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Assessment of Traffic Environment using Fine-tuned Dynamic Vehicle Emission Models

Wei Lei, Xiaoliang Ma* and Hui Chen

Abstract—**In order to assess environmental impacts of local traffic flow, a two-stage parameter tuning approach is proposed for recalibration of the Comprehensive Modal Emission Model (CMEM) using on-road emission measurements collected in Chinese cities. Based on the procedure comprising of grid search and nonlinear simplex optimization, the fuel- and emission-related parameters in the model are estimated to minimize the Mean Square Error (MSE) between model outputs and real measurements. In addition, a regression-based emission model is calibrated using the same data samples to compare performance. It is shown from the numerical results that the tuning process is able of improving the model prediction accuracy, especially concerning the CO emission, when comparing with the original CMEM model and the regression-based model. In addition, the emission models are, after the tuning process, applied together with a traffic simulation model to evaluate dynamic environmental effects of traffic in a case study.**

I. Introduction

The continuous increase of motor vehicles in cities worldwide has led to serious traffic-induced air pollution, a big challenge for urban transport planning and management. To estimate effects of traffic flow, in terms of emission and energy usage, and devise corresponding traffic management strategies, researchers have developed many emission and fuel consumption models, including the aggregated models such as MOBILE6 [1], ARTEMIS [2] and MOVES [3] as well as the micro-scale models, also called dynamic models, such as the CMEM [4], VT-Micro [5] and EMIT [6]. With recent emphasis on dynamic environmental impacts in operational transport projects, the micro-scale models have attracted attentions. In particular, they have been frequently used together with microscopic traffic simulation models for environmental impacts analysis of road traffic [7] [8].

Among all dynamic emission models, the CMEM model, first developed at the University of California at Riverside, has gained its popularity as it incorporates a load-based modal approach and is built upon large amount of emission data samples collected by both dynamometer and on-road tests through the US National Cooperative Highway Research Program (NCHRP). In general, the model calculates tailpipe emissions based on different modules, each of which requires various parameters as inputs. A total of 55 parameters are adopted to characterize tailpipe emissions of each vehicle category/technology. Some of the parameters are determined from measurements whereas the others are obtained based on regression analysis [9]. Although the model has been reported to be successfully applied in transportation projects in US, one key obstacle for the model application is that the complexity and its implementation as a computing program make it difficult to be recalibrated for other countries or regions even if local emission data is available.

In this study, our research focus is on estimation of the CMEM model by tuning essential parameters for various emission factors (HC, CO and NO_x) when second-by-second tailpipe emission measurement data are collected using the OBS-2200, a portable emission measurement system (PEMS), from 28 in-use light-duty vehicles in Beijing. The recruited test vehicles are divided into two categories, namely LDV4 and LDV6, according to the vehicle classification criteria in the CMEM model. The model for each category is estimated separately. In addition, a regression-based model is calibrated using the same data samples for comparison purposes. Finally, both the CMEM and regression-based models are applied in a case study on environmental impact analysis of a signalized intersection where local traffic under different demands is generated from microscopic simulations.

II. Model Tuning

A. Model analysis

The CMEM model is a physical power-demand emission model based on a parameterized analytical representation of emissions production. The emission process is broken down into six modules: 1) engine power demand; 2) engine speed; 3) fuel/air ratio; 4) fuel-rate; 5) engine-out emissions; and 6) catalyst pass fraction. Modules 1) through 4) serve to calculate fuel use rate (*FR*). Module 5) is used to calculate engine-out (*EO*) emissions based on *FR*. Module 6) can estimate catalyst pass fraction (*CPF*), which is defined as the ratio of tailpipe (*TP*) to *EO* emissions. Fig.1 shows the general structure of the CMEM model. The basic idea of the CMEM model for computing vehicle emissions can be briefly described as follows: first of all, it calculates *FR* by some engine operating parameters, e.g. engine power, engine speed, fuel/air ratio etc.; secondly, *EO* emissions are modeled

Wei Lei is a PhD student with Intelligent Transportation System Centre (ITSC), Wuhan University of Technology (WHUT), China; he is currently an exchange PhD student in KTH, Sweden.

