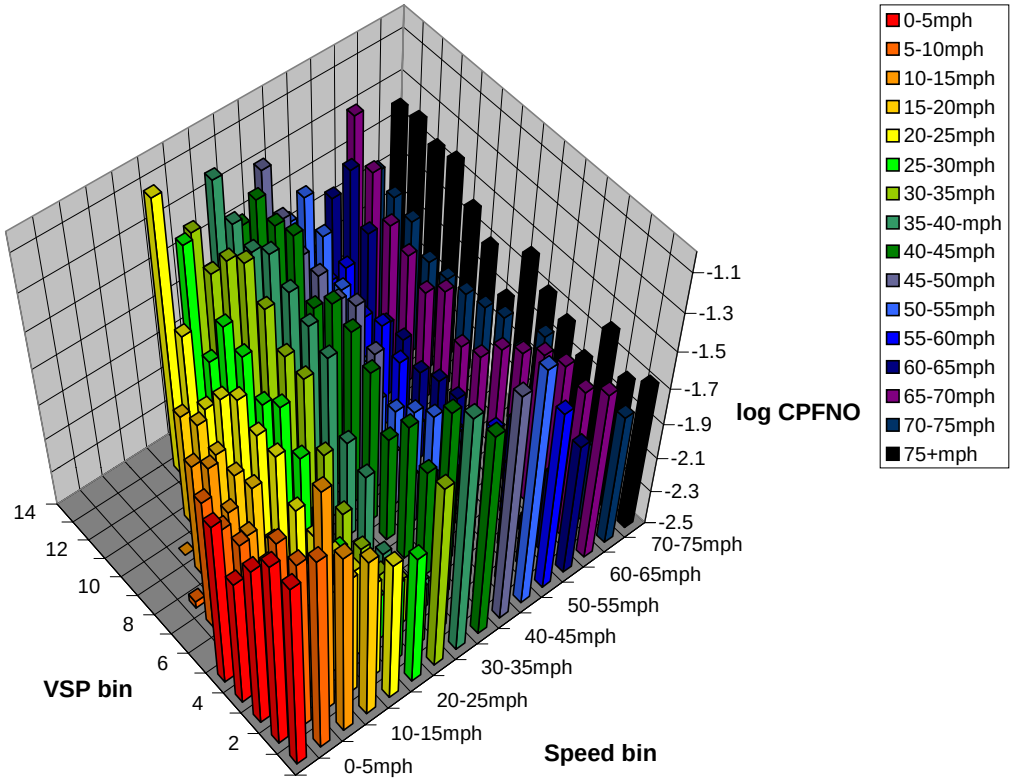

Figure 42. CPF NOx as a function of VSP and speed. The curve is rotated in comparison to the others seen so far to give a better indication of the texture.

To simplify matters, we first look to see if there is a fundamental difference in NOx profiles for the two driving cycles in this data set. Figure 43 shows that the two cycles do not seem to be significantly different (except VSP bin 4). "Significant difference", here is defined as non overlapping confidence intervals.

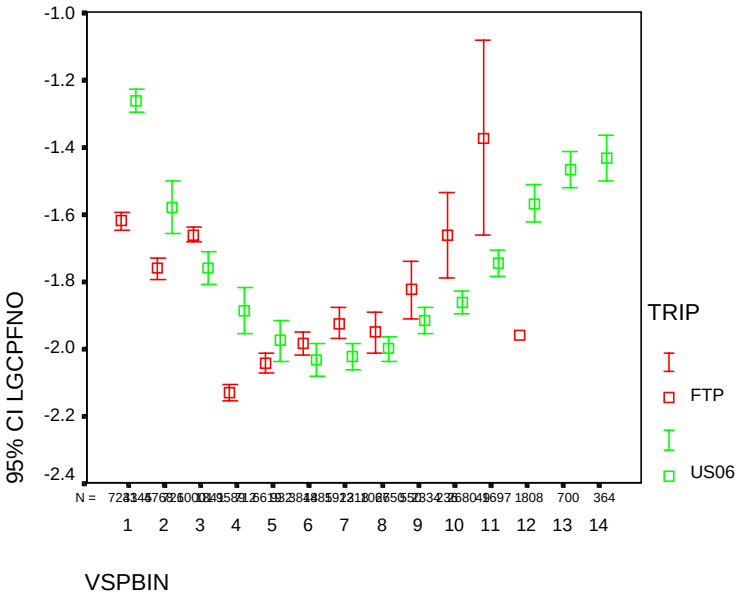

Figure 43. CPF NOx as a function of VSP split by driving cycle.

Due to the low engine out emissions at the lower VSP bins (negative values), it is not as important to accurately depict this region. We can use the same model as above:

$$CPF = (1 - \Gamma_{NOx})*exp[b_{1NOx}*FR] \tag{25}$$

Given these simple algorithms, we can proceed to calibrate and validate the tailpipe portion of the model.

Tailpipe Calibration

The engine out behavior is relatively straightforward and 'unscattered'. Because of this, a least square regression gives parameters, which fit the second by second traces as well as giving relatively accurate total emissions. However the catalyst module is somewhat more complicated.

For the catalyst model, it is advantageous to fit first to the low fuel rate regime (equation 21) and then the high. It is determined that the best method is to calibrate the Γ parameter first, based on idle (VSP bin 3) emissions. This is basically the minimum of the CPF emissions profile and sets the baseline. For NOx, this minimum happens to fall in VSP bin 4, rather than 3. This parameter can be read straight off of the plots.

For CO, table 9 indicates the values of the VSP bin 3 (and lowest speed) values of logCPF along with their uncertainties (variabilities in this case). The uncertainties in Γ are propagated using standard error propagation equations (Taylor, 1982). For error (uncertainty) propagation, we assume normal or log-normal distributions where appropriate. In this case, the uncertainty in CPF was small enough to simply carry over (calculate) the uncertainty in catalyst efficiency (δΓ).

Table 9. Idle (or minimum) catalyst pass fractions (CPF_0) and catalyst efficiencies (Γ) along with their uncertainties (mean standard deviations).

	logCPF0	d(logCPF0)	Γ	$\delta\Gamma$
CO	-2.18	0.006	0.993	0.007
HC	-2.57	0.005	0.997	0.003
NO	-1.55	0.012	0.972	0.028

For NOx, the idle VSP bin does not have the lowest CPF. That is in VSP bin 4 of the FTP cycle. In that bin the Γ = 0.993. We will use this term in the calibration.

Since the catalyst pass fractions are so scattered (being a ratio of two measured quantities), it makes much more sense to fit to the observable tailpipe, rather than the CPF. The question remains whether the parametric fits should be conducted on a linear or logarithmic scale. For this study, it turned out best to fit CO and HC logarithmically and NOx linearly. This will need to be investigated further in a future study.

The next step in calibration is to perform a regression fit to the acceleration modes (equations 21, 23, and 25) using b_1 as an adjustable parameter. *EO* and *FR* are modeled values. Then we can fit to the cruise and or deceleration modes (equations 22 and possibly 24). One could either calibrate to the second by second data directly, or to the aggregate data, or even to the cumulative emissions. In this section, we calibrated to the second by second data, which can be somewhat computationally intensive.

When this is done, the following coefficients along with their uncertainties are obtained:

Table 10. Fitted Catalyst parameters

Parameter	Value	St Dev	95% CI LO	95% CI HI
B1CO	0.749	0.012	0.725	0.773
B2CO	0.0216	0.0002	0.0212	0.0220
GAMMACO	0.993	0.004		
B1HC	0.695	0.004	0.687	0.704
B2HC	0.0162	0.0002	0.0158	0.0167
GAMMAHC	0.997	0.001	0.997	1.001
b1NO	0.456	0.003	0.451	0.461
GAMMANO	0.993			

The following series of figures shows the calibration fits to the combined FTP and US06 driving cycles. From observation, the fits are quite reasonable. A quantitative description of the goodness of fit would require a proper analysis of the uncertainties, however this was not conducted due to the preliminary nature of this model. This will take place in the next stage of model development.

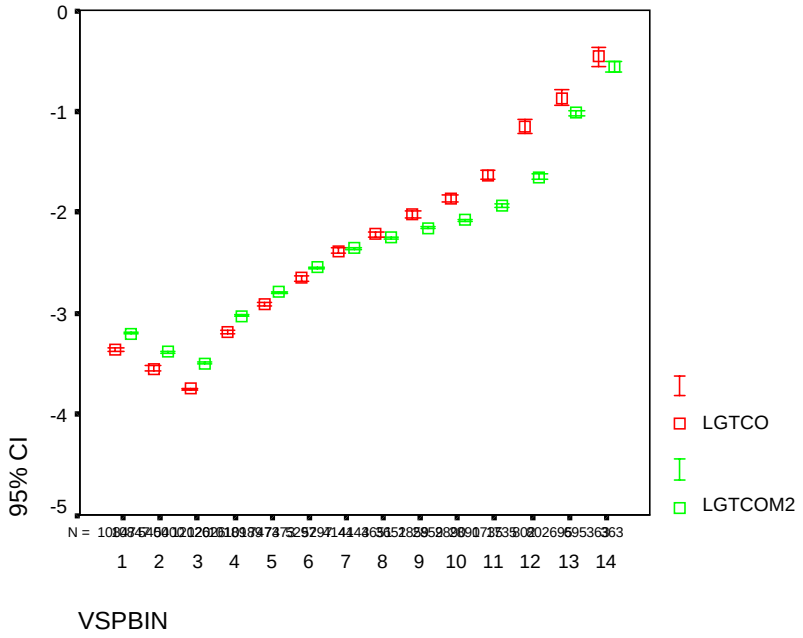

Figure 44. Calibration of TPCO. “M2” is modeled.

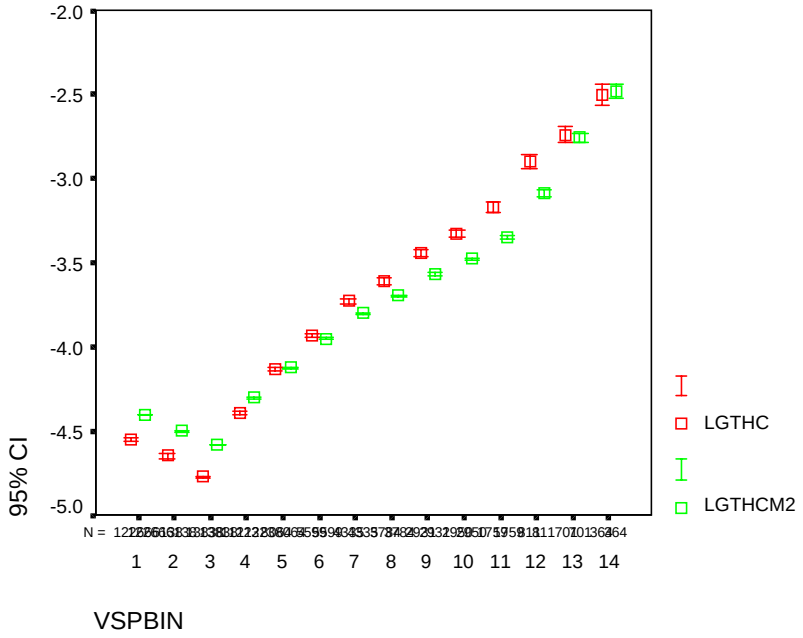

Figure 45. TP HC Calibration to the NCHRP Tier1 data set.

