# Modal Emissions Modeling: A Physical Approach

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Mobile source emission models currently used by state and federal agencies (e.g., Environmental Protection Agency's MOBILE and California Air Resources Board's EMFAC) are often inadequate for analyzing the emissions impact of various transportation control measures, intelligent transportation systems, alternative fuel vehicles, and more sophisticated inspection/maintenance programs contained in most state air quality management plans. These emission models are based on the assumption that vehicle running exhaust emissions can be represented as integrated values for a specific driving cycle, and then later adjusted by speed correction factors. What is needed in addition to these "regional-type" mobile source models is an emissions model that considers at a more fundamental level the modal operation of a vehicle (i.e., emissions that directly relate to vehicle operating modes such as idle, steady-state cruise, various levels of acceleration/deceleration, and so forth). A new modal-emissions modeling approach that is deterministic and based on analytical functions that describe the physical phenomena associated with vehicle operation and emissions productions is presented. This model relies on highly time-resolved emissions and vehicle operation data that must be collected from a wide range of vehicles of varying emission control technologies. Current emission modeling techniques are discussed and the modeling approach and implementation plan for a new, three-year NCHRP Project entitled "Development of a Modal Emissions Model" are described.

Significant improvements are needed in the ability to characterize emissions from vehicles operating in real world conditions and in the models used to generate mobile source emission inventories. Numerous studies have shown that under most on-road operating conditions actual vehicle emissions can differ dramatically from what is predicted by current mobile source emission models (*1–5*). Understanding of the reasons leading to this discrepancy has improved considerably in recent years, and a more systematic approach to determining mobile source emission inventories is needed. This is particularly true given the conformity requirements of the Clean Air Act Amendments of 1990 and the aggressive implementation of transportation control measures, intelligent transportation systems, alternative fuel vehicles, and more sophisticated inspection maintenance programs contained in most state air quality management plans. Using current methods, the uncertainty of mobile source emission inventories is several factors greater than the impact of most mobile source control strategies.

Numerous reasons exist for the present discrepancy between calculated and actual emission inventories: poor mathematical representation of emission control system performance as a continuous function of accumulated mileage or speed; inadequate representation of the active fleet; dated representations of driving patterns and vehicle activities; inadequate treatment of modern closed-loop emission control technology; and a poor mapping of emission data and vehicle operation when compared to present-day driving conditions. In other words, present mobile source emission models currently used by state and federal agencies are based on the assumption that vehicle emissions can be represented by a time-resolved profile of vehicle miles traveled multiplied by emission factors primarily based on the current Federal Test Procedure (*6*). This approach has been shown to be inadequate in many cases, and a more complete and fundamental treatment of the modal operation of the vehicle (i.e., idle, cruise, acceleration/deceleration) is needed. A model that can predict emissions based on vehicle operating mode is critical for evaluating microscale traffic scenarios (i.e., ramp metering, signal coordination, and so forth) and can also help improve macroscale (i.e., regional) emission inventory predictions.

Presented herein is a description of a new modal emissions modeling approach. This model is deterministic in nature and is based on analytical functions that describe the physical phenomena associated with vehicle operation and emissions production. The model relies on highly time-resolved emissions and vehicle operation data that must be collected from a wide range of vehicles of varying emission control technologies. After a brief discussion of current emission modeling techniques, the modeling approach and implementation plan for a new, three-year NCHRP Project entitled "Development of a Modal Emissions Model" is described.

## CURRENT MODEL DEFICIENCIES

The common modeling approach [specifically Environmental Protection Agency's (EPA) MOBILE and California Air Resources Board (CARB) EMFAC models (*7–9*)] used to produce a mobile source emission inventory is based on two processing steps, shown in a simplified fashion in Figure 1. The first step consists of determining a set of emission factors that specifies the rate at which emissions are generated, and the second step is to produce an estimate of vehicle activity. The emission inventory is then calculated by multiplying the results of these two steps together. This methodology has two major shortcomings:

- Inaccurate characterization of actual driving behavior—The current methods used for determining emission factors are based on average driving characteristics embodied in a pre-determined driving cycle, known as the Federal Test Procedure (FTP) (*6*), which is used to certify vehicles for compliance of emission standards and from which most of the emissions data are based. The FTP was established over two decades ago and, at the time, was intended to exercise a vehicle in a manner similar to the operation of a typical in-use urban vehicle. However, it did not include "off-cycle" vehicle operation, which consists of speeds in excess of 57 mph and

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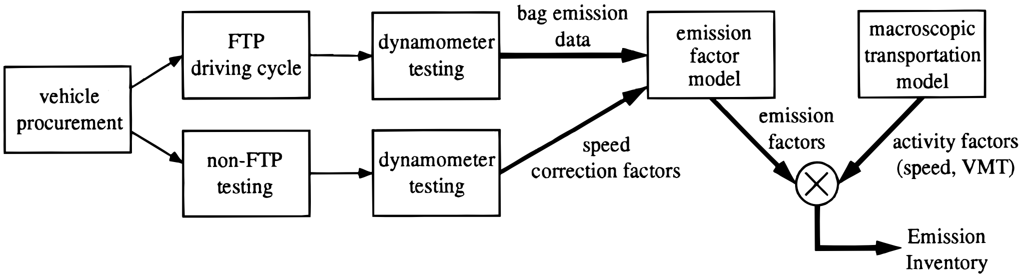

**FIGURE 1 Current emission inventory process.**

acceleration rates above 3.3 mph-s, common events in today's traffic operation. A number of studies show that the FTP does not accurately characterize today's actual driving behavior (*10–12*). Efforts are currently under way to revise the FTP (*10, 13–16*).

- The emissions factor approach is limited—The nonrepresentative nature of the FTP driving cycle tests is exacerbated by the procedure used for collecting and analyzing emissions. The FTP is divided into three segments in which emissions are collected into separate bags. FTP Bag 1 and Bag 3 measurements intend to capture emissions associated with vehicle cold and warm starts, while FTP Bag 2 captures emissions associated with vehicle hot-stabilized running conditions. In MOBILE and EMFAC, these three segments are used as base values to reconstruct statistically the relationship between emission rates and average vehicle speeds. Thus, the models statistically smooth the effect of acceleration and deceleration. Two vehicle trips can have the same average speed but have different speed profiles consisting of drastically different modal characteristics (acceleration, deceleration, idle, and so forth) and thus drastically different emissions output.

Adjustments are made to the base emission rates through a set of correction factors, such as fuel type, temperature, and speed correction. Among these correction factors, the most problematic are the speed correction factors (SCFs), which adjust the emission rates for non-FTP speeds. The SCFs have been derived from a limited set of transient tests (not steady-speed tests) spanning a series of average speeds up to 65 mph. Inherent in the derivation of the speed correction curves is the assumption that averages in the skewed distributions representing the range of emissions at measured speeds can be validly combined to yield emissions factors for other (non-measured) speeds.

The importance of acceleration/deceleration is also underestimated by the models. Studies have shown that a single power acceleration can produce more CO than is emitted in the balance of a typical short (<5 mi) trip (*17*). Other events leading to high engine load can also produce high emissions. For example, vehicles traveling on significant road grades can dramatically increase emissions, and, because of the nature of the current model inputs, grades are not taken into account.

Because of the inherent emissions and vehicle operation "averaging" that takes place in the conventional emission models, they offer little help for evaluating traffic operational improvements that are more microscale in nature. State and federal air quality management plans consist of numerous transportation control measures and more sophisticated inspection/maintenance programs. Further, traffic flow improvements can be accomplished through the advent of intelligent transportation systems. Operational improvements that improve traffic flow (e.g., ramp metering, signal coordination, automated highway systems, and so forth) cannot be evaluated accurately with the conventional emissions models; therefore, a modal emissions approach is necessary.

Even though there are several problems with the current emission models, a new modal emissions model should not be developed with the intent of replacing the older ones. In a sense, the conventional emission models can provide a "top-down" approach to emission inventory modeling at a regional level, and a developed modal emission model is to be considered "bottom-up," more appropriate for microscale evaluation. These two approaches should easily conform with each other, and they meet somewhere in the middle. The two types of models should have a symbiotic relationship in which each benefits from the other.