Xiaoliang Ma Ph.D. is a senior researcher with the Centre for Traffic Research (CTR), Royal Institute of Technology (KTH), Teknikringen 72, Stockholm, 10044, Sweden.

*Corresponding Author, Phone: +46 8 7908426 Email: liang@kth.se.

Hui Chen Ph.D. is a professor with the Centre of System Simulation and Control, Wuhan University of Technology (WHUT), China.

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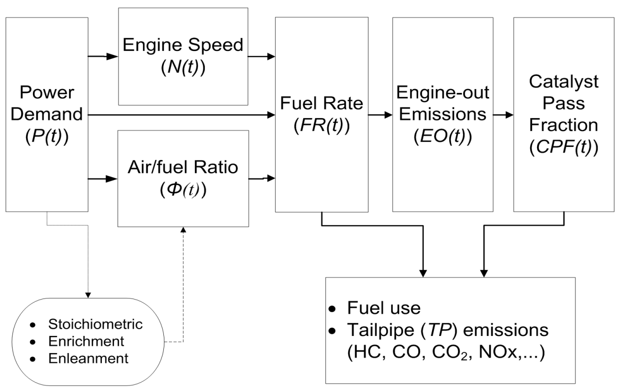

Fig.1 The general structure of the CMEM model and key parameters.

as a mathematical function of *FR* in the engine-out emission module; finally, *TP* emissions are computed as the product of *EO* emissions and *CPF*. Four operating conditions i.e. cold start, stoichiometric, enrichment and enleanment conditions, are considered in the CMEM model. In our study cold-start is not considered because our measurements were collected under hot-stabilized operation condition.

Before presenting the tuning process, it is necessary to get to know some details of the model, especially the principles of the fuel-rate module, engine-out emission module, and catalyst pass fraction module.

1) The fuel-rate module

The *FR* model is mathematically represented by:

$$FR(t)=\begin{cases}\phi(t)\cdot(K(t)\cdot N(t)\cdot V+P(t)/\eta)/44 & \text{for } P>0\\ K_{idle}\cdot N_{idle}\cdot V & \text{for } P=0\end{cases} \tag{1}$$

where t is time in second; $FR(t)$ is instantaneous fuel rate; $P(t)$ is engine power; $K(t)$ is engine friction factor, and K_{idle} is engine friction factor during engine idling; $N(t)$ is engine speed, and N_{idle} is idling engine speed; V is engine displacement; η is a measure of indicated efficiency (approximately equals 0.4). $\Phi(t)$ is fuel/air equivalence ratio.

Engine power $P(t)$ is modeled by:

$$P(t)=P_{acc}(t)+P_{tract}(t)/\varepsilon \tag{2}$$

where P_{tract} is the tractive power requirement; P_{acc} is the engine power demand associated with accessories operation; ε is vehicle drivetrain efficiency, which can be approximated by speed and specific power (SP):

$$\varepsilon=\begin{cases}\varepsilon_1 & \\ \varepsilon_1\cdot[1-\varepsilon_2(1-v/30)^2] & a>0,\ v<30\text{mph}\\ \varepsilon_1\cdot[1-\varepsilon_3(SP/100-1)^2] & SP>100\text{mph}^2/s\end{cases} \tag{3}$$

where ε_1 is the maximum drivetrain efficiency; ε_2 and ε_3 are two coefficients respectively for low speed driving and high-power driving; a and v are vehicle acceleration (mph/s) and speed (mph) respectively. In [9], ε_1 is a significant parameter that affects $FR(t)$. The value of ε_2 is normally fixed whereas ε_3 shows little impact on $FR(t)$ in our sensitivity tests.