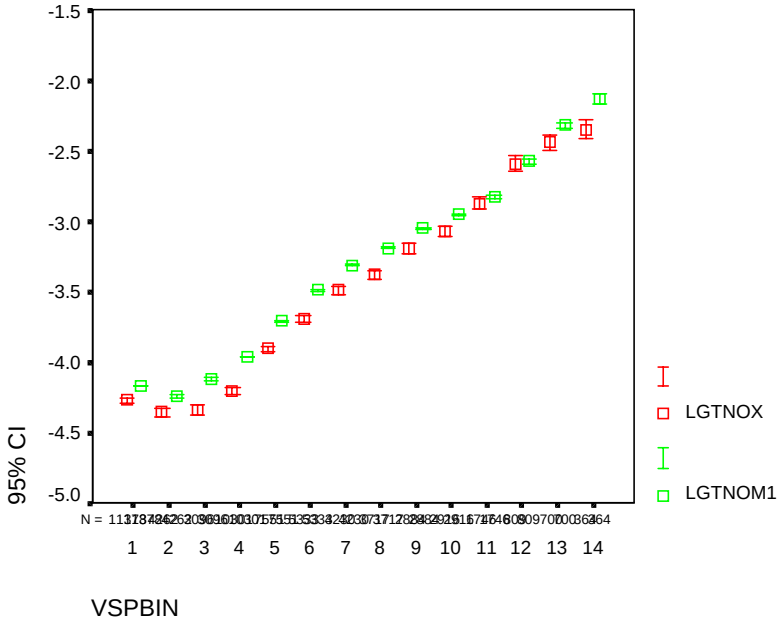

Figure 46. TP NOx Calibration to the NCHRP Tier 1 data set

III - VALIDATION OF PERE

Fuel and CO_2

Validation to MEC

Figure 47 shows the fuel rate comparison of the measured and the modeled. The model is based on equation 6. The only significant deviation lies in VSP bin 14. It is likely that the enrichment model is not capturing all of the vehicles. The error bars are 95% confidence intervals so only reflect the variation in the model (from vehicle weight, etc.), and not the uncertainty. At lower loads this uncertainty is relatively small, but under enrichment conditions, it would be necessary to propagate the uncertainty terms from equation 13. For cumulative fuel consumption, the model overpredicted the vehicle average by 1%.

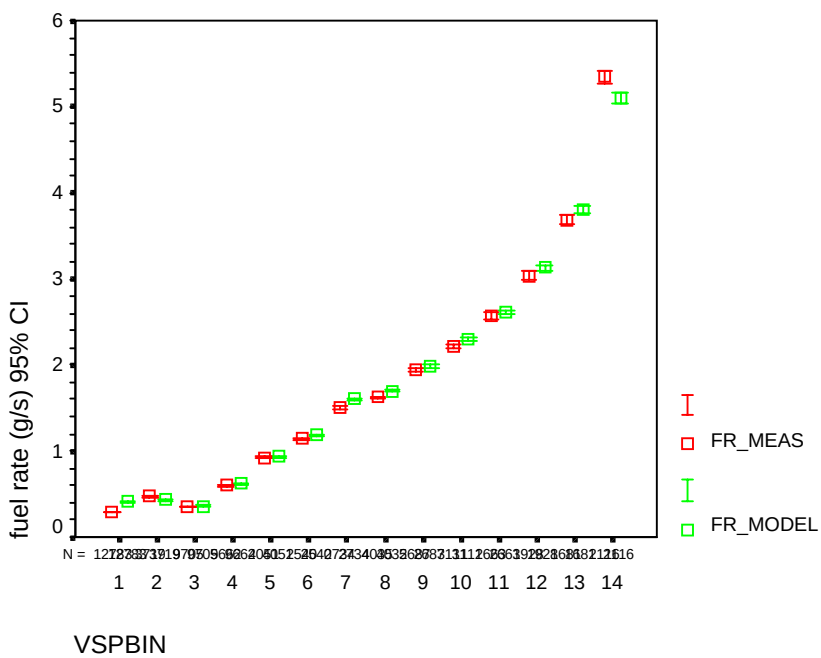

Figure 47. Fuel rate validation for the MEC data. Error bars are 95% confidence interval in the variation.

Figure 48 shows the validation for average CO_2 (calculated from all of the vehicles). This comes directly from fuel rate equation 8. CO and HC terms can be added, but those are relatively small correction terms. The comparison is excellent until the two highest VSP bins, where the model overpredicts due to enrichment. During enrichment, a fraction of the CO and HC is prevented from being oxidized in the catalyst, hence the combustion of fuel into CO_2 and H_2O is less than ideal. The tailpipe CO and HC should correct the model at these higher values in the final form of the model. It is impossible to quantify this uncertainty bar on these points without a CO model, so it is omitted for the purposes of the CO_2 model. It is presented here in this fashion to demonstrate proof of concept for the first portion of MOVES (greenhouse gas). The cumulative CO_2 emissions overpredict by 5% (figure 49). With the measured HC and CO as a correction, this differential drops to 2% (underpredicted).

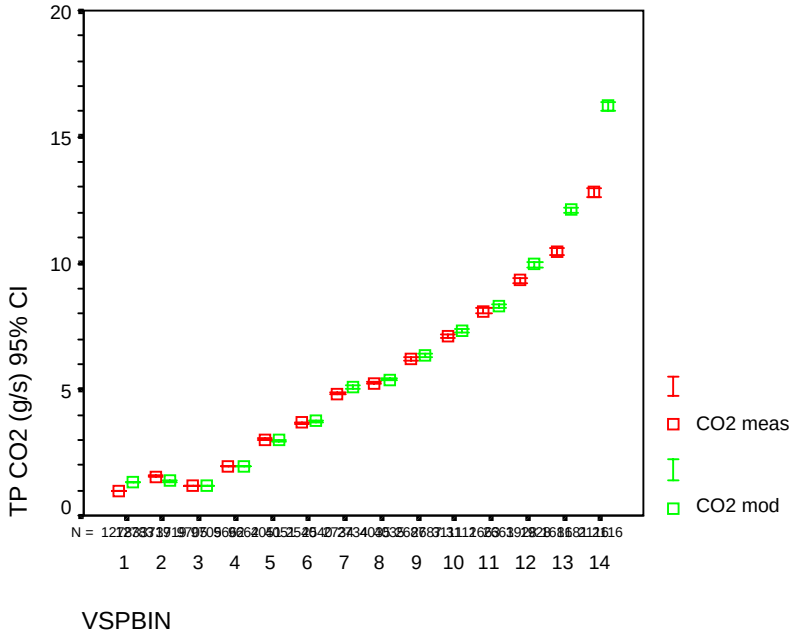

Figure 48. CO_2 validation for the MEC data.

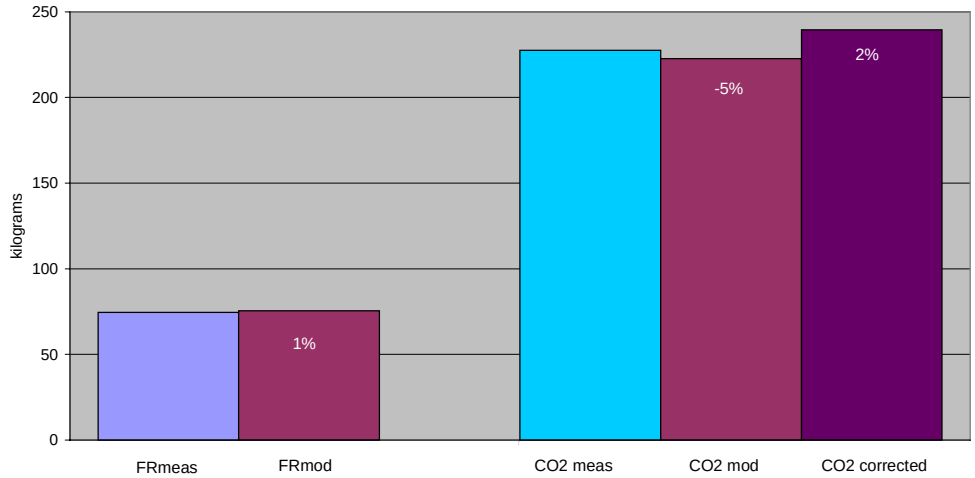

Figure 49. Validation for total FR and CO_2.

Validation to UCC

Frey et al. (2002, p 230) reported a significant speed dependence on CO_2 predictions. By comparing the emissions from the vehicles driven on several CARB Unified driving cycles, it was found that the model was overpredicting on the lower speed cycles and underpredicting on the higher speed cycles.

As part of the proof of concept, 17 vehicles in the CARB dataset were simulated on the 8 UCC driving cycles using PERE. Since the engine size was not supplied as part of the database, the values were obtained from the Kelly Blue Book Website (www.kbb.com). Where there were multiple values for engine size, the smaller value was assumed. However, if the fuel rate

predictions were significantly underpredicting (~20% or more), the higher engine size was chosen and recalculated. The second by second fuel rate and CO_2 were calculated for each driving cycle and car. This value was then "corrected" by subtracting the CO and HC *measurements* to determine the limit of the accuracy of the model (as was done in the previous section. Figure 50 shows the results from PERE compared to those obtained from NCSU. The NCSU model overpredicted at low speeds but underpredicted at higher speeds. The results from PERE were the opposite: it overpredicted as cycle speed increased. However, the speed effect in PERE is less pronounced. It should be noted that the NCSU results only included the smaller engine vehicles (<3.5L) whereas the PERE model used all the vehicles since it is able to accommodate engine size explicitly in the model.

