A Statistical Model of Vehicle Emissions and Fuel Consumption

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Abstract:

A number of vehicle emission models are overly simple, such as static speed-dependent models widely used in practice, and other models are sophisticated as to require excessive inputs and calculations, which can slow down computational time. We develop and implement an instantaneous statistical model of emissions (CO_2, CO, HC, and NOx) and fuel consumption for light-duty vehicles, which is derived from the physical load-based approaches that are gaining in popularity. The model is calibrated for a set of vehicles driven on standard as well as aggressive driving cycles. The model is validated on another driving cycle in order to assess its estimation capabilities. The preliminary results indicate that the model gives reasonable results compared to actual measurements as well as to results obtained with CMEM, a well-known load-based emission model. Furthermore, the results indicate that the model runs fast and is relatively simple to calibrate. The model presented can be integrated with a variety of traffic models to predict the spatial and temporal distribution of traffic emissions and assess the impact of ITS traffic management strategies on travel times, emissions, and fuel consumption.

INTRODUCTION

Vehicle emissions models are necessary for quantifying the impact of traffic flows on air quality. It has been widely recognized that models based on the average speed from fixed driving cycles, such as the US EPA MOBILE6, do not adequately capture the effects of driving and vehicle dynamics on emissions (*1*). Therefore their applicability is limited to estimate and forecast large-scale emissions inventories.

In order to predict traffic emissions more accurately and with a higher spatial and temporal detail, instantaneous or modal emissions models are necessary. They are based respectively on instantaneous vehicle kinematic variables, such as speed and acceleration, or on more aggregated modal variables, such as time spent in acceleration mode and time spent in cruise mode. These models can be classified into emission maps, regression-based models, and load-based models.

Emission maps are matrices that contain the average emission rates for every combination of speed and acceleration in the driving cycle used for the emission test. Although easy to generate and use, emission maps are not satisfactory because they can be highly sensitive to the driving cycle. They are also sparse and not flexible enough to account for such factors as road grade, accessory use, or history effects. Properties and limitations of emission maps are discussed in more detail in (*2*).

Regression-based models typically employ functions of instantaneous vehicle speed and acceleration as explanatory variables. These models overcome some limitations of the emission maps, such as sparseness and non-flexibility, but can lack a physical interpretation and can also overfit the calibration data as they typically use a large number of explanatory variables. Models in the literature that use this approach are presented for example in (*3, 4*).

Load-based models simulate, through a series of modules, the physical phenomena that generate emissions. The primary variable of these models is the fuel consumption rate, which is a surrogate for engine power demand (or engine load). They have a detailed and flexible physical basis, which defines the variables and parameters that should be included when modeling emissions. On the other hand, these models are quite complex and, when applied to the entire flow of vehicles in a network over a period of time, the computational effort can be high. Ultimately, they too can be sensitive to the calibration data, though they are more robust as a result of their physical basis.

It is valuable to design a model that simultaneously obtains realistic results, is fast to run and easy to calibrate in different situations. This paper presents EMIT (EMIssions from Traffic), which is a simple statistical model for instantaneous tailpipe emissions (CO_2, CO, HC, and NO_x) and fuel consumption. In order to realistically reproduce the emissions behavior, the explanatory variables are derived from a load-based approach. The model, due to its simple structure, is relatively easy to calibrate and requires less computational time.

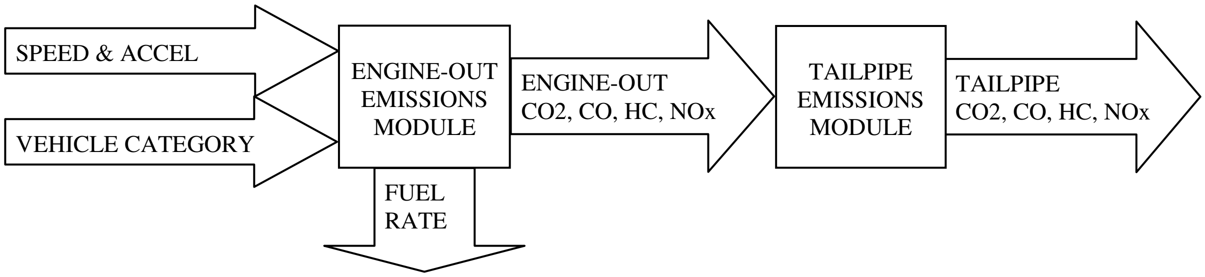
The paper is organized as follows. First, we present the structure of the model. Second, we describe the analysis and the preprocessing of the data used for the model development. The description of the data precedes the description of the model because the data is used to verify some assumptions during the development of the model. We then present the model derivation from the load-based approach its development (notation, rationale, simplifying assumptions, and formulation). The model was calibrated and validated for two vehicle/technology categories. We present calibration and validation results for these two categories. Finally, we present conclusions and directions for future work.

More detail on the development and application of EMIT can be found in (*5*). The first results corresponding to this model can be found in (*6*).

MODEL STRUCTURE

EMIT is a simple statistical model (with a basis in the physical system) for instantaneous emissions and fuel consumption of light-duty composite vehicles. In order to realistically reproduce the behavior of the emissions, the explanatory variables in EMIT have been derived from the load-based approach, using some simplifying assumptions. The model, due to its simple structure, is relatively easy to calibrate and is expected to require less computational time than load-based models.

A block diagram of the structure of EMIT is shown below:



EMIT is composed of two main modules: the engine-out emissions module and the tailpipe emissions module. Although implementing two modules adds a level of complexity to the model, this allows EMIT to predict not only tailpipe, but also its precursor engine-out emissions. This property of the model is useful in practice. For instance, it allows for the modeling of engine and catalyst technology improvements, vehicle degradation, as well as the implications of effectiveness of inspection and maintenance programs. Moreover, it allows for modular and incremental modeling, by identifying model parts that would require improvements, and thus further research.

Given a vehicle category and its second-by-second speed and acceleration, the first module predicts the corresponding second-by-second fuel consumption and engine-out emission rates. These, in turn, are the inputs for the next module that predicts second-by-second tailpipe emission rates.

DATA

The NCHRP Database

The data used for the development, calibration and validation of EMIT is the National Cooperative Highway Research Program (NCHRP) vehicle emissions database, which consists of data relative to chassis dynamometer tests conducted at the College of Environmental Research and Technology, University of California at Riverside, between 1996 and 1999. The NCHRP database was used in the development of CMEM and of other emission models in the literature. The purpose of this section is to provide the principal information on the database. A complete description of the database and the dynamometer testing procedure can be found in (*7*).

The database includes measurements of second-by-second speed and engine-out and tailpipe emission rates of CO_2, CO, HC, and NO_x for 344 light-duty vehicles (202 cars and 142 light trucks). For a limited number of vehicles the measurements of engine speed, throttle position, mass air flow, emission control temperature, gear, and other quantities are also included. Only speed and emissions data are needed in the development of EMIT.

For the development of the NCHRP database, a total of 26 vehicle/technology categories were defined in terms of fuel and emission control technology, accumulated mileage, power-to-weight ratio, emission certification level, and, finally, by normal or high emitter status. The vehicles were randomly recruited, principally in California. For each vehicle category, the sample size was determined based on the approximate percentage contribution of that category to the emissions inventory. The vehicles were tested on chassis dynamometer using three driving cycles: the standard FTP cycle, the high-speed aggressive US06 cycle, and the Modal Emission Cycle (MEC01), an engineered aggressive cycle. The FTP and the US06 are cycles prescribed by the EPA for regulation purposes. The MEC01 cycle was designed at UC Riverside for the development of the NCHRP database and the CMEM model. The MEC01 represents driving conditions with higher speeds and harder accelerations than the FTP cycle, but is less aggressive than the US06 cycle.

The database does not contain the results of all tests. It contains only the data of tests that were successfully completed, since there were cases of vehicle failure. The most common reasons of failure were engine overheating or brake problems. FTP data are available for all vehicles, MEC01 data are available for most vehicles, and US06 data are available for most cars and for a limited number of light trucks.