Engine Friction Factor $K(t)$ is approximated as a function of engine speed $N(t)$ demonstrated by:

$$K(t)=K_0\cdot[1+(N(t)-33)^2\cdot 10^{-4}] \tag{4a}$$

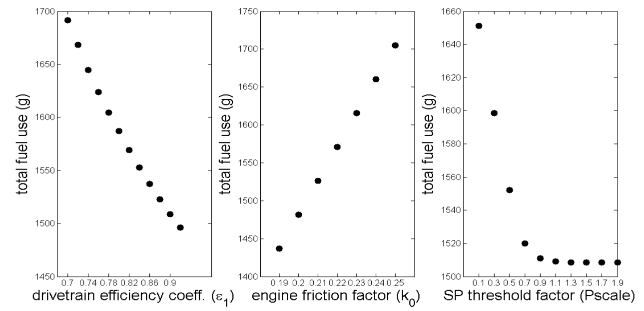

Fig.2 Effect of ε_1, K_0, and P_{scale} on total fuel consumption based on the FTP cycle and the default parameters of the vehicle category IV.

$$K_{idle}=1.5\cdot K_0 \tag{4b}$$

Obviously, K_0 is an important parameter that needs to be tuned for calculation of $FR(t)$.

The determination of fuel-air ratio $\Phi(t)$ can be divided into three regions: lean, stoichiometric, and rich. One critical issue related to estimation of $\Phi(t)$ is how to determine the threshold at which $\Phi(t)$ changes from stoichiometric to enrichment. In CMEM, enrichment is defined occurring when torque demand (Q) is larger than the corresponding enrichment threshold (Q_{th}) estimated by

$$Q_{th}=(P_{th}/0.7457)\cdot 5252/N \tag{5}$$

where P_{th} is the power enrichment threshold modeled by

$$P_{th}=P_{scale}\cdot(9.99\cdot 10^{-5}\cdot M\cdot SP_{\max}+Z_{drag})/\varepsilon_1 \tag{6}$$

where P_{scale} is a dimensionless scaling factor on power; SP_{max} $=192$ mph^2/s is the maximum FTP specific power; M is vehicle mass; Z_{drag} is the power demand to overcome air and tire drag. It can be easily seen from Eq. (5) and (6) that P_{scale} is another essential parameter that determines $FR(t)$.

Therefore, the variables ε_1, K_0, and P_{scale} are essential parameters for the fuel-rate module. Fig.2 shows the effects of ε_1, K_0, and P_{scale} on total fuel consumption based on the FTP cycle and the default parameters of vehicle category 4 defined in the CMEM model.

2) The engine-out emission module

In this module, *EO* emission is calculated under enleanment, stoichiometric, and enrichment conditions. However, the stoichiometric condition is most significant in determination of the EO emission whereas the other operations are negligible. The *EO* emissions of HC, CO, and NO_x under stoichiometric conditions are calculated by

$$EHC=\alpha_{HC}\cdot FR+\gamma_{HC} \tag{7a}$$

$$ECO=\alpha_{CO}\cdot FR \tag{7b}$$

$$ENO_x=\alpha_{NO1}\cdot(FR+FR_{NO1}) \tag{7c}$$

where *EHC, ECO*, and ENO_x are *EO* emission rates for HC, CO and NO_x; α_{HC}, α_{CO} and α_{NO1} are *EO* index coefficients for HC, CO and NO_x respectively; γ_{HC} is a residual term; FR_{NO1} is fuel rate threshold for *EO* NO_x emission. Thus, it is not difficult to tell that α_{HC}, α_{CO}, and α_{NO1} are the essential factors for calculation of *EO* emissions.

3) The catalyst pass fraction module

In the catalyst pass fraction module, the *CPF* for HC, CO, and NO_x under stoichiometric operation condition are demonstrated as follows:

TABLE I
CLASSIFICATION RESULTS OF ALL TEST VEHICLES

Vehicle category	Fuel delivery system	Emission Control Tech.	Mileage (mile)	Power-to-weight ratio	Number of test vehicles
LDV4	FI	3-way catalyst	>50,000	low (<0.039hp /lb)	17
LDV6	FI	3-way catalyst	<50,000	low (<0.039hp /lb)	11

$$CPF(HC) = 1 - G_{HC} \cdot \exp(-b_{HC} \cdot FR) \tag{8a}$$

$$CPF(CO) = 1 - G_{CO} \cdot \exp(-b_{CO} \cdot FR) \tag{8b}$$

$$CPF(NO) = 1 - G_{NO} \cdot (1 - b_{NO} \cdot ENO_x)/100 \tag{8c}$$

where G_{HC}, G_{CO}, and G_{NO} are the maximum catalyst efficiency for each gas normally measured in experiment; b_{HC}, b_{CO}, and b_{NO} are the key coefficients that can be adjusted for *CPF* calculation.