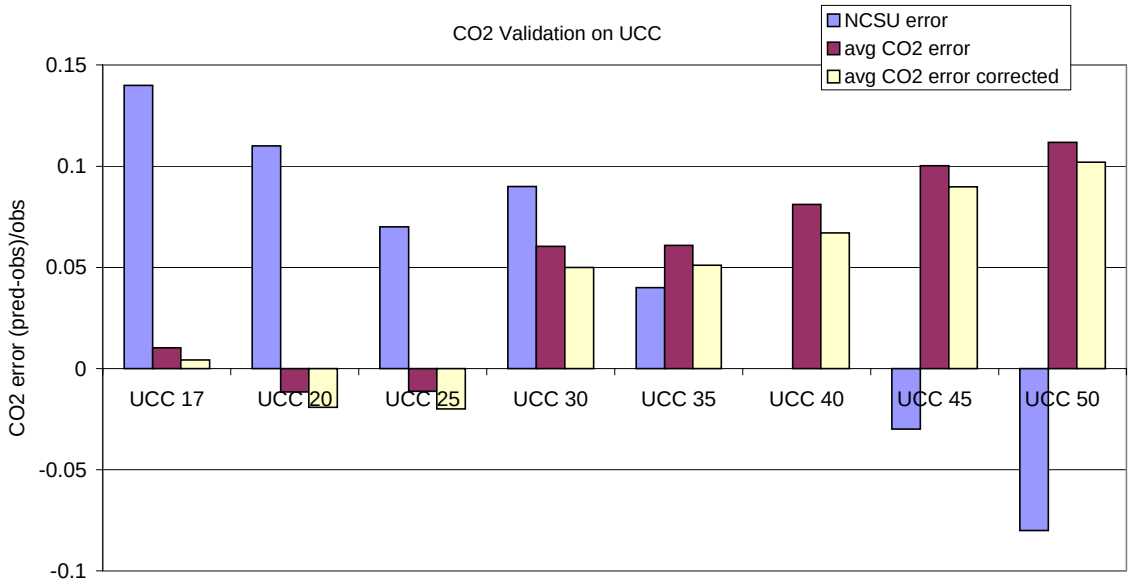

Figure 50. fractional error of the NCSU CO2 predictions compared to PERE predictions.

The results indicate that CO and HC corrections are minor in comparison to a possible speed effect. However, this "speed effect" may be acceptable if a 10% consistency criteria is used. Though the discrepancy seems to increase with increasing average cycle speed, this does not prove that speed is a causal variable, it may only be coincidental. It is possible that the efficiency term (in equation 6) increases with engine speed, which would not be too surprising. This will be investigated in a future study.

Though not shown, the heaviest vehicles (4000 lbs and also with the largest engine size) in the study, overpredicted the fuel consumption by >15% or more for each of the cycles. More heavy vehicles (including light trucks) should be examined in a future study to see if the overprediction trend is real. Other than these vehicles, there was no significant weight effect discerned.

Propagation of Uncertainty

Before presenting the comparison of the engine out model, it is first necessary to discuss the propagation of uncertainty in the model. It has been stated by many of the users of MOBILE, that an estimate of the uncertainty in the model is a necessity. The following is a brief discussion of some methods by which this can be accomplished.

With any measured or modeled value, there is inherent variability and error. An example of natural variability is the distribution of vehicle masses in the modeling data set. This is known and accounted for in the model explicitly. An example of error is the uncertainty associated with the enrichment threshold (FR_{th}) of a given vehicle. This quantity was estimated from the scatter plots as mentioned earlier, without much concern of the "measurement error" because it was assumed that the unknown variability of the vehicles i.e. the difference in the manufacturer's specific enrichment strategies (irrespective of their known weight and engine displacement) would dominate the uncertainty. Thus in equation 13, each of the terms have both inherent variability and error. These are estimated via the uncertainty in the A and B coefficients, which is an output of the linear regression in most statistical software packages. For the purposes of this report, we will use the general term "uncertainty" to denote both measurement error and variability that is NOT known through natural variability. We discount the natural variability that is known, such as the variability in vehicle weights in the study since they are explicitly included in the calculations. We also do not account for systematic uncertainties, which are often significant. Systematic uncertainties often come about due to a failure of the model to account for certain physical effects. These important uncertainties are to be corrected (if significant) when they are discovered.

The question now remains, how can we propagate uncertainties in equations such as 13, to the final emissions calculations? There are a number of standard methods by which uncertainty in the terms of equations 11-17 can be propagated through to the engine out calculation: Monte Carlo, Bootstrap, and Error Propagation. For the sake of simplicity, we use the latter approach. If the probability distributions are normally (or log-normally) distributed, then the error propagation equations simplify since you only need to deal with means and standard deviations (or mean standard deviations) about the mean. This is the most computationally simple of methods, and the method used in this work. However, it may not be suitable for the final MOVES product, and will depend on the circumstances.

Uncertainty in Fuel Rate

It is difficult to estimate the uncertainty in many of the variables in the fuel rate equation 6 (and 1). However, as we have already seen in figure 47, the model performs very well especially when the car is assumed to be operating under stoichiometric conditions. During stoichiometric operation, there are the following unknown uncertainties in K, N, ε, C_R, and C_DA. Thomas and Ross (1997), indicate that some of these parameters are only "adjustable" within a narrow range, such that the uncertainty associated with these variables are relatively small. These include some of the variables comprising the simple engine speed sub model, and all of the above terms with the exception of the engine friction term K. However, since the most of the fuel consumed is needed to overcome road load (moreso than friction), the FR calculation is *probably* relatively insensitive to uncertainties in KNV_d. The accuracy and robustness of the fuel rate model attest to this.

Thus the majority of the uncertainty lies in the enrichment portion of the model. However, due to the *proprietary* nature of each of the vehicle manufacturer's enrichment strategies, the uncertainties in these variables are unable to be estimated. A more thorough study of the uncertainty in the simple models for ϕ, should be reassessed. However, due to the nature of the

model to predict fuel consumption very accurately, even under enrichment conditions, we will assume that the uncertainty in fuel rate is small in comparison to other uncertainties in the model, i.e. $\delta FR \approx 0$.

Uncertainty in Engine Out Emissions

There is a 1:1 correspondence between VSP and FR according to the fit in figure 47. The values are shown in the following table for the average VSP value within the particular bin. The bin definitions are from Frey et al. (2002) and the fuel rate value is the central value in the bin.

Table 11. VSP bins and central VSP and fuel rate values associated with the bins.

VSP bin	Avg VSP	FR
1	<-2	0.419
2	-1	0.339
3	0.5	0.317
4	2.5	0.590
5	5.5	0.857
6	8.5	1.152
7	11.5	1.431
8	14.5	1.643
9	17.5	1.908
10	21	2.100
11	25.5	2.385
12	30.5	2.988
13	36	3.773
14	>39	4.467

Using these bins, we can validate and estimate uncertainties. Some sample calculations are shown in Appendix E.

Engine Out Validation

The next three figures show the comparison of the engine out measurements and the model. There was no effort to separate out speed effects in the engine out portion of the model. Note that the modeled results only vary significantly from measurements at low VSP. Emissions tend to be relatively low at low VSP values, so the error is not as pronounced when compared to total emissions. Also, the regression tends to fit out the higher emission points. The plots are on a log scale to give the reader an idea of the fit at across all VSP values. However, due to the relatively small values of emissions occurring at lower VSP bins, it is probably more important look at the middle and higher VSP bins to gauge the "goodness" of the model.

The model is indeed very good at the engine out level, i.e. most of the modeled points are consistent to within the uncertainty with the measurements at each of the VSP bins. There are some systematic overpredictions for HC in VSP bins 7-10. There is also a systematic overprediction in bin 3 (idle). It is likely that engine strategy is quite different at idle than during normal operation. If idle (light vehicle) emissions becomes an important factor to model in MOVES, it will be necessary to modify or "correct" the idle emissions factors.

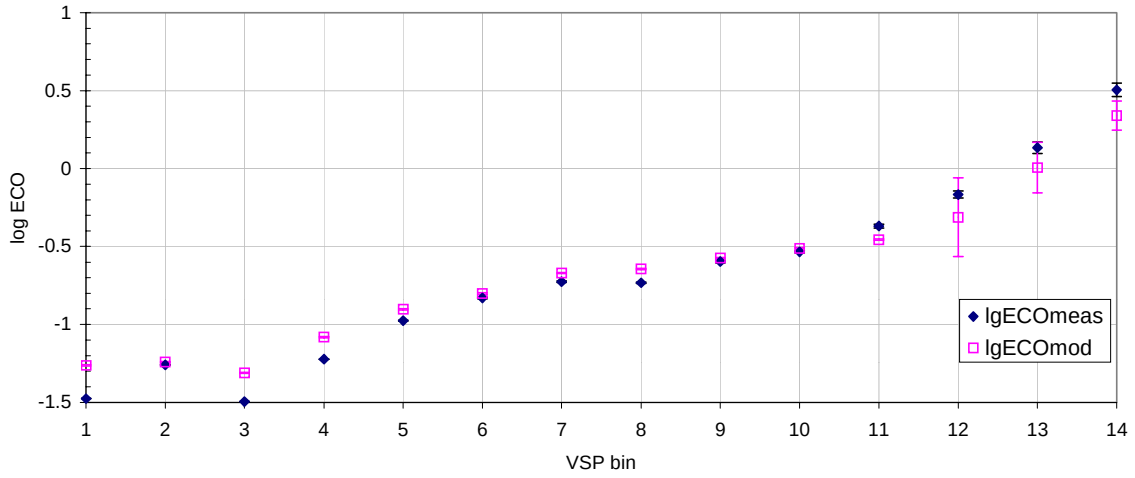

Figure 51. A comparison of the engine out CO measurements from MEC cycle and the model calibrated to the FTP and US06 cycles.

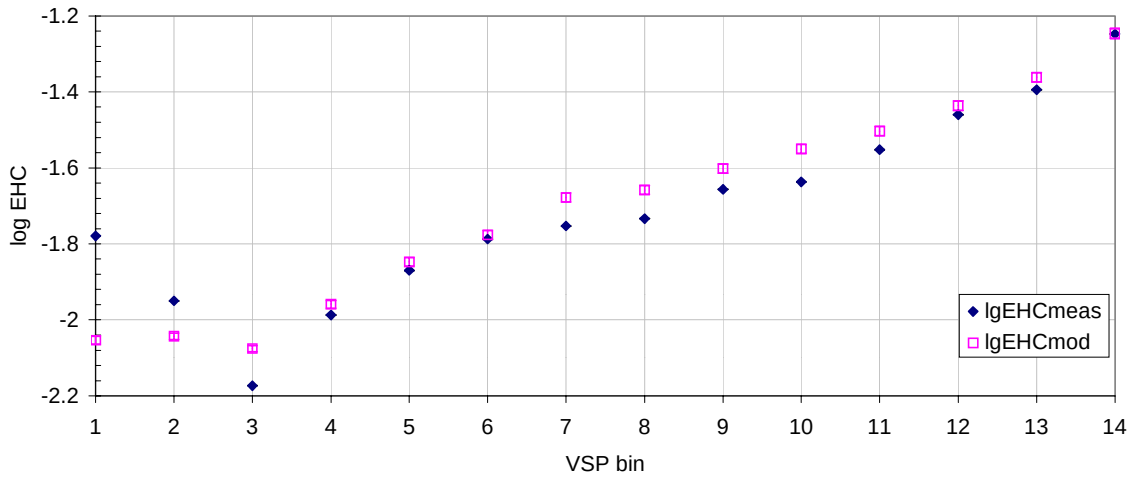

Figure 52. A comparison of the engine out HC measurements from MEC cycle and the model calibrated to the FTP and US06 cycles.