Data Preprocessing

The primary objective of EMIT is to predict emissions from average vehicles, each representative of a vehicle category, rather than from specific makes and models. Thus, for each category, the data were aggregated into composite vehicles data. A compositing procedure similar to that used in (*7*) was implemented. The vehicle classification identified in (*7*) was adopted with some minor modification. The original Category 22 (bad catalyst) includes both cars and trucks. We divided it into two separate categories, given the availability of a large number of vehicles. The other high emitters categories include both cars and trucks, as in the original classification. The classification of individual vehicles was partly revised, with particular attention to high emitters, which we considered misclassified in a number of cases. The revised classification is shown in (*5*).

Only the vehicles for which both the FTP cycle and the MEC01 cycle (version 6 or 7) are available were considered.

The compositing procedure is conducted as follows. For each vehicle category and for each driving cycle, the vehicle tests data are time-aligned by maximizing the R-square among the speed traces. This is performed by time shifting the data and/or cutting few seconds of data. Then, the average second-by-second speed and emission rates are calculated to create the composite vehicle data. Only the first 900 seconds of the MEC01 cycle are averaged because versions 6 and 7 are different after the first 900 seconds.

Acceleration and fuel rate are two variables required in the development of the model, but not reported in the database. We calculate acceleration as the variation between two consecutive second-by-second speeds of the composite vehicle. We calculate fuel rate using the following carbon balance formula:

$$FR = [CO_2 / 44 + CO / 28] \cdot [12 + 1 \cdot 1.85] + HC \qquad (1)$$

where numbers 44, 28, 12 and 1 are the molecular weights of CO_2, CO, C, and H respectively, number 1.85 is the approximate number of moles of hydrogen per mole of carbon in the fuel, and CO_2, CO, and HC are the measured engine-out emission rates. This formula derives the equivalent mass of hydrocarbon from the carbon balance of the emissions measurements (*8, 9*).

Other data used in the model are the following composite vehicle specification parameters: mass, rolling resistance coefficients, and air drag coefficient. These parameters were derived in (*7*), by averaging the parameters of the single vehicles in each category.

In summary, the composite vehicle data used for the development of EMIT are: (1) second-by-second data from the dynamometer tests: speed, engine-out emission rate, tailpipe emission rate, and fuel rate (estimated from Equation 1), and (2) the following composite vehicle specific data: mass, rolling resistance coefficients, and air drag coefficient.

Categories Modeled in EMIT

At the time of writing this paper, EMIT has been calibrated for the following two vehicle categories:

- category 7 (3-way Catalyst ("Tier 0" emission standard), fuel injection, less than 50,000 miles accumulated, and high power/weight ratio),
- category 9 (Tier 1 emission standard, more than 50,000 miles accumulated, and high power/weight ratio).

The characteristics of the vehicles used for the compositing procedure for vehicle categories 7 and 9 are presented in Table 1 (Part a and Part b, respectively).

Because fuel-to-air ratio is not modeled explicitly, EMIT is calibrated using data that cover a large spectrum of operating conditions, including stoichiometric, enrichment and enleanment conditions, in order to capture the emissions variability. The following set of hot-stabilized composite data are used for the calibration: (a) FTP bag 2, (b) FTP bag 3, excluding the first 100 seconds (to account for the catalyst light-off time), and (c) first 900 seconds of the MEC01 cycle. The US06 cycle is used to validate the model. Cold-start conditions are not modeled but can be easily added in a future development, as discussed in the conclusion section.

MODEL DEVELOPMENT

In this section the engine-out and tailpipe emissions modules are derived from the load-based approach.

The Engine-Out Emissions Module

Let i denote the generic emission species (i.e. $i = CO_2, CO, HC, NO_x$). Let EO_i denote the engine-out emission rate of species i in g/s, and EI_i the emission index for species i, which is the mass of emission per mass unit of fuel consumed. By definition of EI_i, engine-out emission rates are given by:

$$EO_i = EI_i \cdot FR \tag{2}$$

where FR denotes the fuel consumption rate (g/s). The following paragraphs describe how FR and EI_i are modeled in a typical load-based formulation.

When the engine power is zero, the fuel rate is equal to a typically small constant value. Otherwise, fuel consumption is mainly dependent on the engine speed and the engine power. This is modeled as follows:

$$FR = \begin{cases} \phi \cdot \left(K \cdot N \cdot V + \dfrac{P}{\eta} \right) & \text{if } P > 0 \\ K_{idle} \cdot N_{idle} \cdot V & \text{if } P = 0 \end{cases} \tag{3}$$

where:

- ϕ : fuel-to-air equivalence ratio, which is the ratio of the actual fuel-to-air mass ratio to the stoichiometric fuel-to-air mass ratio. When $\phi \cong 1$, the mixture is stoichiometric. When $\phi > 1$, the mixture is rich. When $\phi < 1$, the mixture is lean.
- K : engine friction factor (kJ/rev/liter),
- N : engine speed (rev/s),
- V : engine displacement (liters),
- η : engine indicated efficiency,
- K_{idle} : constant idle engine friction factor (kJ/rev/liter),
- N_{idle} : constant idle engine speed (rev/s),
- P : engine power output (kW).

The fuel-to-air equivalence ratio ϕ can be modeled for enleanment, stoichiometric, and enrichment conditions. When engine power is equal to zero, the mixture becomes lean, due to fuel shut-off. Since emissions are not very sensitive to the level of enleanment (except for a fraction of the high emitters), in enleanment conditions it is reasonable to approximate ϕ by a constant. In enrichment conditions, ϕ is a function of engine power and acceleration, but is usually modeled in terms of engine power (or torque) only. When engine power (or torque) is greater than an enrichment threshold, the mixture goes rich. Such a threshold can be modeled in terms of specific power and vehicle parameters. Above the threshold, ϕ can be modeled as a linear function of engine power. When engine power (or torque) is positive but less than the enrichment threshold, the mixture is considered stoichiometric. More details of a model of the fuel-to-air equivalence ratio are described in (*7*).

To link the engine speed N to the wheel speed v, a transmission model is necessary. This can be modeled in a limited fashion as function of vehicle speed, gear shift schedule, gear ratio, and engine peak torque (*10, 7*).

The engine friction factor K can then be modeled as function of engine speed (*7*). Engine power is modeled as:

$$P = \frac{P_{tract}}{\varepsilon} + P_{acc} \tag{4}$$

where:

- P_{tract}: total tractive power requirement at the wheels (kW),
- ε: vehicle drivetrain efficiency,
- P_{acc}: engine power requirement for accessories, such as air conditioning.

The drivetrain efficiency ε depends on engine speed and engine torque. It can be approximated as a function of vehicle speed and specific power, as discussed in (*7*).

When positive, the tractive power is given by:

$$P_{tract} = A \cdot v + B \cdot v^2 + C \cdot v^3 + M \cdot a \cdot v + M \cdot g \cdot \sin\vartheta \cdot v \tag{5}$$

where:

- v: vehicle speed (m/s),
- a: vehicle acceleration (m/s^2),
- A: rolling resistance coefficient (kW/m/s),
- B: speed correction to rolling resistance coefficient (kW/(m/s)^2),
- C: air drag resistance coefficient (kW/(m/s)^3),
- M: vehicle mass (kg),
- g: gravitational constant (9.81 m/s^2),
- ϑ: road grade (degrees).

When the right hand side of Equation 5 is non-positive, P_{tract} is set equal to zero. All parameters (A, B, C, and M) are known and readily available for each vehicle.

In conclusion, FR can be modeled as function of v, a, ϑ, P_{acc}, and known vehicle parameters, since all other variables in Equations 3, 4, and 5 (ϕ, K, N, P, and ε) can be expressed in terms of v, a, ϑ, and P_{acc}, and vehicle parameters. The vehicle parameters are available from vehicle manufacturers or can be calibrated.

Emission indices EI_i are modeled in the literature in various ways as a function of ϕ (*10, 7*), or ϕ and FR (*8*). However, generally, as more fuel is burned, more emissions are formed. As a result, to first approximation EO_i is a linear function of FR:

$$EO_i = \lambda + \mu \cdot FR \tag{6}$$

In particular, every emission species has a particular behavior, which is summarized as follows:

- CO_2 is the principal product of complete fuel combustion; thus, it is mainly proportional to FR.
- CO is sensitive to ϕ. Under enrichment conditions, the combustion is not complete due to the lack of oxygen. Much of the carbon present in the excess fuel is partially oxidized to CO instead of CO_2. Note that CO is generated even under stoichiometric conditions, due to possible partial oxidation of HC.