### Modal Emissions Research

In order to investigate vehicle emissions associated with modal events, several recent research studies have been performed using dynamometers and instrumented vehicles while simultaneously measuring emissions at high time resolutions (typically second-by-second). Since early 1980s, these modal emissions research projects have been conducted at CARB (*18–21*). Based on testing a small set of newer technology vehicles, studies found that CO and HC emissions are greatly affected by various acceleration modes. Single accelerations could produce roughly twice the amount of emissions of the total FTP test (*20,21*). More recently, vehicle manufacturers in collaboration with EPA have conducted dynamometer tests of approximately 27 modern technology vehicles as part of the FTP Revision Project (*10,13–16*). Several driving cycles were used involving high-power driving of hot-stabilized vehicles. In addition, many of the same vehicles were tested again using a "non-enrichment" (stoich) chip which avoids command enrichment. The results of these tests are summarized in the FTP revision project reports (*14*).

In addition to dynamometer testing, several research groups use instrumented vehicles to collect emissions data while they are driven on the road. Staab et al. used an instrumented VW Golf to collect emissions under urban, rural, and freeway road conditions (*22*). More recently, Kelly and Groblicki instrumented a GM Bonneville to collect on-road emissions and have performed several experiments in Southern California (*17*). They found that during moderate to heavy loads on the engine, the vehicle ran under fuel enrichment conditions, resulting in CO emissions 2,500 times greater than those at normal stoichiometric operation (HC was 40 times as great). Similarly, Ford Motor Company Chemistry Department Research

Staff has instrumented a 1992 Aerostar van with Fourier transform infra-red instrumentation to measure approximately 20 species of emissions (e.g., CO, $CO_2$, methane, total hydrocarbons, NO, and so forth) at high time resolution while on the road (*23*). These emissions data are coupled with vehicle operating parameters measured with a data acquisition system. CARB is also sponsoring Sierra Research to instrument a 1991 Chevrolet Lumina to collect second-by-second vehicle operating characteristics and CO and HC emissions. Also, researchers at Georgia Institute of Technology have begun to instrument a vehicle for on-road emissions testing (*24*).

Through both dynamometer testing and the use of instrumented vehicles, the amount of highly time-resolved emissions data coupled with vehicle operation parameters is increasing. As this wealth of data increases, it will be possible to further develop and validate emission models that predict emission rates as a function of vehicle operating mode.

Several "modal-emission" models have recently been developed. For example, the line source dispersion model CALINE4 (*25*) uses modal factors prior to calculating roadway emissions dispersion. The EPA created a mathematical model called "The Automotive Exhaust Emission Modal Model" to estimate light-duty vehicle CO, HC, and $NO_x$ emissions (*26*). Both transient and steady-state operation were investigated. More recently, St. Denis and Winer have created both a speed-acceleration and a speed-load modal emissions model using data from a single Ford vehicle (*27*). Further, researchers at Sierra Research have extended the model VEHSIM (originally developed at GM to compute engine speed and load) to create model VEHSIME that predicts emission rates for specified driving cycles (*28*). The model computes the second-by-second engine speed and load required to drive the cycle, then, using an emissions map (with interpolation), second-by-second emissions are approximated. The EPA has similarly extended the VEHSIM model to create a modal emissions model called VEMISS (*29*). Researchers from the University of California, Riverside have developed a power demand-based modal emission model that predicts second-by-second emissions given specified vehicle operation (*30*). Also, researchers at the University of Michigan have developed a physical model that predicts fuel economy given any driving cycle or trip characteristics, and they have recently extended the model to predict CO emissions (*31,32*). Researchers at the University of California, Davis have also created a CO modal emissions model based on the SCF database used by EMFAC and MOBILE, as well as second-by-second data from an Australian vehicle (*33*).

## Modeling Methodologies

When discussing and comparing emission modeling methodologies, three components associated with the modeling process should be considered: (1) the vehicle test, (i.e., how are vehicles tested when measuring their emissions); (2) the emissions representation, (i.e., how are the emissions represented in the model); and (3) the vehicle activity factor, (i.e., what parameters of vehicle activity are used when determining an emission inventory—either large regional scale, or small roadway scale). As summarized in Table 1, these components apply to several modeling methodologies, including the modal emission model approach.

