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A Numerical Optimization Approach for Calibration of Dynamic Emission Models based on Aggregate Estimation of ARTEMIS

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***Abstract*—In this paper, we propose a numerical approach to calibrate dynamic emission models when on-road or in-lab instantaneous emission measurements are not fully available. Microscopic traffic simulation is applied to generate dynamic vehicle states in the second-by-second level. Using aggregate estimation of ARTEMIS as a standard reference, a numerical optimization scheme on the basis of a stochastic gradient approximation algorithm is applied to find optimal parameters for the dynamic emission model. The calibrated model has been validated on several road networks with traffic states generated by the same simulation model. The results show that with proper formulation of the optimization objective function the estimated dynamic emission model can reasonably capture the trends of online emissions of traffic fleets.**

I. INTRODUCTION

With rapid increase of travel demand on road networks, emission pollution of traffic flow has become a great concern worldwide. The emission gases include NO_x, CO, HC etc., which contribute to be a major source of urban air pollution and lead to deterioration of social environment and human health. Therefore, traffic emission is an important factor in decision making on sustainable transportation planning and management. To support this process, accurate estimation of vehicular emission plays critical roles for comparison of environmental impact of planning and management strategies. To fulfill the objectives, many traffic emission models have been developed. They can be classified into two main categories: aggregate and microscopic emission models.

Aggregate emission models, such as COPERT[1], ARTEMIS[2] and MOBILE [3], normally incorporate average speed, traffic fleet composition and vehicle travel distance as input factors and estimate emissions in levels of large networks or even regions. Among these models, ARTEMIS is one of the most widely known aggregate emission models jointly developed by European Union (EU) countries. The model is developed based on both on-road and in-lab emission measurements in Europe. It can be applied for estimation of both general and short-term dynamic emission quantities. The essential estimation procedure in the ARTEMIS model relies on a database program. However, to be compatible with previous approaches, the model provides alternative modules to calculate emissions directly based on the fleet composition and dynamic traffic states. In Sweden, experiments were conducted to compare on-road emission measurement with model estimation [4]. It was observed that the estimation of ARTEMIS is quite close to real measurements.

On the other hand, microscopic emission models normally take vehicle operating condition as inputs e.g. instantaneous speed, acceleration and engine states, and aim to give micro-scale vehicular emission estimation in the second-by-second level. Widely known microscopic emission models include CMEM [5], VT-Micro [6], and VSP models [7]. Recently, there is special attention on microscopic emission models since by integrating with traffic models they can be used in estimating short-term dynamic emission quantities. In order to assess environmental impacts of local traffic flow, one key question is how to calibrate the microscopic emission models. Usually, such calibration is based on the data collected by the chassis dynomometer or Portable Emissions Measurement System (PEMS). However, both the chassis dynamometer and PEMS systems are expensive equipments. Meanwhile, on-road measurement using PEMS is a rather delicate experiment. In addition, it is challenging to process the measured data. This paper demonstrates our recent research effort on developing a calibration approach for microscopic emission models given that dynamic emission measurement is not fully available. The main idea is to calibrate microscopic emission model according to the aggregate emission estimation of ARTEMIS at a rougher resolution on both time and space i.e. minimizing a statistical measure of the output difference between the summation of dynamic emissions of individual vehicles and the aggregate emission estimated by ARTEMIS for all road segments i.e.

$$\min \; L(\boldsymbol{\theta}) = N^{-1} \cdot \sum_{i=1}^{N} \left(\frac{M_i(\boldsymbol{\theta}) - A_i}{A_i}\right)^2 \qquad (1)$$

where $M_i(\boldsymbol{\theta})$ is the emission amount computed by microscopic emission models at time interval i; A_i is the emission estimated by ARTEMIS at the time interval; N is the number of time segments; $\boldsymbol{\theta}$ is the parameter vector of the microscopic emission model. Although such formulation is not uncommon, it misses a fact that most microscopic emission models have been calibrated by local on-road PEMS or chassis dynomometer test measurement. Although data used for calibration, e.g. collected in US, might be different from the European case, the model estimated from data may reflect a latent structure of dynamic emission of