- HC is a product of incomplete combustion and is also usually proportional to FR. Under enleanment conditions, HC emissions can be higher, in particular during long deceleration events (*11*). During decelerations, the dramatic drop in fuel results in a cessation of combustion, and hence virtually all of the remaining fuel (what little is left) is emitted unburned. However this fuel excess is typically oxidized in the catalyst. This is an example where history effects can be significant.
- NO_x is mainly dependent on the combustion temperature, because the dissociation and subsequent recombination of atmospheric N_2 and O_2 that generate NO and NO_2 is induced by high temperatures (*12*). For small values of FR, very little NO_x is emitted. During stoichiometric conditions, the combustion temperature, and consequently the emission, increase as more fuel is burned. In lean conditions, the excess oxygen facilitates the formation of more NO.

EMIT has been developed and calibrated for hot-stabilized conditions with zero road grade ($\vartheta = 0$), and without accessory usage ($P_{acc} = 0$). The model does not represent history effects, such as cold-start emissions and hydrocarbon enleanment puffs. These factors can be included in future developments, as discussed in the conclusions section. Nevertheless, considering only hot-stabilized conditions is not a critical limitation for highway applications, since most vehicles are hot by the time they reach the highways. Moreover, the hydrocarbons puffs do not significantly affect tailpipe emissions in normal emitting vehicles, since the catalytic converter is usually effective under enleanment conditions (*11*).

The following are assumptions adopted in the development of EMIT:

- Although, as discussed, ϕ, K, N, and ε can be expressed in various functional forms of v and a, their effects on fuel rate can be aggregated into the effects of v, v^2, v^3, and $a \cdot v$, which are the independent variables in Equation 5.
- Since emission rates can be approximated as a linear function of fuel rate (Equation 6), the variables that govern emission rates are the same variables that govern fuel rate.
- Since we do not consider accessory usage ($P_{acc} = 0$), P_{tract} is used as a surrogate for P to test if the vehicle is in idle mode.

Given the previous assumptions, combining Equations 3, 4, and 5, we have:

$$FR = \begin{cases} \alpha_{FR} + \beta_{FR} v + \gamma_{FR} v^2 + \delta_{FR} v^3 + \zeta_{FR} a v & \text{if} \quad P_{tract} > 0 \qquad (7a) \\ \alpha'_{FR} & \text{if} \quad P_{tract} = 0 \qquad (7b) \end{cases}$$

and, from Equation 6:

$$EO_i = \begin{cases} \alpha_i + \beta_i v + \gamma_i v^2 + \delta_i v^3 + \zeta_i a v & \text{if} \quad P_{tract} > 0 \qquad (8a) \\ \alpha'_i & \text{if} \quad P_{tract} = 0 \qquad (8b) \end{cases}$$

where P_{tract} is calculated with Equation 5, using A, B, C, and M from (*7*).

For CO, the effect of enrichment is too distinct to be incorporated in the same equation. For enrichment conditions the emissions are modeled as a linear function of the corresponding stoichiometric emissions:

$$EO_{CO} = \begin{cases} EO_{CO}^{stoich} = \alpha_{CO} + \beta_{CO} v + \delta_{CO} v^3 + \zeta_{CO} a v & \text{if} \quad 0 < P_{tract} \le P_{tract}^{enrich} \qquad (9a) \\ \kappa + \chi \cdot EO_{CO}^{stoich} & \text{if} \quad P_{tract} > P_{tract}^{enrich} \qquad (9b) \\ \alpha'_{CO} & \text{if} \quad P_{tract} = 0 \qquad (9c) \end{cases}$$

The enrichment threshold P_{tract}^{enrich} is determined empirically based on the cut-point in the trend of EO_{CO} versus FR.

Equations 7, 8 and 9 are calibrated for each vehicle category using least square linear regressions.

The Tailpipe Emissions Module

Tailpipe emission rates TP_i (g/s) are modeled as the fraction of the engine-out emission rates that leave the catalytic converter:

$$TP_i = EO_i \cdot CPF_i \tag{10}$$

where CPF_i denotes the catalyst pass fraction for species i.

Catalyst efficiency is difficult to predict accurately, and varies greatly from hot-stabilized to cold-start conditions. As stated previously, at this time cold-start conditions are not considered.

Hot-stabilized catalyst pass fractions are modeled in the literature in various ways as a function of ϕ, FR, and/or engine-out emissions (*7, 8*). Since the physical and chemical phenomena that control catalyst efficiency are challenging to capture, often these functions are purely empirical.

EMIT calculates:

- The tailpipe CO_2 (which is not much different from engine-out CO_2), directly using the equations:

$$TP_{CO_2} = \begin{cases} \alpha_{CO_2} + \beta_{CO_2} v + \gamma_{CO_2} v^2 + \delta_{CO_2} v^3 + \zeta_{CO_2} av & if \quad P_{tract} > 0 \qquad (11a) \\ \alpha'_{CO_2} & if \quad P_{tract} = 0 \qquad (11b) \end{cases}$$

- The tailpipe CO, HC and NO_x with Equation 10. The catalyst pass fractions are modeled empirically as piecewise linear functions of engine-out emission rates under different operating regimes. The most general function is composed of three pieces:

$$CPF_i = \begin{cases} m'_i \cdot EO_i + q'_i & if \quad 0 \le EO_i < z'_i \\ m''_i \cdot EO_i + q''_i & if \quad z'_i \le EO_i < z''_i \\ m'''_i \cdot EO_i + q'''_i & if \quad EO_i \ge z''_i \end{cases} \tag{12}$$

MODEL CALIBRATION

Engine-out Emissions Module

Previous calibration of Equation 7a indicates that the coefficient of v^2 is negative, which is counterintuitive, but not statistically significant. This second order speed term is expected to be small, since it mainly represents a higher order correction to the rolling resistance term. The term in v^2 is then dropped in the calibration process. Dropping it, the goodness of fit of the regression is practically unaffected (adjusted R-squared~0.96) and all coefficients are positive and statistically significant.

All regressions of Equations 8 give satisfactory results in terms of statistical significance as well as adjusted R-squared. For Equation 9a, it is necessary to employ a more 'robust' calibration, by removing a few outliers (~3% of the data) from the calibration data. For HC, the emissions puffs are omitted in the calculation of α'.

The calibrated parameters are shown in Table 2. Engine-out emission rates (EO_i) are expressed in g/s, vehicle speed (v) is expressed in km/h, speed times acceleration (av) is expressed in m^2/s^3, and power is expressed in kW.

We note the following:

- All coefficients have high t-statistics, except for β_{HC} in both categories, and β_{CO} in category 9, which have been dropped.
- All coefficients are, as expected, positive, except for α_{NOx} in both categories and β_{CO} in category 7.

Tailpipe Emissions Module

Equation 11 is calibrated for each vehicle category using least square linear regressions. The calibrated parameters are shown in Table 3 (Part a). Engine-out emission rates (EO_i) are expressed in g/s, vehicle speed (v) is expressed in km/h, speed times acceleration (av) is expressed in m^2/s^3, and power is expressed in kW.

Equation 12 is calibrated for CO , HC and NO_x by minimizing the sum of the squared differences between the predicted and measured tailpipe emission rates. The predicted tailpipe emission rates are obtained as the product of the modeled catalyst pass fraction and the measured engine-out emission rates (to minimize error propagation). The calibrated coefficients are reported in Table 3 (Part b and Part c).

CPF_{HC} and CPF_{NOx} are challenging to model (*8, 13*). CPF_{HC} is scattered especially for medium levels of engine-out emissions, where the highest values are related to high power episodes. CPF_{NOx} is especially noisy for very low engine-out emissions, with values ranging from nearly zero to ~0.95 in category 9 and more than 1 in category 7.

Results

The quality of the calibrated model is assessed using a variety of statistics and graphical analyses.

Let TME denote the total measured emission (in grams) of a given species (or fuel consumption) over the cycle. Let TPE denote total predicted emission (or fuel consumption) over the cycle. We calculate the following statistics for each emission species (or fuel consumption):

- Average error (g/s), which is the difference between TME and TPE , divided by the duration of the cycle (in seconds).
- Relative average error, which is the ratio between the average error and the measured average emission (or fuel consumption) rate.
- Correlation coefficient ρ , which is the ratio between the covariance of the predicted and measured emission (or fuel consumption) rates and the product of their standard deviations.
- R-square (R^2) between the measured and the predicted emission (or fuel consumption) rates.