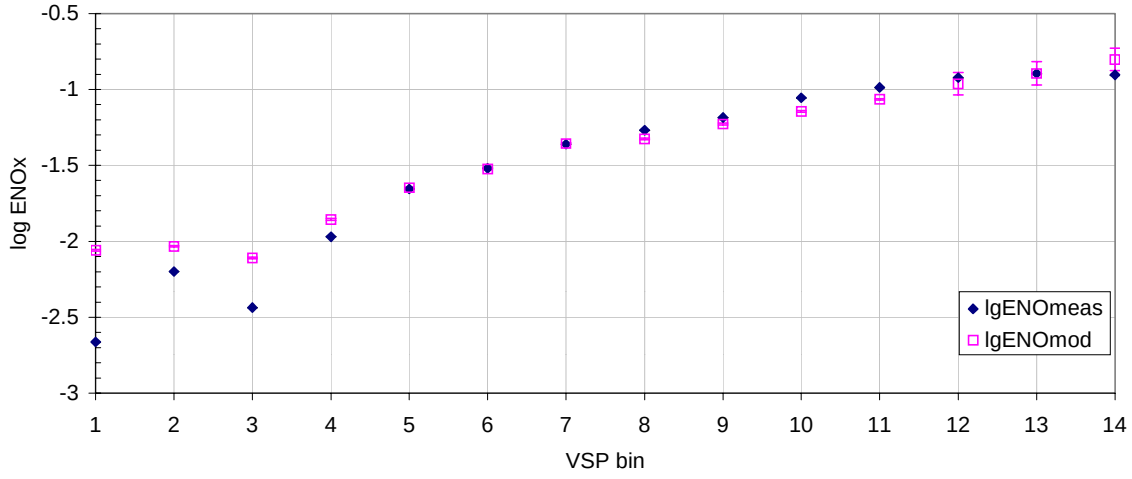

Figure 53. A comparison of the EO NO measurements from MEC cycle and the model.

The cumulative emissions are shown in figure 54. The error was not propagated to this value at this time.

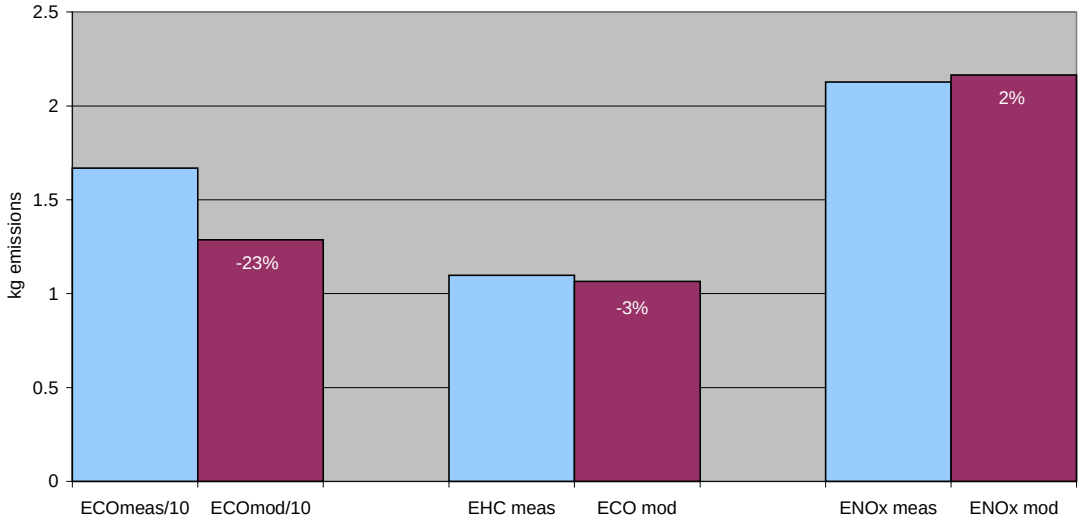

Figure 54. Measured and modeled cumulative emissions.

Tailpipe Validation

The tailpipe validation plots are shown in the next 3 figures. An uncertainty analysis of the tailpipe calculations was not conducted in this study, due to the incomplete nature of the post-catalyst model. However, qualitatively, the model appears to perform reasonably well. The HC and CO consistently underpredict in the middle VSP regions and this must be considered before proceeding.

Cumulative emissions did not compare as well as the engine out. In the next step of this study, it will be important that both the load based behavior and the total emissions are consistent. In our case, it was clear that the two driving cycles used to calibrate were insufficient to calibrate (or develop) the model. Some of the cruise driving effects were not accurately captured.

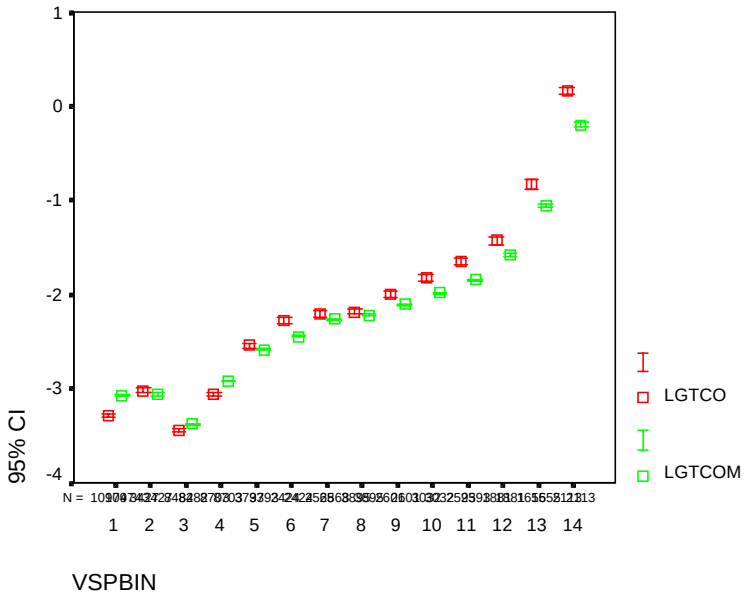

Figure 55. MEC TPCO validation

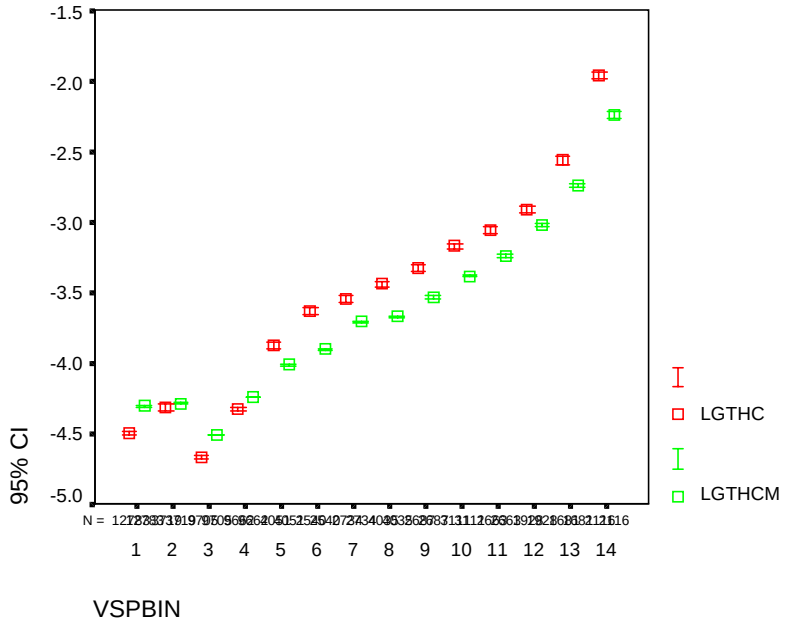

Figure 56. MEC TPHC validation

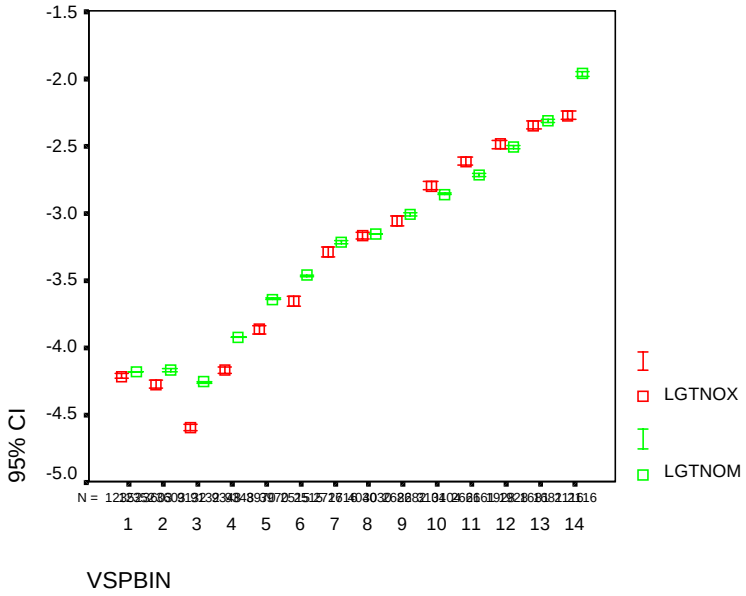

Figure 57. MEC TPNOx validation.

IV - CONCLUSION

We have demonstrated in this report that a physical emissions model can be a powerful addition to MOVES. The advantages are as follows:

- Extrapolations to future model years and deterioration may be modeled in more detail (though new standards and powertrain technologies may require a different approach)
- It might be capable of modeling some new technologies
- Some fuel effects can be modeled explicitly
- Off-road engines can be modeled (though data is needed)
- Fuel and CO_2 are estimated from physical principles directly, rather than empirically determined
- Many of the variations and anomalies in the data can be explained
- New data can be checked for quality or new trends
- A separate pre and post catalyst (engine out and tailpipe) model for criteria pollutants can help isolate or pinpoint the source of emissions
- OBD and IM issues can be modeled explicitly

A purely empirical model is incapable of handling many of the above issues in a meaningful manner without introducing a host of ad hoc correction factors. There are other physical approaches that can be taken, but the one proposed in this paper, is complex enough to handle many present and future emissions issues without overburdening the computational loads.

We first compared Vehicle Specific Power with fuel rate (or fuel consumption), and established the link (and correlation) between the two. The fuel rate approach is the one taken by the CMEM model developed at the University of California, Riverside (CE-CERT). A fuel rate based model is not to be confused with other more macroscopic fuel-based models in the literature.