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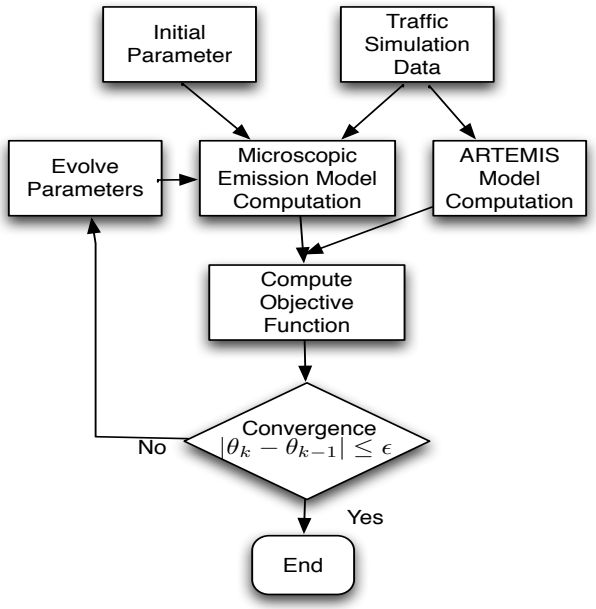

Fig. 1: Flow Chart of Calibration Process

traffic flow. Therefore, this information can be useful if it is incorporated in our calibration methodology. Therefore, we reformulate the objective function by taking into account of the difference of the estimated model parameters from their counterparts derived from the PEMS data i.e.

$$\min\ O(\boldsymbol{\theta}, \lambda) = L(\boldsymbol{\theta}) + \lambda \cdot P(\boldsymbol{\theta}) \quad (2)$$

$$P(\boldsymbol{\theta}) = \sum_{i=1}^{n} \left| \frac{\theta_i - \hat{\theta}_i}{\hat{\theta}_i} \right|^2 \quad (3)$$

where $O(\boldsymbol{\theta}, \lambda)$ is the new objective function and $P(\boldsymbol{\theta})$ is the penalty function representing the difference of the calibrated parameters from those obtained by estimation on PEMS data; λ a non-negative penalty weight, which has a significant impact on the optimization result; θ_i and $\hat{\theta}_i$ are the i_{th} element of the calibrated parameter vector $\boldsymbol{\theta}$ and the reference vector $\hat{\boldsymbol{\theta}}$ estimated by PEMS data respectively.

The remainder of the paper is organized into three parts. In the second section, the calibration methodology will be presented in details. In the third section, numerical results on calibration and validation are shown. At last, we will summarize the paper and point out future research directions.

II. Calibration Method

The process of calibration are presented in a flow chart in Fig.1. The iterative optimization process starts with an initial guess on the parameter vector $\boldsymbol{\theta}_0$. For each iteration k, emissions of the ARTEMIS and microscopic emission model will be estimated by corresponding computational modules with $\boldsymbol{\theta}_k$ using microscopic traffic states generated from a traffic simulation model. Then these emission outputs and the parameter vector $\boldsymbol{\theta}_k$ will be used to compute the objective function $O(\boldsymbol{\theta}_k, \lambda)$ in the equation (2). If a convergence standard is fulfilled, then $\boldsymbol{\theta}_k$ will be the final optimal solution and the searching process terminates; otherwise, the optimization process continues to the next iteration.

TABLE I: SPSA coefficients

Variable	Literature	Applied
a	$\frac{a}{A^\gamma} \cdot \lvert\hat{\mathbf{g}}_0\rvert \approx M_d$	$\frac{a}{A^\gamma} \cdot \lvert\hat{\mathbf{g}}_0\rvert \approx 0.1$
A	10% iteration	100
c	related to std. dev. of noise in $O(\theta, \lambda)$	0.01
α	1.0 or 0.602	0.602
γ	1/6 or 0.101	0.101

A. Model analysis

The VT-Micro model [6], a simple regression based microscopic emission model, will be used in the study. The model was developed by the Virginia Tech using PEMS data collection. The model has been demonstrated capable of estimating second-by-second vehicle emissions with a small margin of error in comparison to in-laboratory measurements. A natural logarithm transformation is used in model to avoid unreasonable negative results and enhance the model representativeness in the low-speed and/or low-acceleration regimes. Furthermore, it separates emission computations for acceleration and deceleration because of significant different emission profiles in the stages. Mathematically, the model is expressed by

$$MOE_e = \begin{cases} exp(\sum_{i=0}^{3} \sum_{j=0}^{3} (L_{i,j}^e \cdot v^i \cdot a^j)) & a \geq 0 \\ exp(\sum_{i=0}^{3} \sum_{j=0}^{3} (M_{i,j}^e \cdot v^i \cdot a^j)) & a < 0 \end{cases} \quad (4)$$