Furthermore, we look at a graphical comparison between the predicted and the measured second-by-second emission (or fuel consumption) rates over time for category 7. Results for category 9 are not presented due to space limitations, and they can be found in (*5*). (*5*) also contains a graphical analysis of predicted versus measured emission (or fuel consumption) rates and a graphical analysis of the residuals (second-by-second differences between the predicted and measured emission rates).

Table 4 shows, for the engine-out and the tailpipe modules of both vehicle categories, the measured average emission (or fuel consumption) rates, average error, relative average error, ρ , and R^2.

Figures 1 through 4 show the fit of the EMIT outputs for category 7 with the measured second-by-second emission (or fuel) rates used for the calibration. The plots show also that the EMIT outputs are comparable with those obtained with the load-based model CMEM Version 2.01 (*14*) for the same vehicle categories. EMIT and CMEM are calibrated using very similar sets of data. From the documentation (*7*), it can be inferred that for category 7 CMEM is calibrated using the data relative to the same 7 vehicles used by EMIT.

A comparison between Figures 1, 2 (FTP bag 2) and Figures 3, 4 (MEC01) shows that the model can capture the emissions variability in a wide range of magnitudes.

The estimated fuel consumption and CO_2 match the measurements satisfactorily (0.0% error and R^2>0.97).

For CO, the model fits the measurements quite well (R^2 between 0.84 and 0.90), with the exception of some MEC01 peaks (Figure 3), resulting in a percentage error equal to or less than –3.5% in engine-out and –8.3% in tailpipe.

For HC, the model has a less desirable performance (R^2 between 0.53 and 0.63). For engine-out, as expected, the principal problem is represented by the enleanment puffs, which are not modeled, resulting in an underestimation of approximately -12%. For tailpipe, there is a tendency to overestimate the low emissions and underestimate the highest MEC01 peaks (Figure 4). The resulting percentage error (-12.1% for category 7 and -23.6% for category 9) is due not to enleanment puffs (which are not present in the measured tailpipe emissions), but to the underestimation of the MEC01 peaks. Probably the model is not able to capture the decreased catalyst efficiency during these enrichment events.

For NO_x, engine-out emissions fit well, while the fit for tailpipe emissions is lower (R^2 drops from 0.86 to 0.79 for category 7 and from 0.87 to 0.67 for category 9), due to the scattered behavior of CPF_{NOx}, which is highly sensitive to the variability of air-to-fuel ratio. In particular, as in the case of CO, there is underestimation of the MEC01 highest speed peak (Figure 4). However, the percentage error is very small (less than 2% in absolute value).

MODEL VALIDATION

The validation of the calibrated model is carried out on the composite US06 data, to test the capability of EMIT to predict emissions and fuel consumption from input data different from those used in calibration. The US06 cycle is a difficult test cycle for model predictions (*7*). The results, as shown in Table 5, are, as expected, poorer than those obtained on the calibration data, but in general quite satisfactory.

Figures 5 and 6 show how the EMIT outputs for category 7 fit the measured second-by-second emission (or fuel consumption) rates. The EMIT outputs are comparable with those obtained with CMEM for the same vehicle categories.

Fuel consumption and CO_2 are estimated within 5.3% and –2.6% respectively, with a very high R^2 (~0.95). For CO, both engine-out and tailpipe modules overestimate some medium peaks and underestimate some high peaks (Figure 5). R^2 is between 0.36 and 0.50, and the percentage error is less than -17% for category 7 (and was less than 7% for category 9). The HC model has the poorest performance (R^2 between 0.22 and 0.32). In engine-out the principal problem is related to enleanment puffs that, however, disappear in the measured tailpipe emissions. Tailpipe emissions are largely overestimated in category 7 (83.4%). For NO_x, the prediction of the engine-out emissions is reasonable, while the fit for tailpipe emissions is lower (R^2 drops from 0.83 to 0.63 for category 7 and from 0.83 to 0.53 for category 9), due to the scattered behavior of CPF_{NOx}. The tailpipe percentage error is 19.8% for category 7 and -3.0% for category 9.

CONCLUSIONS

In this paper, we presented EMIT, a dynamic model of emissions (CO_2, CO, HC, and NO_x) and fuel consumption for light-duty vehicles. The model was derived from the regression-based and the load-based emissions modeling approaches, and effectively combines some of their respective advantages. EMIT was calibrated and validated for two vehicle categories.

The results for the two categories calibrated indicate that the model gives reasonable results compared to actual measurements as well as to results obtained with CMEM, a state-of-the-art load-based emission model. In particular, the model gives results with good accuracy for fuel consumption and carbon dioxide, reasonable accuracy for carbon monoxide and nitrogen oxides, and less desirable accuracy for hydrocarbons.

The structure and the calibration of EMIT are simpler compared with load-based models. While load-based models involve a multi-step calibration process of many parameters, and the prior knowledge of several readily available specific vehicle parameters, the approach presented in this paper collapses the calibration into few linear regressions for each pollutant. Compared to a multi-step calibration, here the parameters directly optimize the fit to the emissions, avoiding error accumulations. Furthermore, due to its relative simplicity, the computational time required to run the model is expected to be less compared to load-based models.

Questions for future research related to EMIT are the following:

1. The tailpipe module for HC, which currently gives the least satisfactory results, needs to be improved.
2. The model needs to be calibrated for the other categories present in the NCHRP vehicle emissions database. Moreover, in order to represent the actual emissions sources present on roadways, other databases should be acquired and used for the model calibration, including data on heavy trucks, buses, more recent vehicles than those represented in the NCHRP database, and on-road measurements.
3. The model can be extended to other emission species, such as particulate matter and air toxics, when data are available.
4. Least square regression benefits from calibration data with extreme values. Therefore, it is recommendable to calibrate EMIT using, in addition to the data presently used, also data from aggressive cycles, like the US06. This is not currently possible, since US06 data are not available for many vehicles from the NCHRP vehicle emissions database.
5. EMIT has been developed and calibrated for hot-stabilized conditions with zero road grade, and without accessory usage. The model does not represent history effects, such as cold-start emissions and hydrocarbon enleanment puffs. Future research should address how to overcome these limitations, in order to provide greater generality to the model. In the following, we suggest some easily realizable modifications to the model to include road grade, cold starts and hydrocarbon enleanment puffs, while how to make the model take account of accessory usage appears to be a more challenging question.
   - Road grade ϑ can be easily introduced adding a variable a_g to the vehicle acceleration a in Equations 7, 8, 9, and 11. The variable a_g is the component of the gravitational acceleration g (9.81 m/s^2) along the road surface ($a_g = g \cdot \sin \vartheta$).
   - In order to model cold-start emissions, two approaches could be pursued. The first approach would consist in simply recalibrating the model using cold-start (e.g. FTP bag 1) data. In this case, EMIT would be composed of two sub-models, one for cold-start and one for hot-stabilized conditions. The second approach would be more general, allowing for intermediate soak times and gradual passage from cold to hot conditions. In this case, it would be necessary to introduce in the model history variables, such as soak time, time elapsed since the beginning of the trip, and possibly cumulative fuel consumption.
   - Hydrocarbons puffs do not significantly affect tailpipe emissions in normal emitting vehicles. On the other hand, they can constitute a significant portion of the total tailpipe emissions in high emitters. In order to model hydrocarbons puffs in EMIT, it would be necessary to introduce in the model history variables, such as the duration of deceleration since its inception up to the current time.

Given its capability of generating time-dependent emission estimates, EMIT is suitable for integration with a variety of traffic models to assess the impact of traffic management strategies on air quality. For instance, we have recently investigated the integration of instantaneous emission models such as EMIT with non-microscopic traffic models. We have proposed a methodology for this type of integration (*5*). The methodology has been applied to integrate EMIT with a mesoscopic dynamic traffic flow model, which is developed in (*15*). The integration is realized through an acceleration model, based on the statistical distribution of real-world acceleration data, which is developed in (*16*). The combined traffic-acceleration-emission model has been applied to a hypothetical case study to illustrate its potential to estimate the effects of route guidance strategies, which are one of numerous examples of dynamic traffic management strategies, on traffic travel times and vehicle emissions. The first results of this application are presented in (*5*).