Before modifying, or simplifying CMEM, it was first necessary to demonstrate that engine out emissions have remained relatively constant since the introduction of three way catalysts and improved fuel control. This was necessary since engine out emissions are difficult to measure. Based on the analysis performed, we can go on the assumption that engine out data will only be required to be taken on occasion, to make checks on the engine model. Using a detailed data set taken at UC Riverside, which includes engine out data, a Physical Emissions Rate Estimator (PERE) was introduced. The model is a modification of CMEM in many respects. In some ways it is simplified, in others, it is more detailed (out of necessity). The fuel rate, CO_2 and engine out models were developed and calibrated to the FTP and US06 cycles. A validation to a different driving trace (the MEC01 cycle) was performed. A separate validation was performed for CO_2 on some of the California unified cycles. The catalyst model was more of a challenge. Due to the complication of a speed history effect (seemingly independent of VSP), a model was introduced but not fully developed. Further analysis of the effects of driving cycles is required before the final algorithms are established. However, the trends described herein, give some indications that this can be accomplished.

In summary, some of the conclusions drawn in the report are:

- Under many operating conditions, VSP and Fuel consumption are well correlated as long as the full (rather than the approximated) VSP equation is used.
- There are strengths and weakness to both binning and parameterizing data. During the model development process, it is often beneficial to parameterize to obtain the most information. However, if the noise in the data is too large (as in catalyst modeling) binning provides a convenient way to average (and filter) the data. In either case, for the final solution the data must be binned so that PERE is compatible with the empirical arm of MOVES.
- The powertrain model was mainly captured from previous work in the literature. For the purposes of MOVES, further analysis and simplification will be required. In particular, the engine speed model will need to be simplified.
- For Tier 1 cars, engine out (pre-catalyst) emissions for criteria pollutants appears to be fairly constant across manufacturers, age, and power to weight ratio.
- Therefore, an engine out model should be able to be calibrated with a relatively sparse (but accurate) data set.
- Comparison of the engine model calibration to the measurements indicate that HC is modeled accurately across FTP and US06 type of driving. The model also indicates that the calibration for all species is excellent for the US06 cycle, however CO and NOx overpredict at lower loads (FTP type driving). It is possible that the catalyst model can compensate for this, but it should be investigated further.
- A significant speed effect on emissions was isolated to the catalyst. It was discovered that emissions from the "cruising" and "deceleration" modes deviated from the expected VSP dependence. For CO (at medium and low VSP bins) this deviation approached nearly an order of magnitude. This will require further investigation.
- There is evidence that modes of driving affect emissions, such that when a vehicle is driving in "cruise" mode, the catalyst behavior is dependent on speed as well as VSP, and when it is in "acceleration" mode, the emissions are more road load (or VSP) dependent.
- It was found that the activity represented by the FTP and US06 cycles was insufficient to calibrate PERE. There appeared to be a gap in (cruise) driving in the 40-55 mph range (based on on-road driving of 18 drivers), thus artificially calibrating the model to low and hi speed transients. It is recommended to calibrate future models using a wider driving range.
- During calibration of PERE, it was found that calibrating to second by second (or VSP bin) measurements gave different results than when calibrating to cumulative (total or bag) emissions. It is important that a calibration to second by second or VSP bin also give accurate total emissions. If not, this could hint that the model is not capturing all the physical effects, or that the activity is insufficient in certain operating regions (as mentioned earlier).
- The fuel consumption and CO_2 portions of PERE were validated to an independent driving cycle (MEC01).
- When validating to a series of CARB unified cycles (each having a different average speed), it was found that PERE was overpredicting CO_2 by 5-10% at higher average speeds (>30mph). It is possible that some of the powertrain efficiency coefficients will need to be updated. It is not certain whether speed is the causal variable in this case. The same validation study indicated that the two heaviest vehicles overpredicted CO_2 by about 15%. Both of these anomalies will require further investigation.
- The engine out validation on an independent cycle was very good for HC and NOx for total emissions. HC slightly overpredicted in VSP bins 7-10, however an improved quantification of the uncertainty in these bins may show that the model is "consistent" with the

measurements. There were discrepancies at very low VSP bins (decelerations), however, these bins don't have a large effect on total emissions.

- The engine out CO model underpredicted total emissions by 23% though the VSP behavior was excellent across all bins. This is likely due to more enrichment events in the MEC cycle. It is hoped that the catalyst model can compensate for this underprediction.
- Idle emissions should be separated as a different "mode" since the model failed to accurately capture VSP bin 3 (idle) properly.
- The tailpipe validation was rudimentary since the model is incomplete. However, it shows promise.

The Physical Emissions Rate Estimator has the potential to be a powerful addition to MOVES in its ability to supplement the empirical model. It can be crucial in 'filling in the holes' in the dataset, as well as providing some means of forecasting emissions from vehicles meeting future emissions standards. However this approach is still a proof of concept using a limited vehicle data set. It has yet to be demonstrated for vehicles certified to standards more stringent that Tier 1, which are more difficult to model. For example, due to the extremely low levels of emissions from SULEV and Tier 2 vehicles, a new paradigm might be required. While this is still a work in progress, the initial studies show promise.

V – ACKNOWLEDGMENTS

The author is grateful to Ford Motor Company for permission to take part in this unprecedented and productive collaboration. I would also like to express my appreciation to members of the EPA modeling team for all their assistance and support: John Koupal, Connie Hart, David Brzezinski, Chad Bailey, Carl Fulper and Carl Scarboro. From the academic community, I would like to acknowledge feedback and assistance from Marc Ross, Matthew Barth, Ted Younglove, Carrie Malcolm, and George Scora. Last but not least, I would like to acknowledge my supervisor, David Chock and manager, Ken Hass.

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APPENDIX A – Off Road Engines and Future Technologies

The fuel consumption mode described in this paper is fairly robust across engine types. Many engines will follow the same fuel trends with power. It is hoped that simply adjusting the powertrain and fuel parameters will be sufficient to model the different technologies and fuel types. As we will show below, this is probably an oversimplification of the issue.

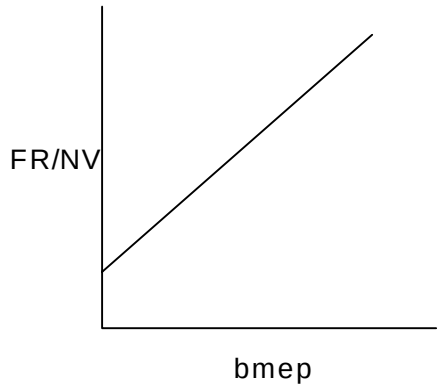

Figure A1. The Willans Line for an internal combustion engine.

Figure A1 shows an example of what is referred to in the literature as a "Willans Line." The y-axis is fuel consumption per stroke per displacement: FR/NV_d. The x-axis is brake mean effective pressure, which is the power per engine stroke (cycle) and displacement unit:

$$bmep = P_b n_R / NV_d \tag{A1}$$

where

n_R =2 for 4 stroke engines and n_R = 1 for 2 stroke engines.

This relationship could be described by a simple linear model such that

$$P_f = P_{f0} + aP_b, \tag{A2}$$

Where

P_{f0} is the offset or idle engine friction term

a is the slope of the line and defines the efficiency of fuel conversion into work.

Quite simply this is the same form as the fuel rate equation 6. We can make the following substitutions or approximations (Ross and An, 1993):

$$P_{f0} = KNV_d/LHV \tag{A3}$$
$$a = 1/\eta LHV$$

This equation can be applied to all internal combustion engines as well as fuel types. Future technologies may increase some of the coefficients in these terms (namely K, N, and η).

Of course, for off-road engines that are not mobile, the brake power needs to be defined by torque and engine speed only:

$$P_b = 2\pi N\tau \tag{A4}$$

For off-road engines, it will be necessary to obtain a calibration of torque or power vs engine speed. Engines that deviate from stoichiometry (such as diesels), may also need a simplified model for φ or air-to-fuel ratio. It is likely that in many cases, a simple adjustment of the FR and powertrain parameters will be insufficient to adjust the emission rates. For example, in our two stroke engine case: the powertrain parameters can be adjusted to change the efficiencies, friction, etc, but none of these changes will reflect the fact that 2 stroke engines inherently have higher hydrocarbon emissions rates due to the scavenging process. Separate emission rates would have to be determined. For the first stages of MOVES, it is recommended to determine the base modal rates empirically until at some future date, an improved model can be developed.

APPENDIX B - Fuel Types

One of the advantages of the fuel approach in this paper, is the possibility of modeling different fuel types explicitly. The physical parameters: LHV (Heywood, p. 915), conversion efficiency (η), and engine friction may vary from fuel to fuel. The hydrogen to carbon ratio in fuels will also vary based on the fuel type, blend and cetane number. For typical gasoline, the ratio is roughly 1.85. The H/C for various fuel types can also be found in Heywood (p. 915).

It is possible that for some fuels, a simple substitution of these parameters will be sufficient to quantify the change in emissions rates. However, it may also be necessary to determine new emissions coefficients (similar to different technologies). There may be factors, which are difficult to theoretically model at this time, which will affect the emissions rates. These factors include, nitrogen content of fuel, oxygenates, other additives, etc. Modal toxic emissions will be especially sensitive to fuel types.

In conclusion, this simple method of quantifying fuel consumption in internal combustion engines may be sufficient to quantify the change in emissions in comparison to “standard” gasoline, but there may also be many exceptions where separate emission rates (or corrections) will be required. For future engine technologies, this technique will need to be reexamined on a case by case basis. Efficiency improving mechanisms such as variable valve, cam, cylinder number, and compression ratio may all affect the Willans line, but their affect on the emission rates is unknown without more data.

APPENDIX C – CMEM Parameters: Simplification and Sensitivity

This section describes the CMEM powertrain, engine-out and catalyst parameters, and lists which may be omitted due to various reasons. A full statistical analysis was not accomplished in this very brief study, and may perhaps be warranted in a future study.

Powertrain Parameters
The following are fixed parameters in the CMEM second by second powertrain model. They only vary according to vehicle technology classes. The parameters obtained from readily available databases are marked "known", the rest are estimated based on publications etc. The parameters, which have little affect on emissions (as long as reasonable values are chosen), are marked with an "x". Some parameters are only sensitive when enrichment is concerned. Those are specifically marked.