For a modal emissions model, a convenient method to characterize vehicle operating modes of idle, cruise, and different levels of acceleration/deceleration is to set up a speed/acceleration matrix, as shown in Table 2. The matrix measures emissions associated with each bin or mode. This emissions matrix can be multiplied with a similar matrix that has vehicle activity broken down so that each bin contains the time spent in each driving mode. The result is the total amount of emissions produced for the specified vehicle activity with the associated emissions matrix. The problem with such an approach is that it does not properly handle other variables that can affect emissions, such as road grade or use of accessories. "Correction factors" can be used so that these other variables are taken into account, but this can be problematic since their effect will typically be based on secondary testing not associated with the core model (e.g., similar to the speed correction factors in CARB's EMFAC).

Another modal emissions modeling method develops an emissions map based on engine power and speed. Second-by-second emission tests are performed at numerous engine operating points, taking an average of steady-state measurements. By basing emissions on engine power and speed, the effects of acceleration, grade, use of accessories, and so forth can be taken directly into account. When creating an emission inventory, the vehicle activity parameters of engine power and speed must be derived from second-by-second velocity profiles. Recently, EPA performed extensive mapping of emissions as a function of power and speed for 29 different vehicles—a time-consuming, expensive procedure—and there have been data difficulties (*34*). Another problem with using an emissions mapping approach is substantial time dependence in the emissions response to the vehicle operation (e.g., the use of a timer to delay command enrichment or oxygen storage in the catalytic converter).

**TABLE 1 Modeling Components of Several Emissions Modeling Methodologies**

| Emission Modeling Methods | Vehicle Test | Emission Representation | Vehicle Activity Factors |
|---|---|---|---|
| current models (i.e., EMFAC, MOBILE) | FTP driving cycle (& ancillary speed correction factor tests) | total emissions for entire cycle | vehicle speed (with speed correction factors) |
| multiple driving cycles | multiple driving cycles by roadway type and congestion level | total emissions for each driving cycle | average congestion speed for each roadway type |
| velocity-acceleration matrix | second-by-second emissions testing for all modes | average emissions for each mode of velocity-acceleration | time spent in velocity-acceleration matrix |
| emission mapping | second-by-second emissions testing | emissions map for modes of engine power and speed | engine power and speed (must be translated from sec-by-sec velocity profile) |
| parameterized physical model | short driving cycle to determine key parameters | parameterized analytical representation | sec-by-sec profile and/or parameterized trip characteristics |

**TABLE 2 Speed/Acceleration Matrix Containing Modes of Idle, Cruise, and Different Levels of Acceleration/Deceleration**

| | DECELERATION/ACCELERATION (mph/s) | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Speed (mph) | -6 | -5 | -4 | -3 | -2 | -1 | 0 | 1 | 2 | 3 | 4 | 5 | 6 |
| 0 | | | | | | | IDLE | | | | | | |
| 5 | | | | | | | | | | | | | |
| 10 | | | | | | | | | | | | | |
| 15 | | | | | | | | | | | | | |
| 20 | | | | | | | | | | | | | |
| 25 | | | | | | | | | | | | | |
| 30 | | | | | | | CRUISE | | | | | | |
| 35 | | | | | | | | | | | | | |
| 40 | | | | | | | | | | | | | |
| 45 | | | | | | | | | | | | | |
| 50 | | | | | | | | | | | | | |
| 55 | | | | | | | | | | | | | |
| 60 | | | | | | | | | | | | | |
| 65 | | | | | | | | | | | | | |

Another problem associated with both the speed-acceleration matrix and emission mapping approaches is the error generated by either averaging emission rates within each bin or extrapolating/interpolating among them in the emission map grids. Without knowing the underlying relationship for emission rate versus vehicle speed and acceleration rates, or engine speed and engine load, the most widely used methodology assumes a simple two-dimensional linear relationship among them. Due to measurement difficulties, most speed-acceleration matrices or emission maps have only a very limited number of bins or measurement points, resulting in the repetitive use of the above procedure in real applications. The error associated with a single bin or engine operational point could be accumulated into major computing errors in the final results. The key to eliminating this kind of error is to establish a correct analytical formula among the important variables.