where MOE_e is the emission rate (g/s) of a pollutant specie e; e can be CO, HC and NO_x; v and a represents the instantaneous vehicle speed and acceleration separately; $L_{i,j}^e$ and $M_{i,j}^e$ are the model coefficients. Both $M_{i,j}^e$ and $L_{i,j}^e$ represents 16 parameters that need to be calibrated. The large dimension of the parameter vector makes the optimization problem quite challenging. In particular, the optimization objective involves calculation of aggregated emission using ARTEMIS in a large time interval in which a database query instead of analytical equation is applied. Therefore, the optimization procedure has to be based on gradient-free approaches or numerical approximation of gradients. In this study, we consider numerical approximation of gradient for solving the optimization problem.

B. SPSA

Among many numerical optimization methods, the Simultaneous Perturbation Stochastic Approximation (SPSA) approach [8] is a numerical scheme using first-order approximation of gradients of the optimization objective function. It shows obvious advantages over the traditional finite difference method (FDM) since it is computationally much more efficient especially for high-dimension multivariate optimization problems. This is mainly because only two evaluations

of the objective function per iteration are necessary in SPSA while the FDM algorithm needs $2 * n$ evaluations (n is the dimension of the parameter vector). On the other hand, the SPSA achieves the same level of accuracy as the FDM algorithm if the same number of iterations are performed.

The SPSA algorithm can be mathematically expressed as follows:

$$a_k = \frac{a}{(k+A)^\alpha} \quad (5)$$

$$c_k = \frac{c}{k^\gamma} \quad (6)$$

$$\boldsymbol{\theta}_k^+ = \boldsymbol{\theta}_k + c_k \cdot \Delta \quad (7)$$

$$\boldsymbol{\theta}_k^- = \boldsymbol{\theta}_k - c_k \cdot \Delta \quad (8)$$

$$\hat{\mathbf{g}}_k = \frac{O(\boldsymbol{\theta}_k^+, \lambda) - O(\boldsymbol{\theta}_k^-, \lambda)}{2 \cdot c_k \cdot \Delta} \quad (9)$$

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - a_k \cdot \hat{\mathbf{g}}_k \quad (10)$$

where a_k and c_k are gain sequences at step k; Δ is a n-dimension random perturbation vector fulfilling the Bernoulli distribution; $\hat{\mathbf{g}}_k$ is the estimated gradient vector at step k; a, A, α, γ, c are user-defined coefficients for the algorithm. In literature, an instruction on numerical analysis has been proposed [8] [9]:

- α, γ can be set as 0.602 and 0.101, respectively, the asymptotically optimal values of 1.0 and 1/6 may also be used.
- A is chosen such that it is much less than the maximum number of iterations allowed or expected, normally, takes 10% of maximum iteration number.
- Choose a such that $\frac{a}{A^\gamma}$ times the magnitude of elements in $\hat{\mathbf{g}}_0$ approaches smallest desired change in the first few iterations of θ, which requires some extra replications in early iterations.

According to our numerical tests, the SPSA algorithm is very sensitive to the coefficients in our optimization problem. With carefully numerical experiment according to the guidance above, we adopt the coefficients as listed in table I where M_d is the least desired change magnitude among the parameters in the early iterations.

C. Enhancements on SPSA

Although basic SPSA algorithm has proved to be powerful in solving optimization problems, enhancement on the algorithm is still necessary to make it more suitable for numerical analysis in our study.

1) Scaling: In the dynamic emission model, model parameters may variate from each other by a large scale. For example, in the estimation of the VT-Micro model [10], the coefficient with largest absolute value is -8.27978, and the smallest one is $3.98E-08$. In practice, this will bring numerical difficulties in optimization. According to literature [11], proper scaling parameters can dramatically improve the efficiency of SPSA. Moreover, transforming them into same regions can also improve the algorithm performance [12]. In this study, a simple scaling is implemented for each parameter to transfer them into a value between 1 and 10. When applying parameters for emission computation in SPSA, an inverse scaling has to be performed.