Table C1. Powertrain Parameters

Parameter	Known	Insensitive
M (mass)	Yes	
Vd (Engine Displ)	Yes	
Trlhp (dyno)	Yes	
S (N/v)	Yes	x
Nm (rpmpeak)	Yes	Enrichment
Qm (torquepeak)	Yes	Enrichment
Pmax (peak power)	Yes	Enrichment
Np (rmax)	Yes	x
Nidle		x
Ng (Ngears)	Yes	x
K0 (friction)		x
ε1 (efficiency)		x
ε2		x

Engine-Out Emission Parameters
The following tables lists fitted parameters in the CMEM engine-out second-by-second model. The "Set Constant" column indicates which of the parameters could be fixed, based on previous studies, which have demonstrated that these parameters do not seem to vary significantly from model to model and year to year. However, they may vary from LDV to LDT, or very different technology classes.

Table C2. Engine-Out Parameters

Parameter	Set Constant	Insensitive
C_0	x	
aCO		
aHC		
rHC		
a1NO		
a2NO		
FRNO1		

FRNO2		
hcmax		x (enleanment)
hctrans		x (enleanment)
r_R	x	x (enleanment)
φmin	x	x (enleanment)
δSPth		x (enleanment)
rO2	x (enleanment)	

The enleanment portion of the model can be omitted since the catalyst takes care of these events in most cases. In certain types of hi-emitters, this may have more of a significant effect, but it is probably not worth the extra complication of the model to include this for only a very small portion of the fleet. In this approach, only (the first) ~8 coefficients are necessary to fit.

Catalyst Parameters

The catalyst model is the weakest link in this or any emission model. An aggregate model such as VSP subsumes a catalyst model since it is a modal tailpipe model. In this sense it is a aggregate or "lumped parameter" model. It is necessary to greatly simplify a catalyst model in order to be of use in MOVES. The "Soak" and "Cold Start" parameters are specified below. These two regimes are more simply modeled in an aggregate fashion as we shall describe below.

Table C3. Catalyst Parameters

Parameter	Set Constant	Insensitive
CsoakCO		Soak
CsoakHC		Soak
CsoakNO		Soak
βcatCO		Soak
βcatHC		Soak
βcatNO		Soak
βCO		Cold Start
βHC		Cold Start
βNO		Cold Start
Tcl		Cold Start
φcold		Cold Start
CSHC		Cold Start
CSNO		Cold Start
ΓCO		
ΓHC		
ΓNO		
bCO		
cCO		
bHC		
cHC		
bNO		
cNO		
γ (tip in)		x
φ_0 (max)		Enrichment

Pscale (threshold) Enrichment

The primary catalyst fitted coefficients are the b, c and Γ parameters. On a second-by-second (sbs) correlation (as opposed to bag), these fits can be very poor for specific vehicles (even if the validation is conducted on the same vehicles used to calibrate). We can conclude from this that these parameters are not capturing the complexities of catalyst action. It is likely that it is impossible to capture sbs behavior of a catalyst with only 9 fitted coefficients, or even 90! Catalyst (and air fuel ratio) behavior is very stochastic in nature. For that reason, it is just as reasonable to use a simpler lumped parameter model, this is outlined in the paper. Moreover, since emissions are so sensitive to catalyst behavior, it is usually easier to model hi-emitters.

APPENDIX D - Second by Second Tailpipe Emissions

We have seen that, to first order (for a given vehicle), engine out emissions are correlated with fuel rate or quantities proportional to it: VSP, air flow, throttle, RPM*load, etc. In fact, the correlations have been quite good with fuel rate in particular. Therefore, any analysis technique that determines the significance of a causal variable (such as Hierarchical Tree Based Regression, neural network, or design of experiment) should result in these "load type" variables being the most important. Frey et al., (2002) also proved that VSP gives the first split for tailpipe emissions using HTBR. However, the same correlation with load cannot be made with catalyst behavior. The scatter in the second by second tailpipe emissions is most likely due to catalyst effects. It is generally accepted by modelers that engine out emissions are relatively easy to model, in comparison to catalyst pass fractions. The latter tends to be very sensitive to parameters, which are very difficult for modelers to obtain, such as an accurate measure of air to fuel ratio, oxygen storage rates, temperature of the catalyst, flow, precious metal loading, honeycomb geometry, etc.

One of the goals of the present study is to determine if engine out and tailpipe should be separated. Some of the examination above supports this need. However, it is interesting to examine tailpipe trends directly for comparison. The following sections demonstrate the tailpipe trends as a function of fuel rate and VSP. This discussion addresses decision node 4 on the flow chart.

Tailpipe CO

The following figures show the trend of tailpipe CO as a function of FR and VSP. We have already seen that some of the scatter at the higher CO values is due to enrichment events. The correlation coefficients are:

$$\rho_{TCO/FR} = 0.48, \quad \rho_{TCO/VSP} = 0.31$$

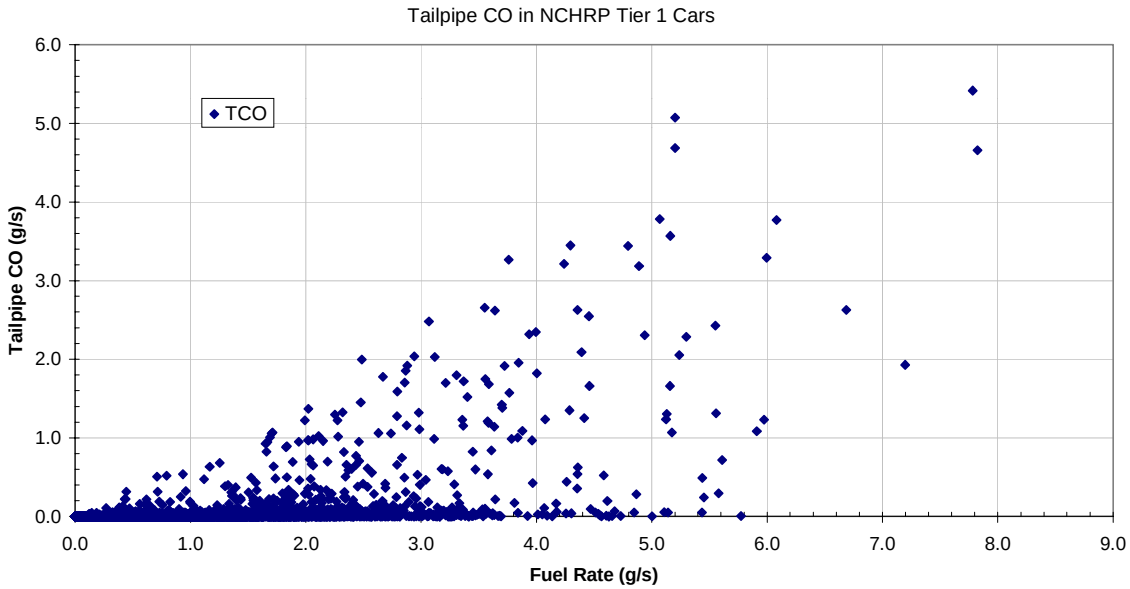

Figure D1. Tailpipe CO as a function of FR.

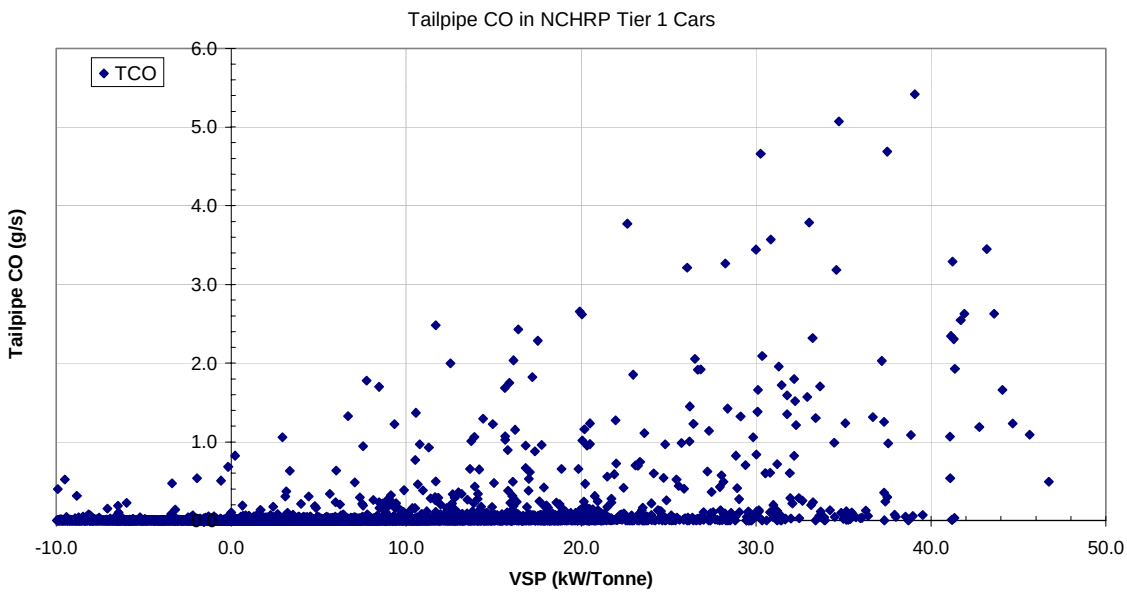

Figure D2. Tailpipe CO as a function of VSP.

Figure D3 shows the same except binned by VSP. The bin sizes are determined from Frey et al. (2002). Note that the bin sizes are not identical. The 95% confidence intervals are measures of the confidence of the mean values within the bins, i.e. the mean is correct to within 95%. The emissions are plotted logarithmically due to the skewness of the distribution. Figure D4 shows the same data but with the error bars plotted as the standard deviation. This gives a measure of the variability of the data (not the uncertainty of the mean). Figure D5 shows that much of the variability originates from the two different driving styles. This is somewhat problematic, and more will be discussed about this in the CPF section. It is not shown, but the fuel rate and the CO_2 do not demonstrate this (significant) split by driving cycle.

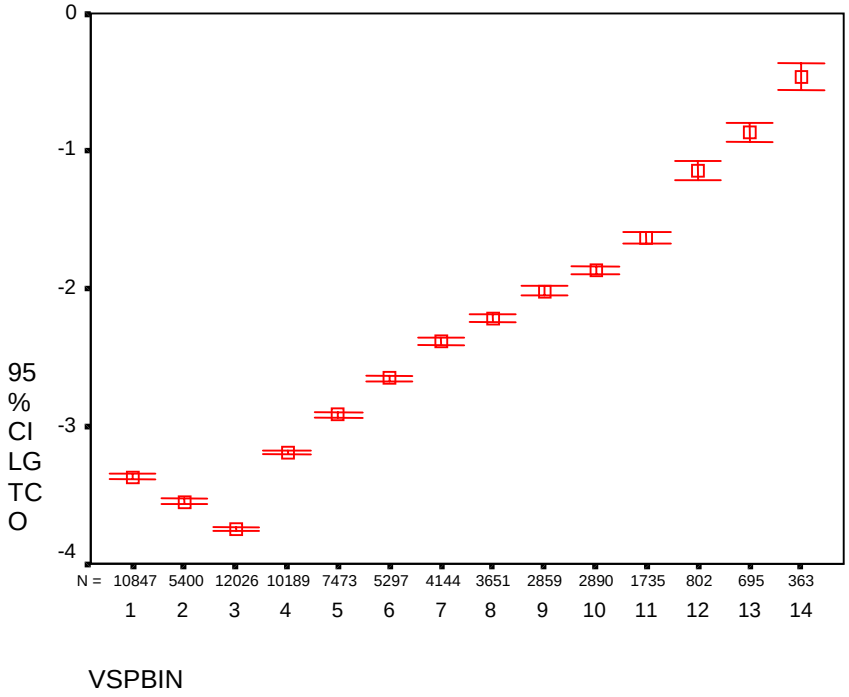

Figure D3. Tailpipe CO binned by VSP on a log scale.