B. Vehicle classification

Classification of all test vehicles into appropriate vehicle categories is an important procedure for recalibrating the CMEM model. In our study, the 28 test vehicles are allocated to two main categories, LDV4 and LDV6, based on the classification criteria of CMEM. Table I shows the final results of vehicle classification. Furthermore, data from ten LDV4 vehicles and eight LDV6 vehicles are randomly chosen to build up composite calibration datasets for the corresponding vehicle classes.

C. Parameter tuning procedures

It is revealed from model analysis that the CMEM model calculates *FR*, *EO* and *TP* emissions through different stages. It is reasonable to sequentially calibrate parameters related to these modules. Nevertheless, on-road *EO* emissions are not measurable for the PEMS systems whereas *FR* and *TP* emission measurements can be obtained directly. Therefore, the *EO* emission-related parameters cannot be calibrated in a separate optimization stage. In this study, the *EO* and *TP* related parameters are estimated simultaneously in a single stage based on the *TP* emission measurements. Next, a two-stage tuning method is proposed for the calibration of the CMEM model using *FR* and *TP* emission measurements.

In the first stage, the essential parameters of the *FR* module, ε_1, K_0, and P_{scale}, are recalibrated by minimizing the MSE between modeled fuel rate and corresponding measurement i.e.

$$\min MSE = \sum_{t=1}^{N} (f(t) - \hat{f}(t))^2 / N \tag{9}$$

where $f(t)$ is the measured instantaneous fuel rate (g/s); $\hat{f}(t)$ is the prediction of fuel rate from the CMEM model (g/s); N is the size of composite data samples. To escape from numerical problems such as traps of local minima, an integration of numerical grid search (GS) and nonlinear simplex optimization (NSO) has been applied in the tuning process. The size of mesh grid for each parameter depends on the magnitude of the default value.

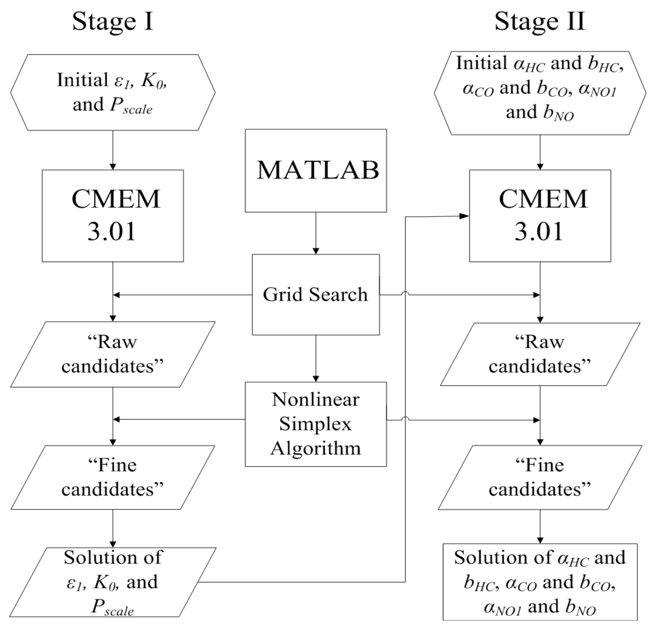

Fig.3 The flow chart of the two-stage tuning method for the CMEM model.

The NSO algorithm [10] is one of the most widely used optimization methods without computation of gradient information. The GS procedure is referred to "raw search", serving to find some good "candidates" of ε_1, K_0, and P_{scale}. Furthermore, these "raw candidates" will be taken as starting points. A "fine search" by running the NSO algorithm from "raw candidates" will lead to "fine candidates", among which the parameters with the least MSE will be the final solution.