2) Gradient Average: In principle, averaging a few gradient estimations can improve the precision of the estimate of gradient information [13]. This is also emphasized by [14]. Thus in our implementation, we consider incorporating several independent SPSA gradient approximations at each iteration. That is, we replace the original calculation of $\hat{\mathbf{g}}_k$ in equation (5) by

$$\hat{\mathbf{g}}_k = r^{-1} \cdot \sum_{j=1}^{r} \hat{\mathbf{g}}_k^{(j)} \quad (11)$$

where r is the replication number of independent SPSA approximations. According to report in [9], the averaged gradients mechanism does not give significant performance augment in comparison with using standard SPSA algorithm when the sample size is small. Along with the increase of sample size, the advantage of gradient average becomes obvious. Even though a larger size of replications may produce better performance, the computation needs extra calculations on gradients per iteration. When the evaluation of the objective function is expensive, the computational cost on replications will increase dramatically. Thus, a trade-off has to be made between optimization speed and quality. In the implementation, r is normally set to 4 which gives empirically satisfactory results.

3) Multiple Initial Guesses: Although SPSA algorithm has shown to be powerful in literature, it still belongs to a gradient search algorithm. It is widely known that gradient-based approaches may suffer from existence of local optima. In this problem, we consider a classical mechnism by introducing multiple random initial guesses. Therefore, the smallest optimum will be our final solution after running the SPSA algorithm from each initial guess.

D. Calibration Procedure

Some crucial steps in the calibration is summarized as follows:

1) Step 1: Select proper vehicle category to be estimated according to the referenced ARTEMIS model; In ARTEMIS, vehicles are classified based on vehicle type and emission standards such as EURO I, EURO II etc. To formulate a complete dynamic emission model, it is necessary to estimate the microscopic model according to the aggregate emission estimation for each category of ARTEMIS;

2) Step 2: Determine a sensible range of the penalty weight λ in objective function. In principle, λ can be any positive value. When λ approaches zero, it tends to minimize $L(\boldsymbol{\theta})$. When λ is large, it tends to minimize $\lambda \cdot P(\boldsymbol{\theta})$. In our calibration process, it is not possible to test all penalty weights. Therefore it is necessary to justify a sensible range for λ so that the effects of smaller or larger penalty weights can be completely reflected;

3) Step 3: Determine appropriate SPSA coefficients for the problem. Based on preliminary numerical tests, proper coefficients for SPSA can be justified to achieve good performance in terms of convergence and calibration result;

4) Step 4: Perform the optimization procedure by SPSA. Multiple initial guesses are generated to run the SPSA algorithm and find a group of optimal parameter vectors for the microscopic emission model; the parameters resulted in the minimal value of the objective function are the solution to the optimization with the selected λ.

III. Numerical Experiments and Results

In our further numerical experiments, traffic data generated by a microscopic traffic model is applied for calibration and validation of the dynamic emission model. Two road networks are used for dynamic emission model calibration:

- A single one-way road segment with a length of 150 meters: traffic states generated by 10 minutes of simulation are applied for numerical test of the SPSA coefficients;
- A road network of large unsignalized intersection in Fig.2: traffic state data generated by simulation of 10 minutes and one hour is applied separately for calibration of dynamic emission model in accordance with aggregate estimate of ARTEMIS.

One group of referenced model parameters belongs to the vehicle class with close characteristics of the ARTEMIS category of passenger car Euro II standard. Thus the VT-Micro emission model is calibrated for this category. Because of the relative convenience of solving optimization problem on a small network, it is applied in numerical tests for determining appropriate coefficients for the SPSA algorithm. With coefficients settled for SPSA, the intersection network is used in a full calibration to find optimal parameters for the dynamic emission model. In particular, the parameter vector estimated from real on-road emission measurement [15] is adopted as the referenced parameter vector.

As it is important to analyze the effect of penalty weight λ on the result of the optimization problem, we have done extensive numerical tests and find that λ has a sensible range of $[10^{-6}, 10^{-4}]$. This means $\lambda < 10^{-6}$ or $\lambda > 10^{-4}$ does not give solution on optimization significantly different from $\lambda = 10^{-6}$ or $\lambda = 10^{-4}$ respectively. Thus in the rest of the study, λ values in the grid of $[10^{-6} : 10^{-6} : 10^{-4}]$ are applied in the model calibration.

With a fixed λ weight, the model calibration problem is solved by sampling N random initial guesses and then run the SPSA with each of those points. The parameters with smallest objective function will be considered as the solution with the fixed λ. By this process, we try to overcome potentially frequent existences of local minima. Although the increase of sampling points may make it more likely to find a global solution, the computational time might be amplified by a large scale. In our study, $N = 1000$ is selected to compromise the chance for a global solution and computation time.