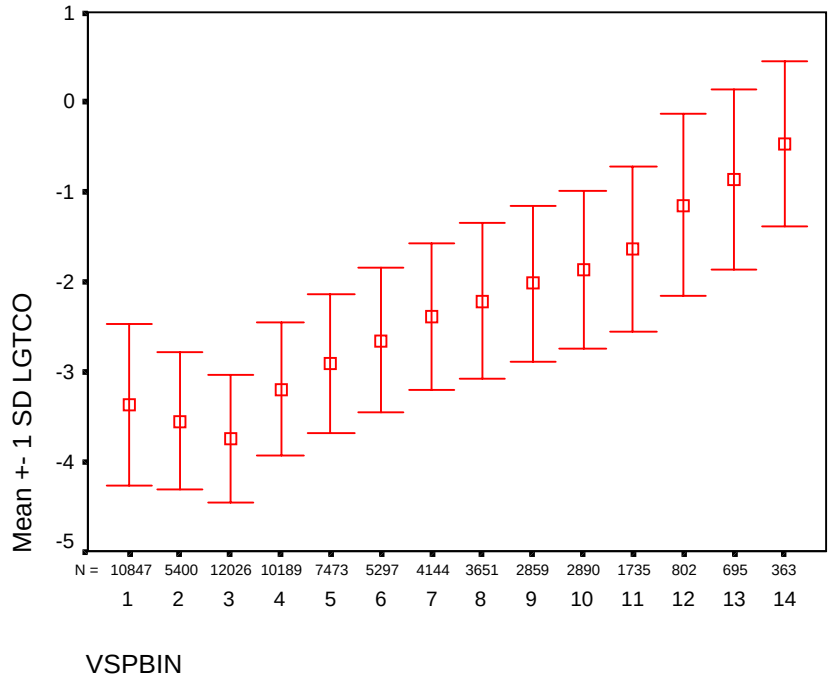

Figure D4. Tailpipe CO plotted logarithmically as a function of VSP bin. Bars are 1 standard deviation.

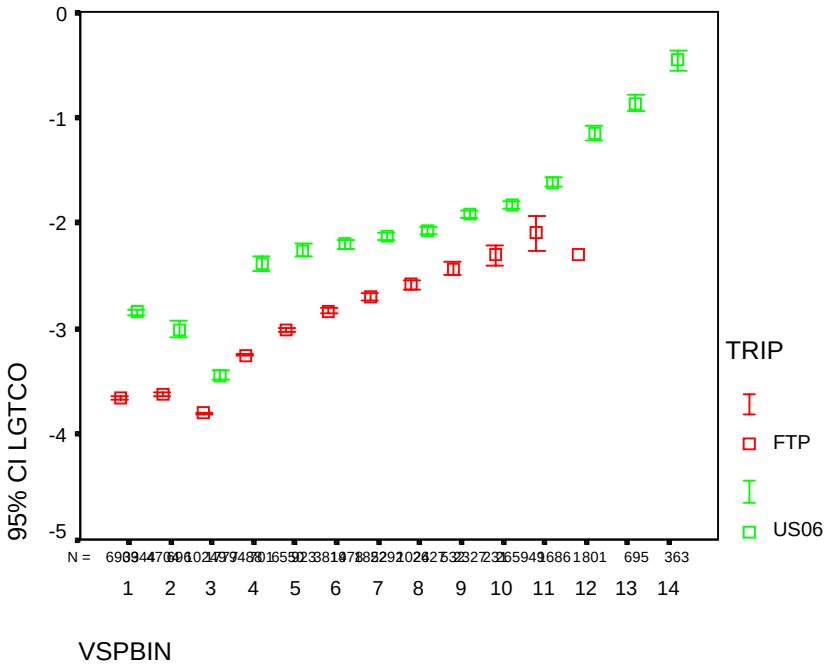

Figure D5. Tailpipe CO binned by VSP and separated by driving cycle.

Tailpipe HC

The following figures show the trend of tailpipe HC as a function of FR and VSP. The correlation coefficients are:

$$\rho_{THC/FR} = 0.33, \qquad \rho_{THC/VSP} = 0.23$$

The correlation is significantly worse than those obtained from engine out values.

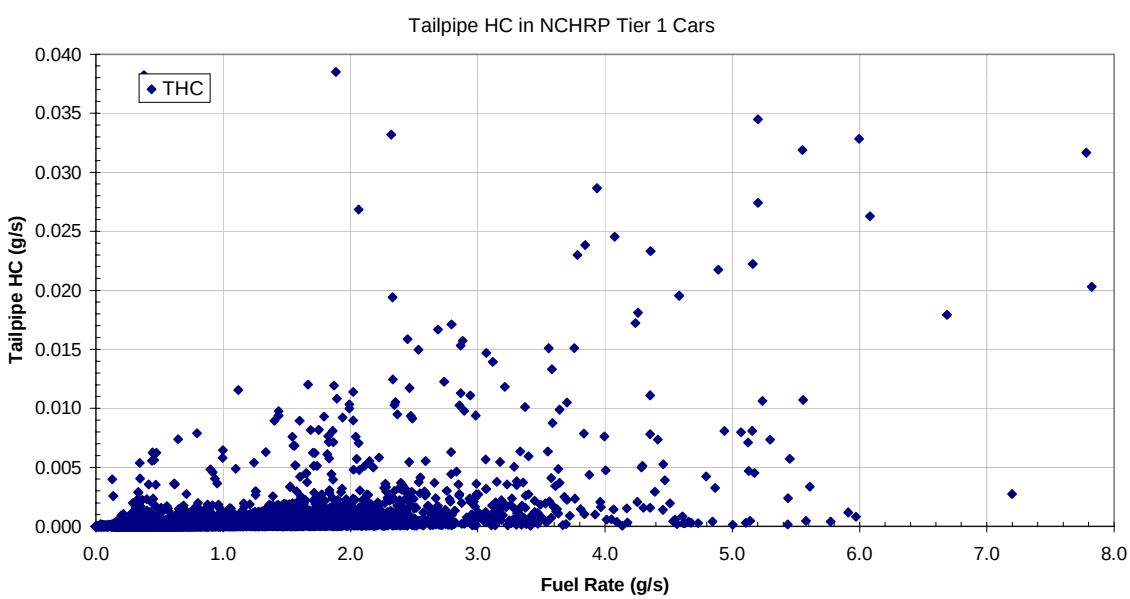

Figure D6. Tailpipe HC as a function of fuel rate.

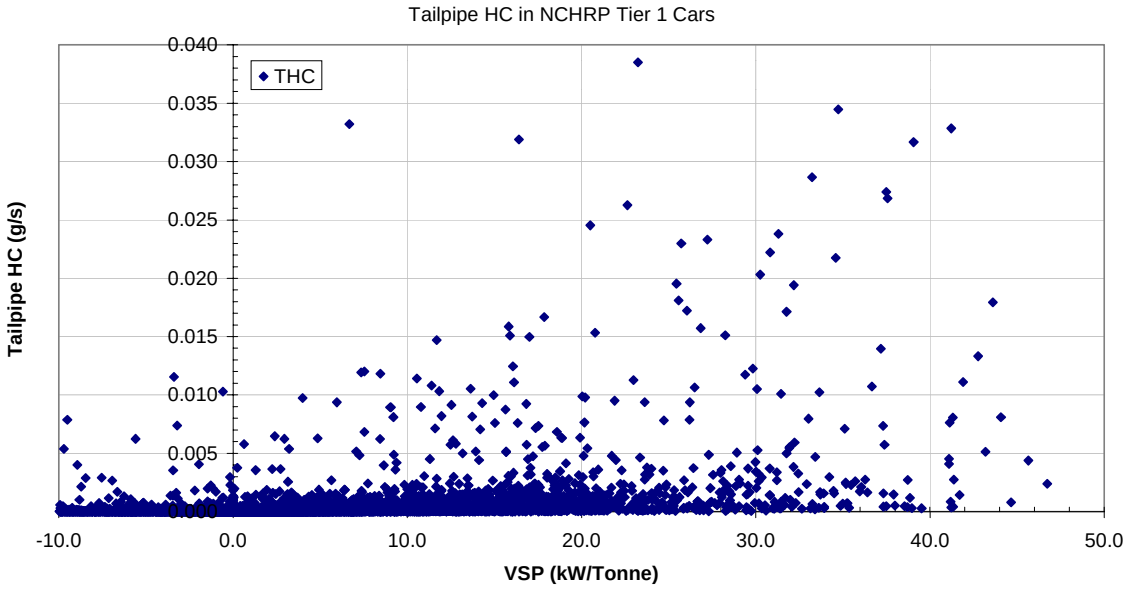

Figure D7. Tailpipe HC as a function of VSP.

Figure D8 shows the same data binned by VSP. The variability and the discrepancy between the cycles match that of CO (above).

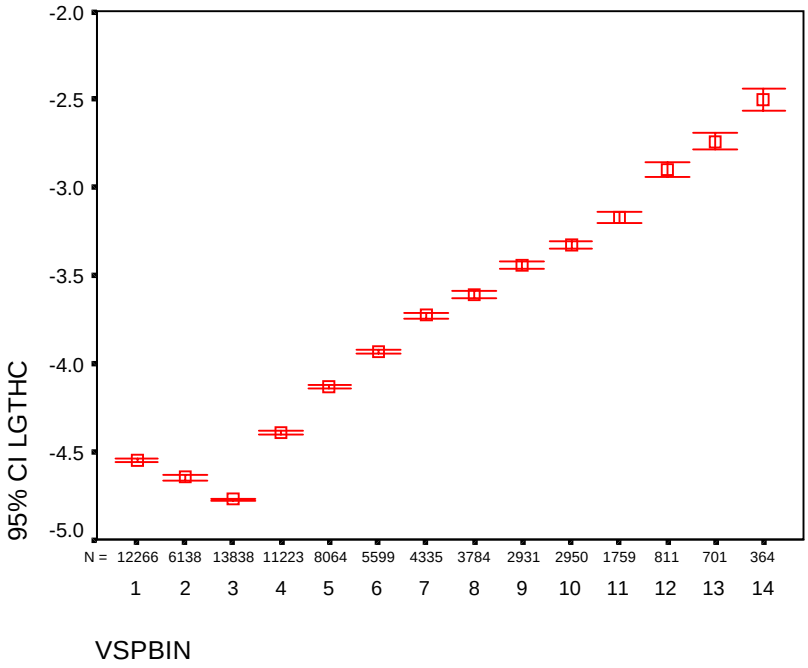

Figure D8. Tailpipe HC binned by VSP.