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TABLE 1: Vehicles Used for the Category 7 (Part a) Composite Vehicle and the Category 9 (Part b) Composite Vehicle.

Part a

Vehicle ID	Model Name	Model Year	Mass (lb)	Odometer (miles)
126	Suzuki Swift	92	2,125	48,461
136	Nissan 240SX	93	3,125	43,009
147	Mazda Protege	94	2,875	40,201
169	Mercury Tracer	81	2,500	6,025
248	Saturn SL2	93	2,500	42,264
257	Nissan Altima	93	3,250	32,058
259	Honda Accord LX	95	3,000	49,764

Part b

Vehicle ID	Model Name	Model Year	Mass (lb)	Odometer (miles)
187	Toyota Paseo	95	2,375	56,213
191	Saturn SL2	93	2,625	63,125
192	Honda Civic DX	94	2,375	57,742
199	Dodge Spirit	94	3,000	57,407
201	Dodge Spirit	94	3,000	56,338
229	Honda Civic LX	93	2,625	61,032
242	Saturn_SL2	94	2,625	64,967
260	Toyota Camry LE	95	4,000	51,286
281	Honda Accord EX	93	3,250	72,804

TABLE 2: Calibrated Parameters for the Engine-Out Emissions Module (Equations 7, 8, and 9) for Category 7 (Part a) and Category 9 (Part b). The t-Statistics Are Reported in Parentheses.

Part a

	CO_2	CO	HC	NOx	FR
α	.907 *(42.9)*	.0633 *(21.2)*	.0108 *(23.1)*	-.00522 *(-5.2)*	.326 *(26.3)*
β	.0136 *(24.4)*	-3.43 e-04 *(-4.2)*	*(dropped)*	.00038 *(14.4)*	.00228 *(6.9)*
δ	1.86e-06 *(53.8)*	1.73 e-07 *(30.9)*	1.20e-08 *(15.6)*	1.64e-08 *(10.8)*	9.42e-07 *(46.2)*
ζ	.231 *(216.3)*	.00977 *(43.5)*	.00124 *(52.3)*	.00282 *(55.9)*	.0957 *(152.4)*
α'	.862	.0369	.00552	.00326	.300
κ		-3.66 *(-11.2)*			
χ		12.5 *(16.4)*			
P_{tract}^{enrich}		30			

Part b

	CO_2	CO	HC	NOx	FR
α	1.02 *(40.8)*	.0316 *(22.8)*	.00916 *(58.1)*	-.00391 *(-3.7)*	.365 *(26.1)*
β	.0118 *(20.7)*	*(dropped)*	*(dropped)*	.000305 *(11.4)*	.00114 *(6.5)*
δ	1.92e-06 *(48.4)*	1.09e-07 *(49.9)*	7.55e-09 *(33.3)*	2.27e-08 *(14.0)*	9.65e-07 *(44.0)*
ζ	.224 *(195.5)*	.00883 *(43.0)*	.00111 *(60.5)*	.00307 *(64.9)*	.0943 *(150.3)*
α'	.877	.0261	.00528	.00323	.299
κ		-6.10 *(-14.3)*			
χ		21.8 *(18.9)*			
P_{tract}^{enrich}		34			

TABLE 3: Calibrated Parameters for the Tailpipe CO_2 Emissions Module (Equation 11) (Part a) and the Catalyst Pass Fraction Functions (Equation 12) for Category 7 (Part b) and Category 9 (Part c).

Part a (t-statistics are reported in parentheses)

	Category 7	Category 9
α	1.01 (41.49)	1.11 (47.0)
β	0.0162 (25.22)	0.0134 (19.3)
δ	1.90e-06 (47.62)	1.98e-06 (47.0)
ζ	0.252 (205.18)	0.241 (42.0)
α'	0.985	0.973

Part b

m'_{CO}	0.927	q'_{CO}	0.048	z'_{CO}	0.816
m''_{CO}	0.0538	q''_{CO}	0.749		
m'_{HC}	0	q'_{HC}	0.045	z'_{HC}	0.022
m''_{HC}	9.16	q''_{HC}	-0.152		
m'_{NOx}	0.127	q'_{NOx}	0.110		

Part c

m'_{CO}	0	q'_{CO}	0	z'_{CO}	0.005
m''_{CO}	1.15	q''_{CO}	-0.006	z''_{CO}	0.705
m'''_{CO}	0.045	q'''_{CO}	0.746		
m'_{HC}	0	q'_{HC}	0.011	z'_{HC}	0.011
m''_{HC}	3.69	q''_{HC}	-0.031	z''_{HC}	0.047
m'''_{HC}	23.39	q'''_{HC}	-0.977		
m'_{NOx}	0.124	q'_{NOx}	0.067		

TABLE 4: Calibration Statistics for the Engine-Out Module for Category 7 (Part a) and Category 9 (Part c), and the Tailpipe Module for Category 7 (Part b) and Category 9 (Part d).

Part a

	CO_2	CO	HC	NO_X	FR
Measured average rate (g/s)	2.26	0.157	0.0147	0.0208	0.806
Average error (g/s)	-0.00111	-0.00551	-0.00170	0.000244	0.0000522
Relative average error (%)	0.0	-3.5	-11.7	1.2	0.0
ρ	0.99	0.93	0.76	0.93	0.98
R^2	0.98	0.87	0.58	0.86	0.97

Part b

	CO_2	CO	HC	NO_X
Measured average rate (g/s)	2.52	0.0780	0.00130	0.00241
Average error (g/s)	-0.000667	-0.00602	-0.000158	0.0000404
Relative average error (%)	0.0	-7.7	-12.1	1.7
ρ	0.99	0.92	0.73	0.89
R^2	0.98	0.84	0.53	0.79

Part c

	CO_2	CO	HC	NO_X	FR
Measured average rate (g/s)	2.30	0.124	0.0133	0.0211	0.797
Average error (g/s)	0.000130	-0.00308	-0.00165	0.000181	-0.0000695
Relative average error (%)	0.0	-2.5	-12.3	0.9	0.0
ρ	0.99	0.95	0.79	0.93	0.98
R^2	0.97	0.90	0.63	0.87	0.97

Part d

	CO_2	CO	HC	NO_X
Measured average rate (g/s)	2.49	0.0629	0.000682	0.00160
Average error (g/s)	-0.0000401	-0.00402	-0.000161	-0.0000219
Relative average error (%)	0.0	-6.4	-23.6	-1.4
ρ	0.99	0.94	0.76	0.82
R^2	0.97	0.88	0.58	0.67

TABLE 5: Validation Statistics for the Engine-Out Module for Category 7 (Part a) and Category 9 (Part c), and the Tailpipe Module for Category 7 (Part b) and Category 9 (Part d).

Part a

	CO_2	CO	HC	NO_X	FR
Measured average rate (g/s)	3.87	0.315	0.0243	0.0444	1.40
Average error (g/s)	0.000785	-0.0516	-0.00455	-0.00111	0.0494
Relative average error (%)	0.0	-16.4	-18.7	-2.5	3.5
ρ	0.98	0.68	0.50	0.91	0.97
R^2	0.96	0.46	0.25	0.83	0.94

Part b

	CO_2	CO	HC	NO_X
Measured average rate (g/s)	4.37	0.154	0.00119	0.00427
Average error (g/s)	-0.113	-0.0256	0.000993	0.000846
Relative average error (%)	-2.6	-16.7	83.4	19.8
ρ	0.98	0.60	0.47	0.79
R^2	0.96	0.36	0.22	0.63

Part c

	CO_2	CO	HC	NO_X	FR
Measured average rate (g/s)	3.89	0.197	0.0220	0.0447	1.34
Average error (g/s)	-0.211	-0.00428	-0.00491	-0.000156	0.0713
Relative average error (%)	-0.5	-2.2	-22.3	-0.4	5.3
ρ	0.98	0.71	0.47	0.91	0.97
R^2	0.95	0.50	0.22	0.83	0.95

Part d

	CO_2	CO	HC	NO_X
Measured average rate (g/s)	4.26	0.0786	0.000778	0.00347
Average error (g/s)	-0.0932	0.00513	0.000206	-0.000105
Relative average error (%)	-2.2	6.5	26.5	-3.0
ρ	0.98	0.66	0.57	0.73
R^2	0.95	0.43	0.32	0.53