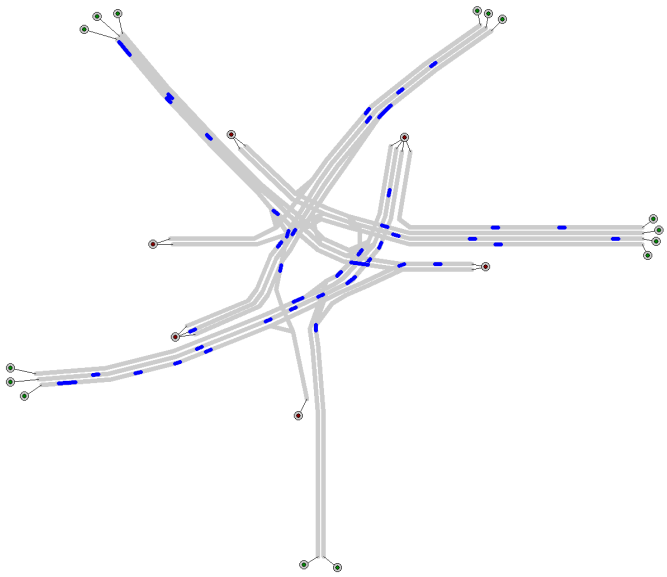

Fig. 2: The configuration of the Intersection network

The numerical study in this section is mainly focused on the emission gas of CO. However, the calibration for other two emission gases such as HC and NO_x can be performed in a same manner. With the CO emission, numerical results are presented with different perspectives:

1) The influence of λ in calibration. In order to analyze the influence of λ on the objective function and its components, an intermediate measure of $L(\boldsymbol{\theta})/O(\boldsymbol{\theta}, \lambda)$ is applied. From the left graph of Fig.3, we can see that λ is inversely proportion to $L(\boldsymbol{\theta})/O(\boldsymbol{\theta}, \lambda)$. In addition, both $O(\boldsymbol{\theta}, \lambda)$ and $\lambda \cdot P(\boldsymbol{\theta})$ are inversely proportional to $L(\boldsymbol{\theta})/O(\boldsymbol{\theta}, \lambda)$. This means with the increase of penalty weight λ, the objective function and the penalty component also raise up. However, it is difficult to conclude the effect of λ on $L(\boldsymbol{\theta})$. In particular, with λ tends to be zero, the optimization effort is more and more on $L(\boldsymbol{\theta})$. But this does not necessarily lead to an optimal $L(\boldsymbol{\theta})$ in comparison with other magnitude of λ.
2) Validation of dynamic emission estimation. Fig.4 shows cross-validation results when different λ e.g. $10^{-6}, 10^{-5}, 2 * 10^{-5}$, and $3 * 10^{-5}$ are applied in calibration. Different λ leads to different objective functions. Among these objective functions $\lambda = 10^{-6}$ results in the least value of $L(\boldsymbol{\theta})$ while $\lambda = 3 * 10^{-5}$ leads to the smallest value of the penalty function part $\lambda \cdot P(\boldsymbol{\theta})$. The calibration and validation are based on two separate 10-min simulations of the Intersection network of Fig.2 and the emission quantities are aggregated in a 30-second period. It is intuitive to see that the model performance is worst when λ is set toward zero. The cross-validation result indicates potential over-fitting risk when the optimization is too much emphasized on $L(\boldsymbol{\theta})$. A good result on fitness

TABLE II: Default coefficient of VTMicro (CO emissions for Passenger Car)

	Cons	Acc	Acc^2	Acc^3
Positive acceleration coefficients				
Cons	-5.0043	1.0743	-0.26622	0.017079
V	0.075802	-0.04131	0.01538	-0.001086
V^2	-0.00130	0.000940	-0.000303	1.8784e-5
V^3	9.414e-6	-3.7408e-6	9.696e-7	-3.689e-8
Negative acceleration coefficients				
Cons	-7.6691	-0.50039	-0.12064	-0.00652
V	0.11837	0.07740	0.01590	0.000772
V^2	-0.00303	-0.00213	-0.00048	-2.8211e-5
V^3	2.6123e-5	1.6473e-5	4.222e-6	3.0575e-7

TABLE III: Calibrated coefficient for VTMicro (CO for Passenger Car, EURO II)