In the second stage, the fuel-related parameters ε_1, K_0, and P_{scale} calibrated in the first stage will be fixed. The parameters α_{HC}, b_{HC}, α_{CO}, b_{CO}, α_{NO} and b_{NO} will be re-estimated respectively for prediction of *TP* emissions, i.e. HC, CO and NO_x, by minimizing MSE between emission model outputs and measurements i.e.

$$\min MSE = \sum_{t=1}^{N} (e(t) - \hat{e}(t))^2 / N \tag{10}$$

where $e(t)$ is the measured *TP* emission (g/s); $\hat{e}(t)$ is the predictions of *TP* emission from the CMEM model (g/s). Similarly as in the first stage, a combination of numerical grid search and nonlinear simplex algorithm are used to find "raw candidates" and then "fine candidates", and finally the best "find candidate" (with the lowest MSE) will be final solution. Fig.3 shows the general procedure sequences of this two-stage tuning method.

D. Results

The calibration procedure described has been implemented in the MATLAB environment in our study. The main issue makes the tuning process uncommon is that the evaluation of the optimization objective function requires frequent runs of the CMEM software, which has a command-line interface for both UNIX and DOS systems. Since the training dataset is large and the CMEM runs need extensive CPU and I/O operations, the whole numerical optimization is a rather expensive computing procedure.

TABLE II
DEFAULT AND CALIBRATED MODEL PARAMETER VALUES
(a) FUEL RATE

Class	Default			Calibrated		
	ε_1	K_0	P_{scale}	ε_1	K_0	P_{scale}
LDV4	0.9004	0.206	1.3125	0.8947	0.1984	1.9580
LDV6	0.8889	0.222	1.1160	0.9278	0.1993	1.6773

(b) HC EMISSION

Class	Sample size	Default			Calibrated		
		a_{HC}	b_{HC}	MSE	a_{HC}	b_{HC}	MSE
LDV4	20295	0.0149	0.0871	3.495e-5	0.0069	0.5517	3.037e-5
LDV6	19733	0.0112	0.0445	1.352e-5	0.0051	0.1874	1.211e-5

(c) CO EMISSION

Class	Sample size	Default			Calibrated		
		a_{CO}	b_{CO}	MSE	a_{CO}	b_{CO}	MSE
LDV4	20295	0.1205	0.2957	0.1403	0.1540	3.7353	0.1299
LDV6	19733	0.0968	0.1470	0.0286	0.1019	3.6526	0.0270

(d) NO_x EMISSION

Class	Sample size	Default			Calibrated		
		a_{NO1}	b_{NO}	MSE	a_{NO1}	b_{NO}	MSE
LDV4	20295	0.0293	1.7594	2.041e-4	0.0527	2.0179	1.843e-4
LDV6	19733	0.0365	1.0124	3.023e-5	0.0215	3.0011	2.889e-5

In the Table II (a), both default and calibrated results for the fuel-related parameters ε_1, K_0, and P_{scale} are presented. According to the values of MSE, the model with modified fuel-related parameters can significantly reduce the prediction errors. In the Table II (b)-(d), the tuned emission-related coefficients α_{HC}, b_{HC}, α_{CO}, b_{CO}, α_{NO1} and b_{NO} are presented in comparison with the default values. Meanwhile, it is not difficult to tell from the MSE values that the recalibrated parameters achieve significant improvement in performance, comparing to the default parameters.

III. MODEL VALIDATION

After recalibration of the CMEM model using the training datasets randomly assigned from real emission measurement, validation is performed by comparing model prediction with the out-of-sample emission data. The out-of-sample data is composed of continuous emission time series data sets collected from different vehicles of the LDV4 and LDV6 classes. In addition, another dynamic emission model, the VT-Micro model, is also used in the calibration and validation processes to compare the performance with the CMEM model. The VT-Micro model adopts a simple regression-based approach and it can be represented by

$$MOE_e = \begin{cases} \exp(\sum_{i=0}^{3}\sum_{i=0}^{3}(L_{i,j}^{e} \times v^i \times a^j)) & \text{if } a \geq 0 \\ \exp(\sum_{i=0}^{3}\sum_{i=0}^{3}(M_{i,j}^{e} \times v^i \times a^j)) & \text{if } a < 0 \end{cases} \tag{11}$$

where MOE_e (g/s) is the tailpipe emission rate; i and j are powers for v and a, respectively; $L^e_{i,j}$ and $M^e_{i,j}$ are the regression model coefficients; v (km/h) and a (km/h/s) are vehicle speed and acceleration. A data transform by natural logarithm was adopted to avoid negative model outputs. The calibration of VT-Micro can be easily conducted through the multivariate linear regression process which has also been coded in MATLAB.