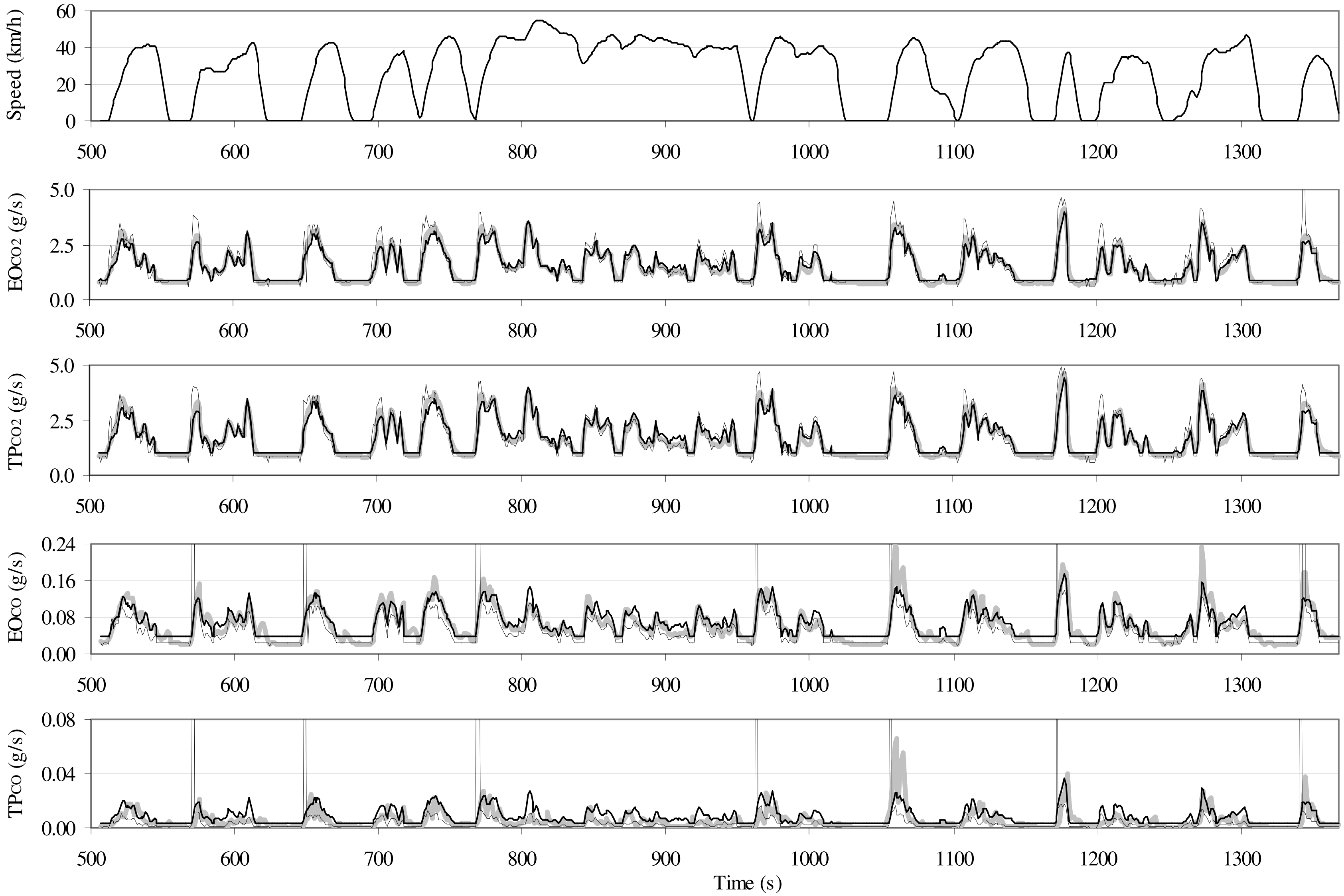

FIGURE 1: Category 7 - FTP bag 2. Second-by-second engine-out (EO) and tailpipe (TP) emission rates of CO2 and CO. Thick light line: measurements; dark line: EMIT predictions; thin line: CMEM predictions. The top plot represents the speed trace.

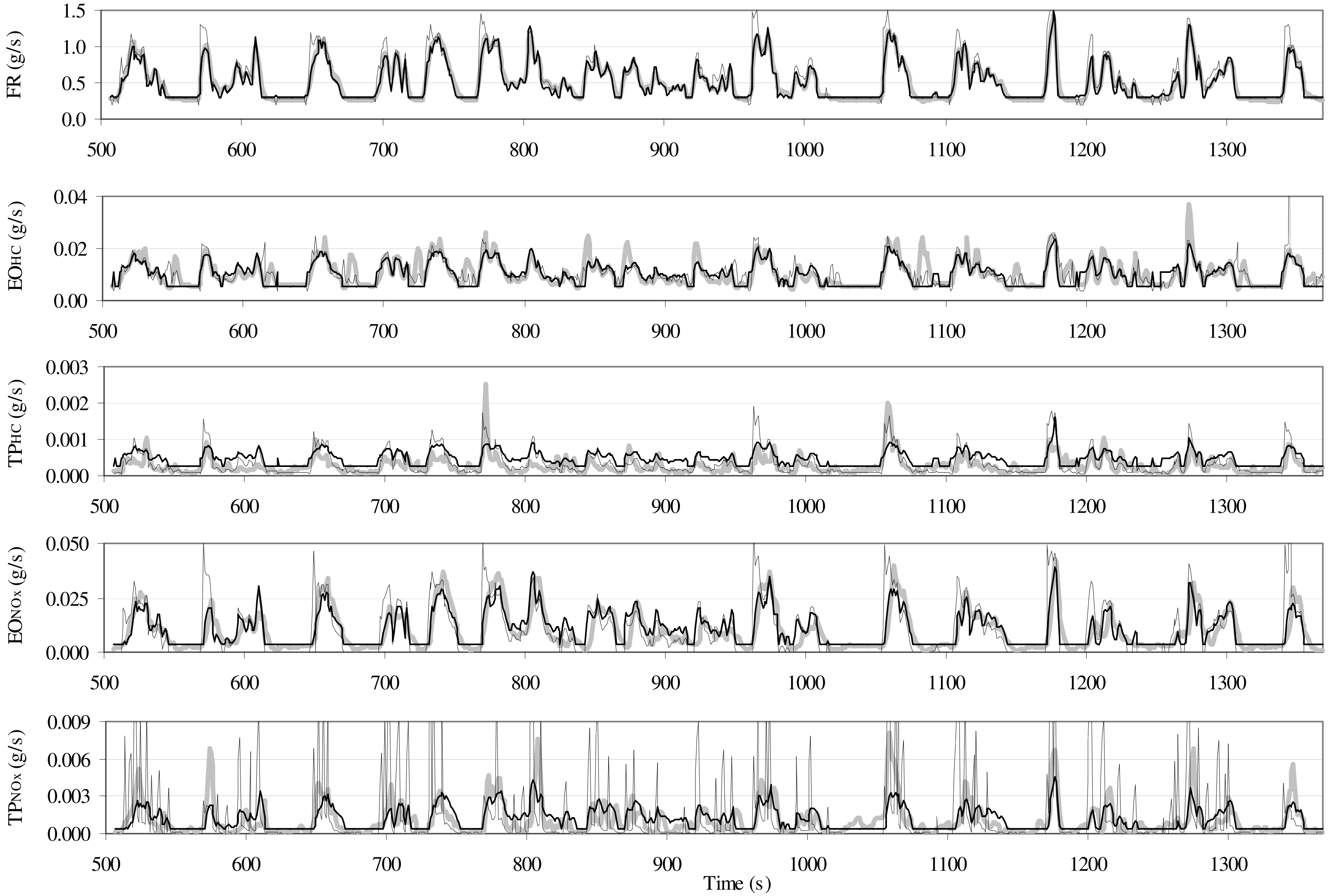

FIGURE 2: Category 7 - FTP bag 2. Second-by-second fuel rate (FR) and engine-out (EO) and tailpipe (TP) emission rates of HC and NOx. Thick light line: measurements; dark line: EMIT predictions; thin line: CMEM predictions.