## PHYSICAL MODELING APPROACH

To avoid the problems associated with the above methods, a physical, power-demand modal modeling approach based on a parameterized analytical representation of emissions production is used. In the physical model, the entire emissions process is broken down into components that correspond to physical phenomena associated with vehicle operation and emissions production. Each component is then modeled as an analytical representation consisting of various parameters that are characteristic of the process. These parameters vary according to the vehicle type, engine, and emission technology. The majority of these parameters are stated as specifications by the vehicle manufacturers and are readily available (e.g., vehicle mass, engine size, aerodynamic drag coefficient, and so forth). Other key parameters relating to vehicle operation and emissions production must be deduced from a comprehensive testing program. The testing involved is much less extensive than creating emission maps for a wide range of vehicle operating points.

This type of modeling is deterministic rather than descriptive. Such a deterministic model is based on causal parameters or variables, rather than based on simply observing the effects (i.e., emissions) and assigning them to statistical bins. Further, the essence of the proposed modeling approach is that the major effort is up front, in the model-development phase, rather than in application. Once the model forms are established, data requirements for applications and for updating to include new vehicles are modest. This limited requirement for data in future applications is perhaps the main advantage of this modeling approach. This approach also provides an understanding of or explanation for the variations in emissions among vehicles, types of driving, and other conditions. Analysts will be able to discuss "whys" in addition to providing numbers. This is in contrast to models based on statistical "surrogate" variables that are not necessarily linked to physical variables that can be measured (*33*).

There are several other key features that make the physical, deterministic model approach attractive.

- It inherently handles all of the factors in the vehicle operating environment that affect emissions, such as vehicle technology, fuel type, operating modes, maintenance, accessory use, and road grade. Various components model the different processes in the vehicle related to emissions.
- It is applicable to all vehicle and technology types. When modeling a heterogeneous vehicle population, separate sets of parameters can be used within the model to represent all vehicle and technology types. The total emission outputs of the different classes can then be integrated with their correctly weighted proportions to create an entire emission inventory.
- It can be used with both micro- and macroscale vehicle activity characteristics. For example, if a second-by-second velocity profile is given, the physical model can predict highly time-resolved emissions. If average vehicle activity characteristics, such as average speed, peak average speed, idle time, or positive kinetic energy (PKE, a measure of acceleration), are given, the physical model can be used based on average power requirements calculated from the activity parameters.
- It is easily validated and calibrated. Any second-by-second driving profile can be applied to the model, while simultaneously measuring emissions. The two results can be compared and the parameters of the model can be calibrated accordingly.
- It is not restricted to pure steady-state emission events, as is an emissions map approach or a speed/acceleration matrix approach. Therefore, emission events that are related to the transient operation of the vehicle are more appropriately modeled.
- Functional relationships within the model are well defined. Therefore, in contrast to a model that operates by sampling numerical data, the analytical approach avoids extrapolation and

interpolation. Moreover, it is possible to describe delay effects, such as with the introduction of timers for command enrichment.

- The model is transparent. Results are easily dissected for evaluation. It is based on physical science, so that data are tested against physical laws, and measurement errors can be identified in the model establishment phase.
- The computations performed in the model consist primarily of evaluating analytical expressions, which can be done quickly with only modest memory requirements.

There are also some potential disadvantages to the approach. Establishment of this type of model is data intensive. A large number of physical variables need to be collected or measured, or both, for the wide variety of vehicle technology types in different states of deterioration. Because the modeling approach is based on the study of extensive emissions measurements in the context of physical laws, a systematic inductive study of physical mechanisms such as energy loss and chemical equilibrium will be necessary. The model development will identify a smaller set of key variables that play an important role in the generation of emissions. Models of this kind have been developed to predict fuel use with data from the 1970s (*31,32*). Through this process one finds that the variations in fuel use and emissions among vehicles and in different driving modes are sensitive to only a few critical parameters. Satisfactory accuracy will be achievable with publicly available parameters and with parameters that can be obtained from brief dynamometer tests.