Tailpipe NOx

The following figures show the trend of tailpipe NOx as a function of FR and VSP. The correlation coefficients are:

$\rho_{TNOx/FR} = 0.40$
$\rho_{TNOx/VSP} = 0.35$

The correlations have consistently been better for FR over VSP for all the pollutants. This demonstrates again, that FR is a better independent variable for emissions characterization.

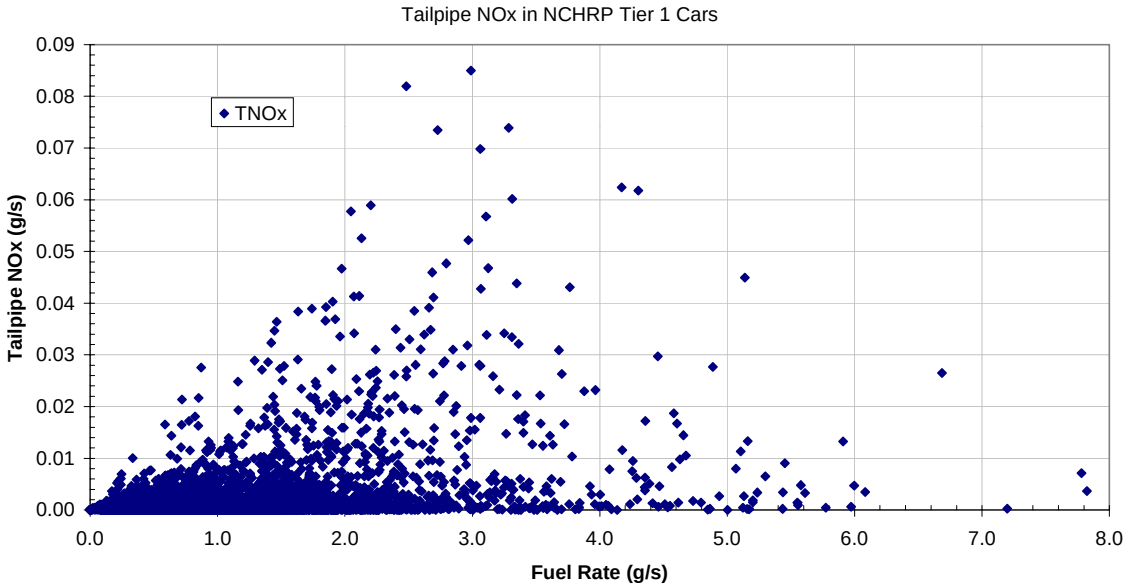

Figure D9. Tailpipe NOx as a function of FR.

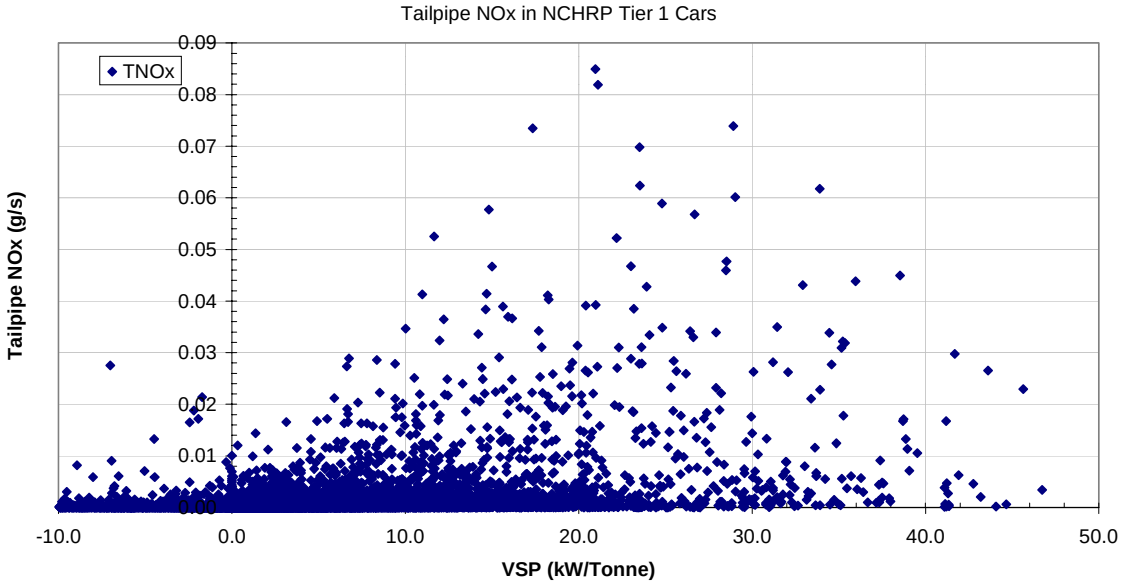

Figure D10. Tailpipe NOx as a function of VSP.

Figure D11 shows the same data binned by VSP. The variability and discrepancy between the cycles is similar to that of CO (above).

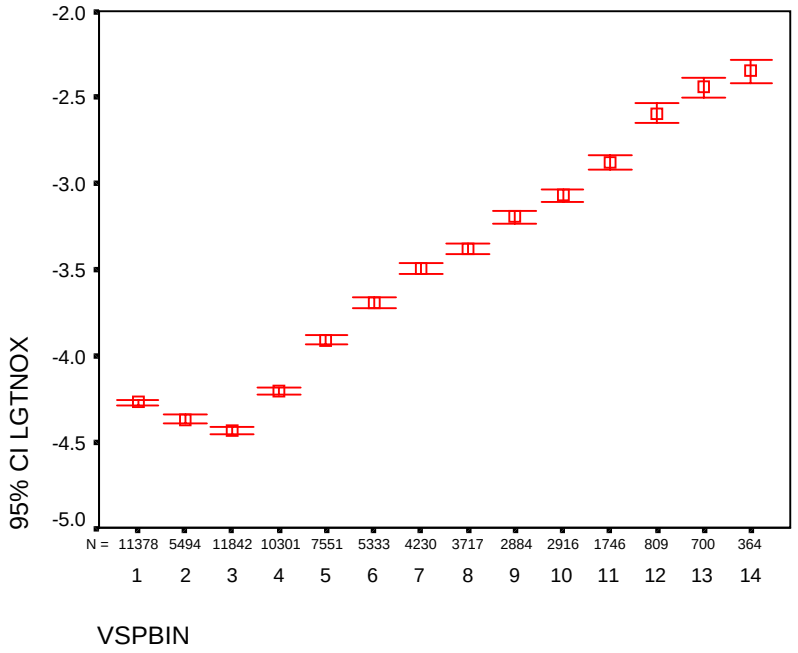

Figure D11. Tailpipe NOx binned by VSP.

In conclusion, we have demonstrated that the correlations for the tailpipe emissions are significantly worse than those of engine out. This is to be expected, but if separate further physical analysis of engine and catalyst out trends can discover the cause of the tailpipe scatter, the predictive capability of the model can be significantly improved. Furthermore, light trucks and cars will meet the same emissions standards, it is likely that this will confound the tailpipe trends presented in this paper. It is thus not recommended to model tailpipe directly using a physical model. The separate modeling of engine out and catalyst would allow for the explicit modeling of phenomena such as hi emitters, degradation, new technologies, etc, thus increasing the versatility and power of the model. The added complexity would not compromise the accuracy of the model at all, but rather can only increase it.

APPENDIX E – Sample Error Propagation Calculations

The uncertainty in equation 13 is as follows (assume $\delta Wt = \delta V_d = 0$):

$$\delta FR_{th} = \sqrt{\left[A * Wt * Vd * \left(\frac{\delta A}{A}\right)\right]^2 + \delta B^2} \tag{E1}$$

This turns out to be larger than the standard error of the measured FR_{th}, so we should take the more conservative estimate of error.
The uncertainty in equation 11 is simply:

$$\delta ECO = \delta a_{1CO} * FR \tag{E2}$$

This assumes that the fractional uncertainty in FR is small compared to that of a. Whether or not this is strictly true, they are both small compared to the next term. Under enrichment, this becomes:

$$\delta ECO = \sqrt{(\delta a_{2CO} FR)^2 + a_{2CO} FR_{th}{}^2 \left[\left(\frac{\delta a_{2CO}}{a_{2CO}}\right)^2 + \left(\frac{\delta FR_{th}}{FR_{th}}\right)^2\right] + a_{1CO} FR_{th}{}^2 \left[\left(\frac{\delta a_{1CO}}{a_{1CO}}\right)^2 + \left(\frac{\delta FR_{th}}{FR_{th}}\right)^2\right]} \tag{E3}$$

The last additive term (in the square root) is very small compared to the other 2 terms and can be ignored if simplification is desired. We propose that relative uncertainties can be ignored if they are an order of magnitude smaller than the relative uncertainties of the other (larger) terms. Only 20% of the enrichment events (modeled) occur in VSP bins 11 or less, so we will use the latter term only in bins 12-14. If there are more low power to weight ratio vehicles in a different study, bin 11 will likely have a larger uncertainty, since they will tend to go into enrichment at a lower VSP value. For the purpose of simplification, the FR_{th} is taken to be identical to the FR at the higher VSP bins.

The uncertainty in EHC is:

$$\delta EHC = \sqrt{(\delta a_{HC} FR)^2 + (\delta r_{HC})^2} \tag{E4}$$

The uncertainty in ENOx is simply:

$$\delta ENOx(FR) = \sqrt{(\delta a_{1NO} * FR)^2 + (\delta a_{2NO} * FR^2)^2} \tag{E5}$$

Under enrichment, it is:

$$\delta ENOx = \sqrt{\left(\delta a_{3NO} FR\right)^2 + a_{3NO} FR_{th}{}^2 \left[\left(\frac{\delta a_{3NO}}{a_{3NO}}\right)^2 + \left(\frac{\delta FR_{th}}{FR_{th}}\right)^2\right] + \left(\delta ENOx(FR_{th})\right)^2} \qquad \text{(E6)}$$

Once again, since the fractional uncertainty in a_3 is nearly an order of magnitude larger than that of a_1 or a_2, the last additive term can be ignored.