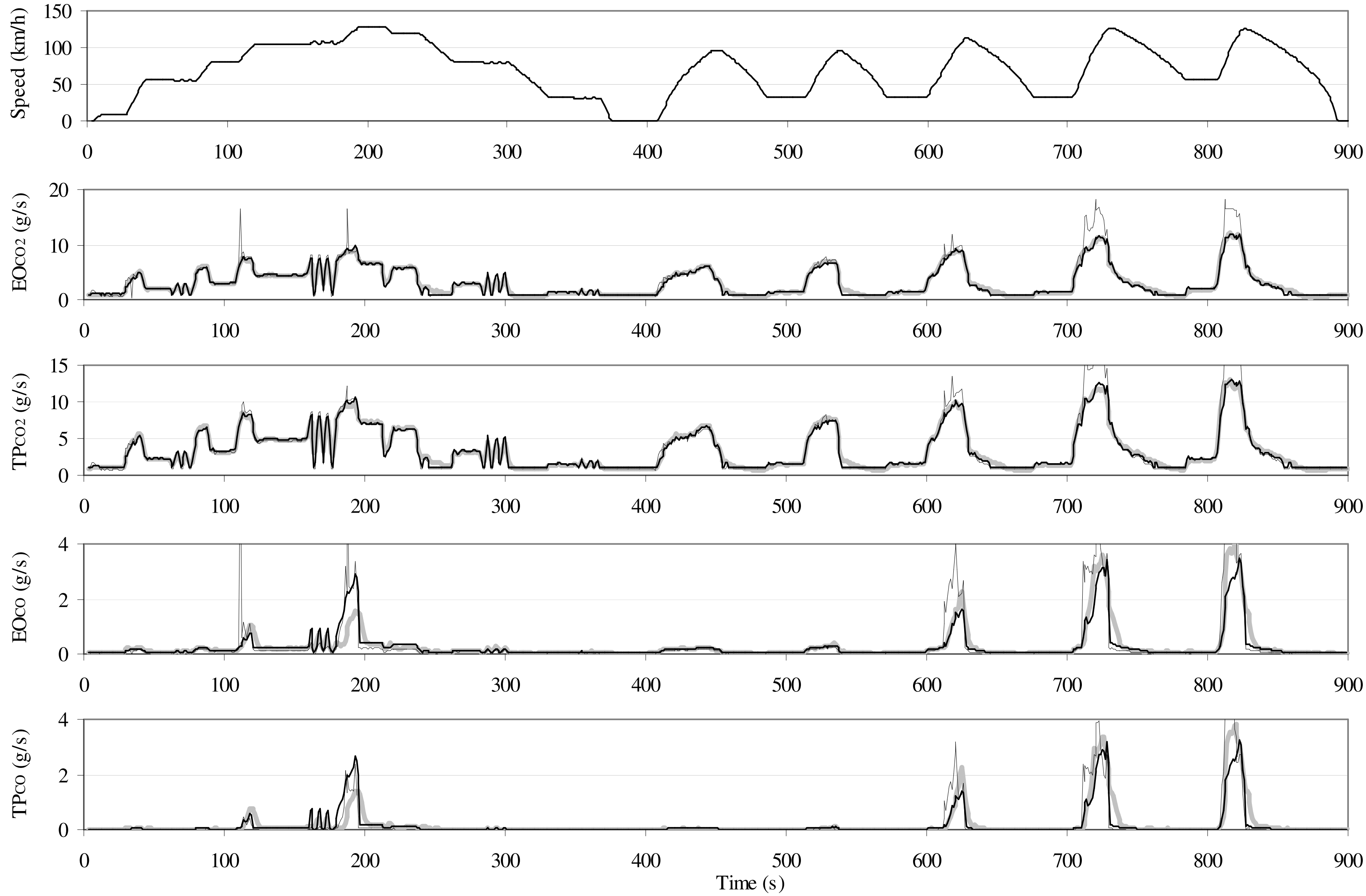

FIGURE 3: Category 7 – MEC01. Second-by-second engine-out (EO) and tailpipe (TP) emission rates of CO_2 and CO. Thick light line: measurements; dark line: EMIT predictions; thin line: CMEM predictions. The top plot represents the speed trace.

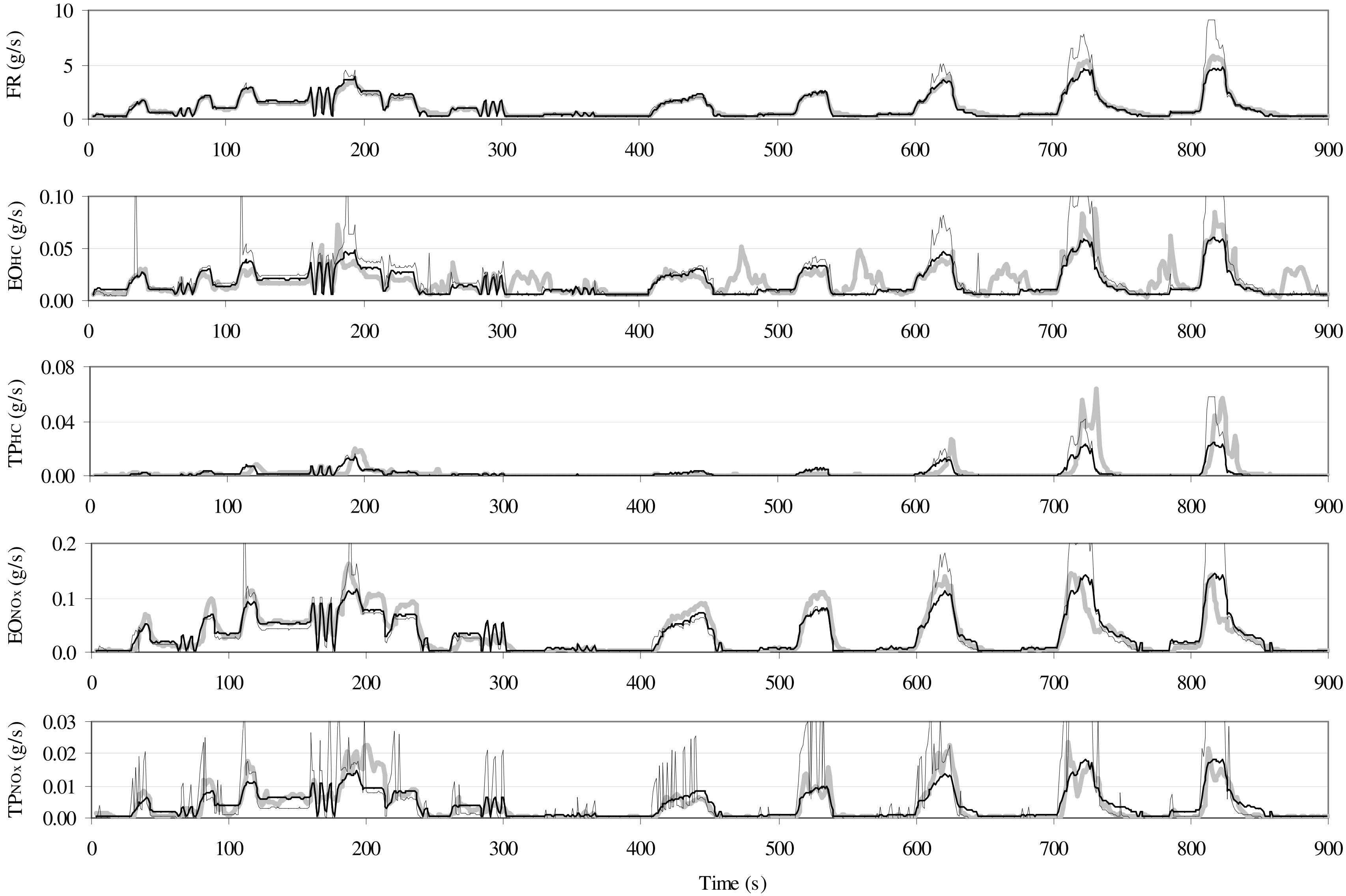

FIGURE 4: Category 7 – MEC01. Second-by-second fuel rate (FR) and engine-out (EO) and tailpipe (TP) emission rates of HC and NOx. Thick light line: measurements; dark line: EMIT predictions; thin line: CMEM predictions.