The statement about the degree of parameterization which is adequate assumes that accuracy is interpreted in absolute terms on the basis of regulatory needs. For example, analytic modeling of extremely low emissions, which can occur for short periods during moderate-power driving, with high relative accuracy might complicate the model to no purpose. Relative accuracy where the emissions are below those of interest for regulatory purposes are not evaluated. Similarly, in current second-by-second data there is some temporal variability to emissions (which may not be real) whose study may not justify more detailed measurements and model making. For regulatory purposes, accurate prediction of emissions over modes of the order 10 seconds and more may be adequate.

Another critical component of the approach is that malfunctions and tampering have to be explicitly modeled. There is evidence that the emissions control devices of a high percentage of in-use vehicles have been tampered with (*35*). Further, problems of high deterioration rates of catalyst efficiency, misfueled vehicles, and so forth, must be accounted for. Modeling components that estimate the emissions of gross-emitters are also an important part of this approach.

## Generic Model

A block diagram of a generic physical model is shown in Figure 2, and each component is described in detail below.

### *Power Demand Function*

An instantaneous power demand function is the fundamental basis of the physical model. By knowing the vehicle's mass and given a prescribed acceleration and velocity on a particular grade, the total tractive power requirements (in kilowatts) placed on a vehicle (at the wheels) is given in simplest form as:

$$P_{\text{tractive}} = \frac{M}{1000} \cdot V \cdot (a + g \cdot \sin\theta) + \left(M \cdot g \cdot C_r + \frac{\rho}{2} \cdot V^2 \cdot A \cdot C_a\right) \cdot \frac{V}{1000} \qquad (1)$$

where

$M$ = vehicle mass (kg)
$V$ = vehicle velocity (m/sec)
$a$ = vehicle acceleration (m/s$^2$)
$g$ = gravitational constant (9.81 m/s$^2$)
$\theta$ = road grade angle
$C_r$ = rolling resistance coefficient
$\rho$ = mass density of air (1.225 kg/m$^3$, depending on temperature and altitude)
$A$ = cross-sectional area (m$^2$), and
$C_a$ = aerodynamic drag coefficient.

To translate this tractive power requirement to demanded engine power requirements, the following simple relationship can be used as a first approximation:

$$P_{\text{engine}} = \frac{P_{\text{tractive}}}{\eta_{tf}} + P_{\text{accessories}} \qquad (2)$$

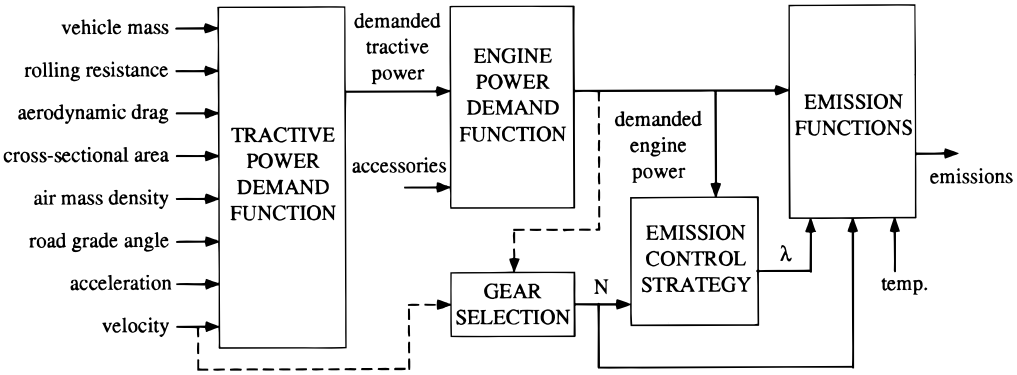

**FIGURE 2 Power-demand emissions modeling methodology.**

where $\eta_{tf}$ is the combined efficiency of the transmission and final drive, and $P_{\text{accessories}}$ is the engine power demand associated with the operation of accessories, such as air conditioning, power steering and brakes, and electrical loads. In the final model, $P_{\text{accessories}}$ may be modeled as a function of engine speed, and $\eta_{tf}$ can be modeled in terms of engine speed and $P_{\text{tractive}}$.