To evaluate the model performance, two widely used statistics indices, the Mean Absolute Percentage Error (MAPE) and the Root Mean Square Error (RMSE) were adopted here to evaluate the model performance. They are mathematically represented by

$$\text{MAPE} = (\sum_{k=1}^{N} |(\hat{y}_k - y_k) / y_k|) / N \tag{12}$$

$$\text{RMSE} = \sqrt{\sum_{k=1}^{N} (\hat{y}_k - y_k)^2 / N} \tag{13}$$

where y_i is measurement (g/s), $\hat{y}_i$ is the CMEM predictions (g/s), and N is the size of composite data samples.

A comparison of the validation results of the default and fine-tuned CMEM model as well as the VT-Micro model is listed in Table III in terms of the two statistics measures described above. It can be seen from the table that the prediction performance of the tuned CMEM model shows an improvement over the CMEM model with default parameters. Meanwhile, it gives better performance than the VT-Micro model, especially concerning the CO and HC emissions.

In Fig.4, example profiles of the second-by-second emission predictions are demonstrated for the CMEM model with both default and well-tuned parameters as well as the VT-Micro model. It is not difficult to identify from the picture that the CMEM model with default coefficients cannot really capture the trends of real-world emissions especially when there are sudden fluctuations. In general, it makes considerable underestimation for all pollutants in comparison to the measurements probably because emissions of in-use vehicles in China produce more pollution than their counterparts in US. However, with the proposed fine-tuning process, the CMEM model show improved performance in capturing trends of the time series even though it tends to overestimates emissions during low emission profiles. Therefore, the CMEM model with recalibrated parameters is better suited for assessing environmental impacts of traffic in Chinese cities. Additionally, after regression against the measurement, the VT-Micro model shows a good performance in predicting emission levels. Although it is inferior in reflecting high emission values, the VT-Micro model seems to give better prediction performance in capturing low emission profiles than the CMEM model.

IV. MODEL APPLICATION

Finally, to evaluate the dynamic environmental impacts of local traffic, integration of microscopic traffic simulation with dynamic emission models has become a widely accepted approach [11] [12]. In this study, we model a traffic intersection in Wuhan (see Fig.5) using VISSIM, a popular microscopic traffic simulation tool. The software will be conducted to generate traffic states based on the current signal plan. In the network, a major traffic flow runs between Huacheng and Xudong (four lanes for each direction) whereas a minor flow goes between Tiejicun and Yujiatou (one lane for each direction). The signal control is based on a fixed stage strategy with a cycle length of 86 seconds.

TABLE III
COMPARISON OF OUT-OF-SAMPLE VALIDATION RESULTS

Vehicle number	Mean Absolute Percentage Error (%)								
	HC			CO			NO_x		
	CMEM (default)	CMEM (calibrated)	VT-Micro	CMEM (default)	CMEM (calibrated)	VT-Micro	CMEM (default)	CMEM (calibrated)	VT-Micro
LDV4-1	94.0	84.2	86.5	83.3	52.8	60.2	89.5	82.1	76.3
LDV4-2	95.1	85.9	88.6	88.2	38.5	57.5	91.4	84.9	87.3
LDV6-1	88.9	79.1	77.3	90.6	62.8	71.1	93.3	88.6	85.7
LDV6-2	81.7	73.2	74.5	91.4	73.7	69.0	82.5	76.1	72.7