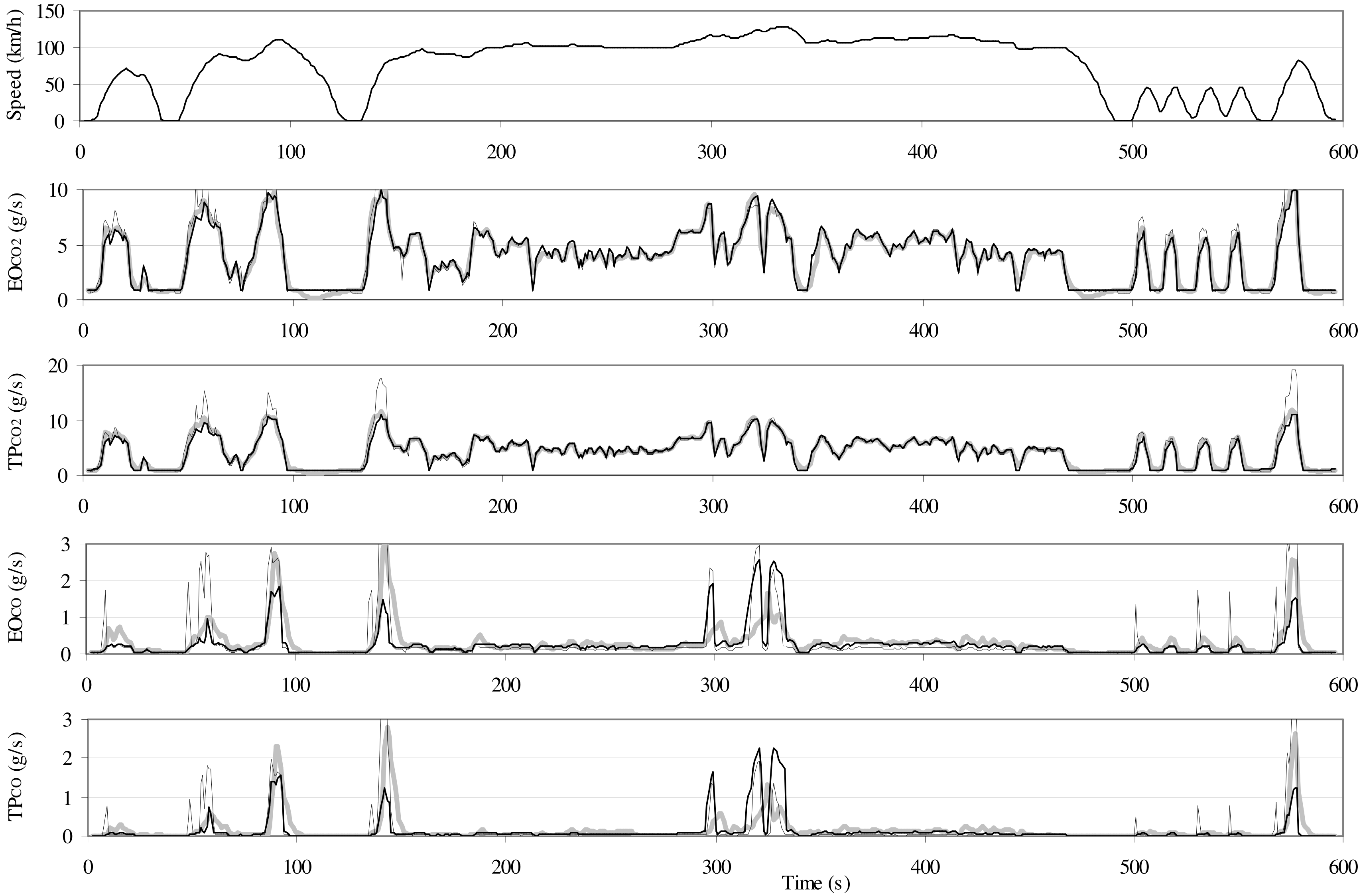

FIGURE 5: Category 7 – US06. Second-by-second engine-out (EO) and tailpipe (TP) emission rates of CO_2 and CO. Thick light line: measurements; dark line: EMIT predictions; thin line: CMEM predictions. The top plot represents the speed trace.

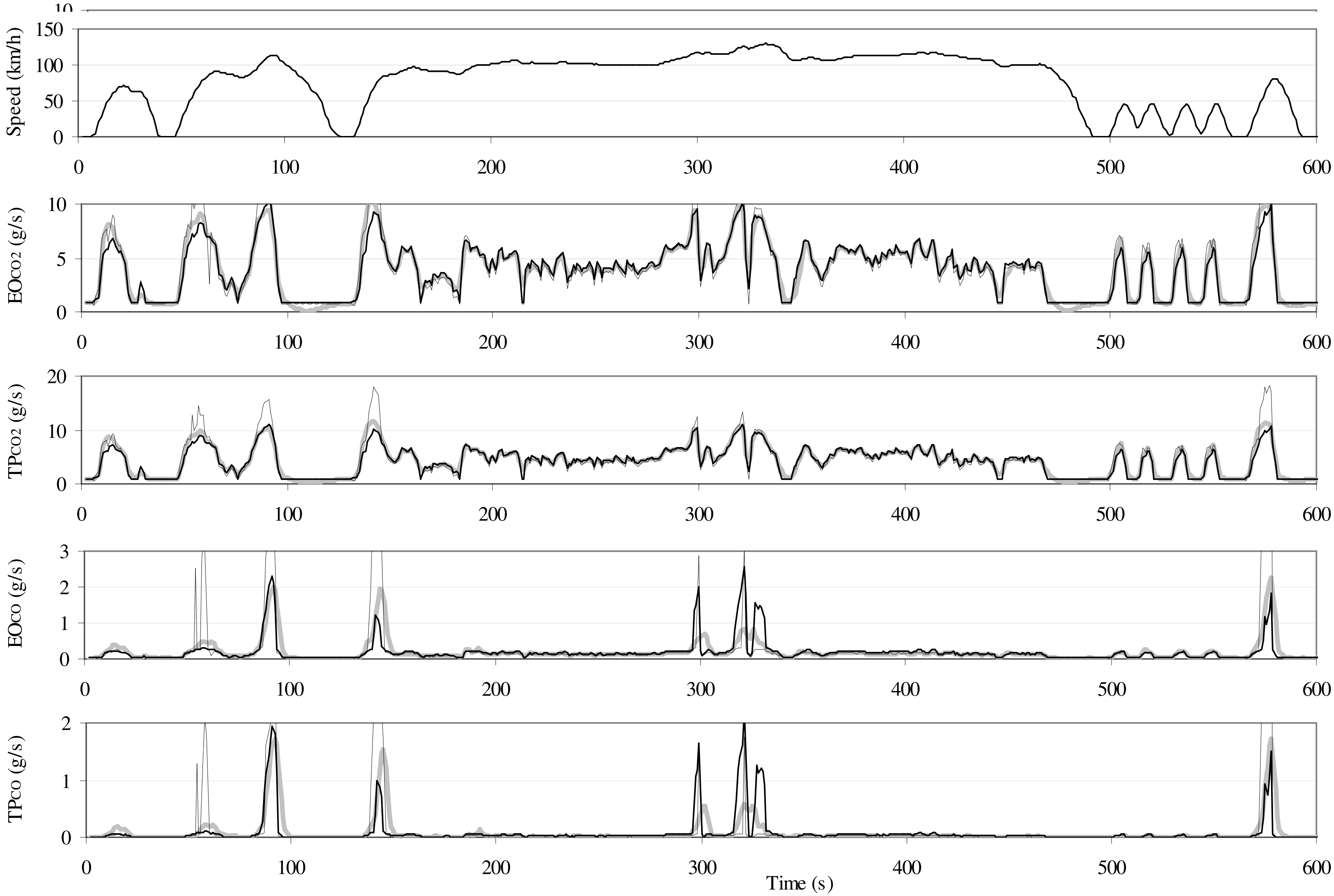

FIGURE 6: Category 7 – US06. Second-by-second fuel rate (FR) and engine-out (EO) and tailpipe (TP) emission rates of HC and NOx. Thick light line: measurements; dark line: EMIT predictions; thin line: CMEM predictions.