### *Gear Selection and Engine Speed*

The speed of the engine in relation to the speed of the vehicle is determined by an internal gear selection strategy (or shift schedule) that depends on inputs such as engine and vehicle speeds and, possibly, other related inputs such as demanded engine power. Engine speed $N$ (rps) plays a role in fuel use and the emission control function. Gear selection and engine speed are complicated by the wide variety of automatic transmissions and their management. It is not necessary, however, for the model to accurately specify engine speed every second. Rather, accuracy is required for longer intervals. For these purposes, simple statistical specification of shift scheduling/engine speed will be adequate. It should prove satisfactory to determine engine speed in terms of immediate prehistory and vehicle speed and the power requirement.

### *Emission Control Strategy and Equivalence Ratio*

One of the most important components of this physical model is approximating the emission control mechanisms of the vehicle. For older vehicles, engine control was accomplished through some combination of mechanical, pneumatic, or hydraulic systems. The engine control regulates fuel and air intake as well as spark timing and exhaust gas recirculation to achieve the desired performance in fuel economy, emissions, and power output. Due to the advent of automotive electronics, modern vehicles have complex emission control systems that closely regulate fuel injectors. For a hot-stabilized engine operating under normal conditions, the fuel mixture is maintained at the stoichiometric ratio, where the performance of the catalytic converter is maximized. However, there are several other vehicle operating modes that can affect the commanded air/fuel ratio. During engine start and warm up, the air/fuel ratio is typically commanded rich to improve combustion stability (older, carbureted vehicles use a choke). Another important operating mode is during high power episodes, such as those induced by hard accelerations and/or steep grades. During such an episode, the air/fuel ratio is again commanded rich for peak demand power and protection of engine and catalyst components.

When modeling the emission control function, we consider $\lambda$ as the regulated output variable, where $\lambda$ is the "equivalence ratio" and is defined as:

$$\lambda = \frac{(A/F)_0}{(A/F)} \qquad (3)$$

where $(A/F)_0$ is the air/fuel ratio at stoichiometry (≈14.7), and $(A/F)$ is the commanded air/fuel ratio. Like engine speed, the equivalence ratio must be modeled in terms of the driving characteristics (especially the engine power required and engine warm-up history) and parameters that describe the vehicle's command enrichment strategies. As with engine speed, it is not necessary to specify accurately equivalence ratio every second; but, since $\lambda$ is a sensitive parameter for emissions control in short, high-powered driving episodes, it must be accurately specified for relatively short periods. A modeling approach based on a power threshold and possible delay with a timer will be tried initially. In a study already under way by the team, CARB data involving several high-power episodes have been modeled with encouraging results (*36*).

### *Fuel Use Model*

A model that determines the fuel use in any driving cycle for any vehicle model has previously been developed (*31*,*32*) and is given as

$$\frac{dF}{dt} \approx \lambda\left(k \cdot N \cdot D + \frac{P_{\text{engine}}}{\eta_{\text{engine}}}\right) \qquad (4)$$

where

$k$ = engine friction factor (representing the fuel energy used at zero power output to overcome engine friction per engine revolution and unit of engine displacement)
$N$ = engine speed
$D$ = engine displacement, and
$\eta_{\text{engine}}$ = measure of indicated engine efficiency.

This equation is a simple but fairly accurate way to determine fuel use rate (in kilowatts).

### *Emission Functions*

A set of analytical functions that describes engine emissions rates can be developed as functions of fuel consumption and air/fuel ratio. Under stoichiometric conditions, engine-out emissions are basically proportional to fuel use. These functions change, however, with non-stoichiometric conditions (e.g., commanded enrichment). Tailpipe emissions can be modeled as:

$$\text{emissions}_{\text{tailpipe}} = \frac{dF}{dt} \cdot \frac{dCO/dt}{dF/dt} \cdot CPF \qquad (5)$$

where

$dF/dt$ = the fuel-use rate in g/s
$dCO/dt$ = the engine-out emissions (for CO) in grams/s, and
$CPF$ = the catalyst pass fraction, a function primarily of temperature and equivalence ratio.