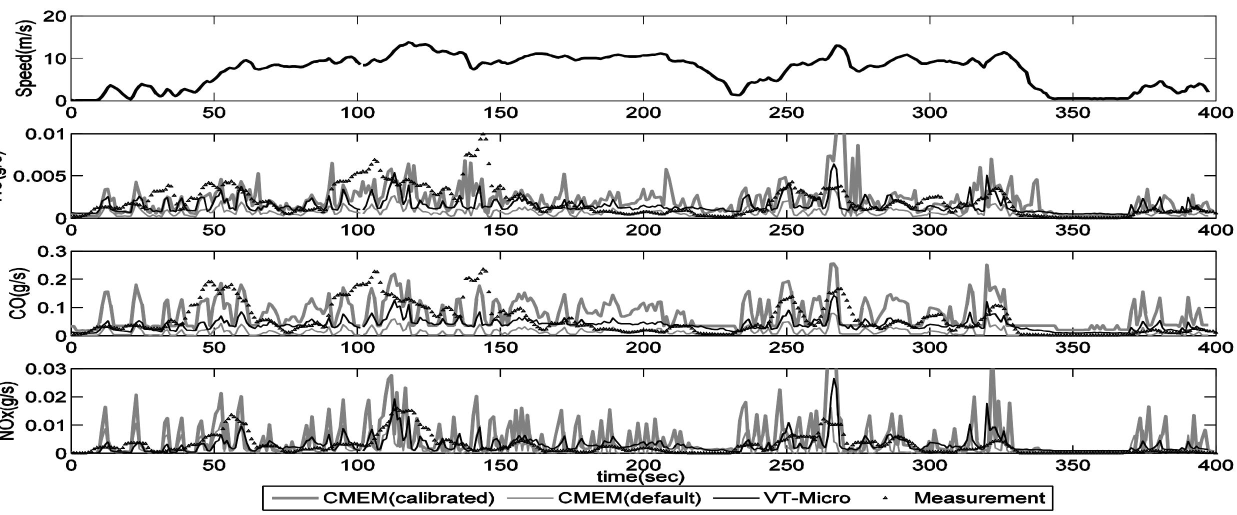

Fig. 4 A comparison of the second-by-second validation results from the default and tuned CMEM model as well as the VT-Micro model for LDV4.

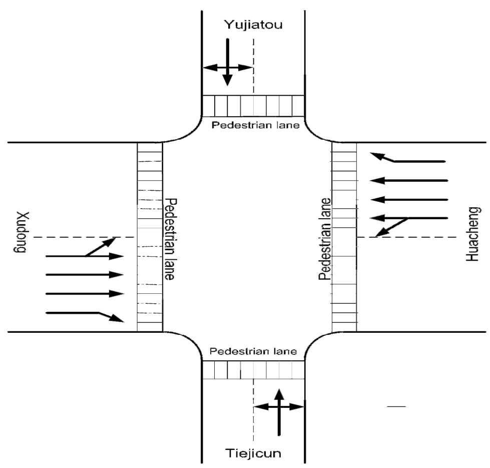

Fig. 5 The geometric layout of the signalized intersection

After coding the intersection in VISSIM, a calibration is conducted for basic driving behavior parameters, mainly the desired speed distribution and desired acceleration distribution, using traffic measurement. Since it is practically difficult to allocate the vehicles observed in real traffic according to the emission categories, we approximate vehicle composition with LDV4 vehicle (50%), LDV6 vehicle (40%), truck (8%), and bus (2%). To produce statistical significant results, the traffic simulation model has been run with replications until the statistical measures in terms of traffic flow rates are stabilized. The number of simulation replications is determined according to a so-called sequential procedure presented in [13].

In order to assess the environmental impacts under different traffic conditions, we set three levels of travel demand, i.e. low, medium, and high, for the simulation runs. This is simply done by multiplying the common demand on the four directions by a factor of 50% (low), 100% (medium), or 125% (high). The output of the VISSIM simulation model (speed and acceleration per second) is processed and then taken as inputs for the CMEM model with fine-tuned coefficients to estimate dynamic traffic emission. In addition, the default CMEM model and the VT-Micro model re-estimated by real emission are also used for the impact assessment to compare performance. In the study, only emissions from the LDV4 vehicles and LDV6 vehicles are calculated, although other types of vehicles are simulated in the road network.

In Fig.6, a comparison of dynamic average emission factors (g/km) per vehicle for the CMEM model with both default and tuned parameters as well as the VT-Micro model is presented under the low, medium and high demands. Similar as in the validation process, the CMEM model with default parameters always underestimate emission factors, especially for HC and CO. Meanwhile, the calibrated VT-Micro model gives similar prediction performance comparable to the fine-tuned CMEM model in most cases, which is in accordance with the validation result. In addition, with the increase of traffic demand, it is not difficult to observe that the HC and CO emission factors tend to increase as the average speed level drops. However, the average emission factor for NOx does not change much when traffic demand increases, which probably implies that NOx emission is less affected by the increase of stop-and-goes than the HC and CO emissions.