## **Parameterization**

Using this physical model approach, models for different engine/emissions technologies that are represented in the national vehicle fleet need to be established. This will include the appropriate combinations of engine type (spark ignition, diesel), fuel-delivery system (carbureted, fuel injection), emission-control system (open-loop, closed-loop technology), and catalyst usage (no catalyst, oxidation catalyst, three-way catalyst). The generic model outlined above only considers the different components for a modern, closed-loop emission-controlled vehicle having a spark ignition engine.

There are several other vehicle/technology/year combinations that will require variations of this generic model.

After the models corresponding to the different technologies have been approximated, identifying the key component parameters of the models that characterize vehicle operation and emissions production is necessary. These parameters can be classified into several categories: (1) readily available (public domain) static vehicle parameters (e.g., vehicle mass, engine size, and so forth); (2) measurable static vehicle parameters (e.g., vehicle accessory power demand, enrichment power threshold, and so forth); (3) deterioration parameters (e.g., catalyst aging, and so forth); (4) fuel-type parameters; and (5) vehicle operating parameters.

When the physical models and associated parameters are established for all vehicle/technology/year combinations, they must be combined with vehicle operating parameters that are characteristic of real-world driving. These vehicle operating parameters consist of static environmental factors such as ambient temperature and air density, as well as dynamic factors such as commanded acceleration (and resultant velocity), road loads such as road grade, and use of vehicle accessories (e.g., air conditioning, electric loads, and so forth).

Combining the physical models with vehicle operating parameters results in highly time-resolved emission rates. These predicted rates can then be compared directly to measured emissions data, and the parameters of the modeling components—or the modeling components themselves—can be adjusted to establish an optimal fit. This calibration/validation process can occur iteratively until the models are well developed.

As previously mentioned, deterioration factors are considered within this model. These deterioration factors correspond to the effects of emission equipment failure, tampering, and long-term reductions of efficiencies (e.g., catalyst aging). They can be represented as modeling components within the physical model itself or as simple additional parameters with the current components, or both. The incorporation of these components is critical to model development since their contribution to emissions production has been shown to be significant (*37*).

### Extension of Microscale Model for Macroscale Use

The developed modal emissions model is microscale, meaning it can readily be applied to evaluating emissions from specified driving cycles or integrated directly with microscale traffic simulations (e.g., TRAF-NETSIM, FRESIM, and so forth). However, its use for estimating larger, regional emissions is somewhat more complicated. Because microscale models typically model at the vehicle level and have high accuracy, they require extensive data on the system under study and are typically restricted in size due to the nonlinear complexity gain incurred with larger networks. To produce emission inventories of greater scope, it is possible to develop link-level emission functions for different roadway facility types (e.g., freeway section, arterials, intersections, rural highways, freeway on-ramps, and so forth) using the modal emissions model. At the microscale level, emissions can be estimated as a function of vehicle congestion on each facility type, with different degrees of geometrical variation. Statistical emission rates are then derived from the microscale components as a function of roadway facility type and congestion level. These rates are then applied to individual links of a macroscale traffic assignment model.

## FUTURE WORK

Using this modal emissions modeling approach, a three-year project to develop a comprehensive modal emissions model will be undertaken. This research project will be done in three phases. The first phase consists of collecting data and literature from recent related studies, analyzing these data and other emission models as a starting point for the new model design, and developing a new dynamometer emissions testing protocol to be used for the vehicle-testing phase of the project.

Phase 2 is the vehicle-testing phase and consists of acquiring approximately 300 vehicles that are representative of the national fleet of on-road vehicles; performing emission tests on these vehicles using a 48-in. single-role electric dynamometer, running the previously designed testing protocol; developing a working modal emissions model in an iterative fashion as test data are acquired; and validating the model using different drive cycles as well as using on-road emissions data collected from an instrumented vehicle.

Phase 3 of the project demonstrates how the developed modal emission model can be integrated with both microscale and macroscale transportation models.

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