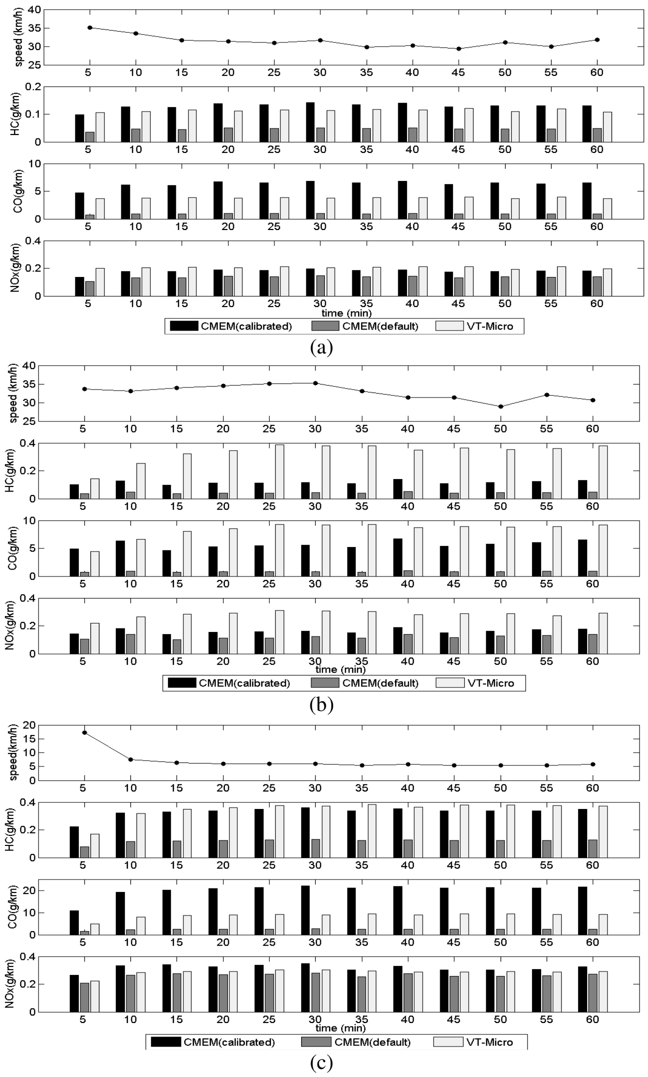

Fig. 6 Dynamic traffic emissions at the simulated intersection under conditions: a) low demand; b) medium demand; and c) high demand.

V. SUMMARY AND FUTURE WORK

In this study, we have proposed a two-stage tuning approach for calibrating the CMEM model based on the collected PEMS data from light duty vehicles running under the hot-stabilized condition. In the first stage, the fuel-rate module is calibrated upon fuel consumption measurement by tuning three critical parameters: ε_1, K_0, and P_{scale}. In the second stage, the engine-out emission module and the catalyst pass fraction module are calibrated by simultaneous tuning of three sets of model parameters, α_{HC}, b_{HC}, α_{CO}, b_{CO}, α_{NO1} and b_{NO} respectively. Both numerical grid search and nonlinear simplex algorithm play important roles in the optimization process. The validation results show that the prediction performance, in terms of MAPE and RMSE, of the CMEM model is significantly improved, especially for the CO emission. The tuning procedure has been conducted for two vehicle classes in the standard CMEM model: LDV4 and LDV6. In addition, the VT-Micro model, a regression-based approach, shows performance comparable to the fine-tuned CMEM model, although they cannot capture high emission values. At last the CMEM model with fine-tuned parameters is applied in a case study to assess the dynamic emissions factors at a signalized intersection with traffic states generated by microscopic traffic simulation. Different demands are applied to analyze the relation between congestion and emissions.

Many issues need to be investigated in our future study to improve the accuracy of dynamic emission models. For example, emission data under cold start conditions should be collected for estimating cold-start parameters. In addition, it is anticipated the scope of test vehicles should be extended to other categories, such as light-duty trucks (LDT), heavy-duty vehicles (HDV), and other high emitting vehicles.

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