	Cons	Acc	Acc^2	Acc^3
Positive acceleration coefficients				
Cons	-5.8247	4.1856	-0.68593	0.01685
V	0.0222	-0.0865	-2.49E-5	6.676E-6
V^2	-1.127E-4	-3.253E-5	1.261E-4	-8.193E-6
V^3	4.501E-5	2.392E-4	-2.381E-5	6.6138E-7
Negative acceleration coefficients				
Cons	-9.6370	-0.5897	-0.0624	-0.00029
V	0.1058	0.0161	7.319E-4	1.234E-6
V^2	-0.00643	0.0068	8.402E-5	-7.761E-6
V^3	2.612E-5	-1.448E-5	1.698E-6	-1.238E-7

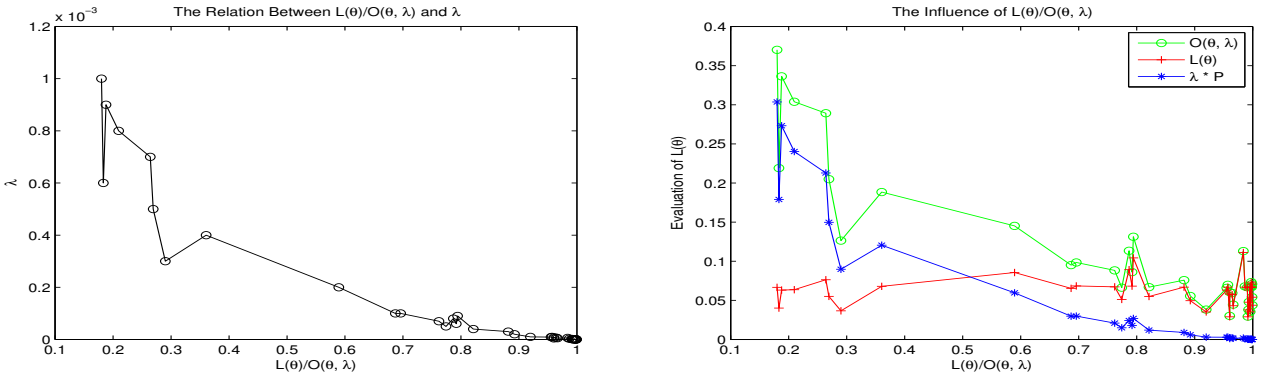

Fig. 3: Influence of $L(\theta)/O(\lambda, \theta)$ on λ and the objective function $L(\theta)$.

seems to be achieved when $\lambda = 2 * 10^{-5}$ is applied.

3) Calibrated coefficients of the VT-Micro model. Table II and III show the referenced and estimated parameters with $\lambda = 2 * 10^{-5}$. From the tables, it can be noticed that the calibrated parameters are in similar magnitude as the counterpart referenced parameters.
4) Validation on the total emission. Table IV shows validation results with respect to total emission on road networks based on the microscopic emission model re-estimated. Especially, emission from a large road network of Göteborg is analyzed with a 20-minutes traffic simulation data. From error percentage in the table, the model shows good prediction performance in general.

TABLE IV: Validation result on more road networks

Road Network	ARTEMIS(g)	VTMicro(g)	Diff Percent(%)
Intersection	1942.912	1856.897	4.42
Göteborg	6743.584	7329.682	8.69
Single road	119.396	125.227	4.88

IV. Summary and Further Research

This paper describes a numerical approach to calibrate microscopic emission model based on aggregate emission estimation. An aggregate emission model ARTEMIS developed by EU countries is applied for estimating aggregate emission quantities. Based on the aggregate estimation from ARTEMIS and referenced parameters estimated previously for a similar vehicle category, a microscopic emission model, VT-Micro, is calibrated by minimizing a joint objective combining

- a measure on the aggregate output difference between the two types of models;
- a measure on the Euclidean distance between the calibrated and referenced parameter vectors.

The standard SPSA algorithm with several critical enhancements is applied to solve the multivariate optimization problem. Extensive numerical experiment has been conducted to analyze the effect of penalty weights. A group of parameters for the VT-Micro model are proposed for the CO emission estimation of the "ARTEMIS EURO II passenger car" and validated by

- traffic data generated at the same road network for calibration and validation;
- traffic data on different road networks with various traffic flow characteristics.

From the validation result, the calibration approach shows its capacity in estimating dynamic vehicle emission model especially given the on-board emission measurement is not available.

In this study, only a self-developed microscopic simulation tool is applied to generate second-by-second traffic states. Currently, we extend our study in evaluating the methodology

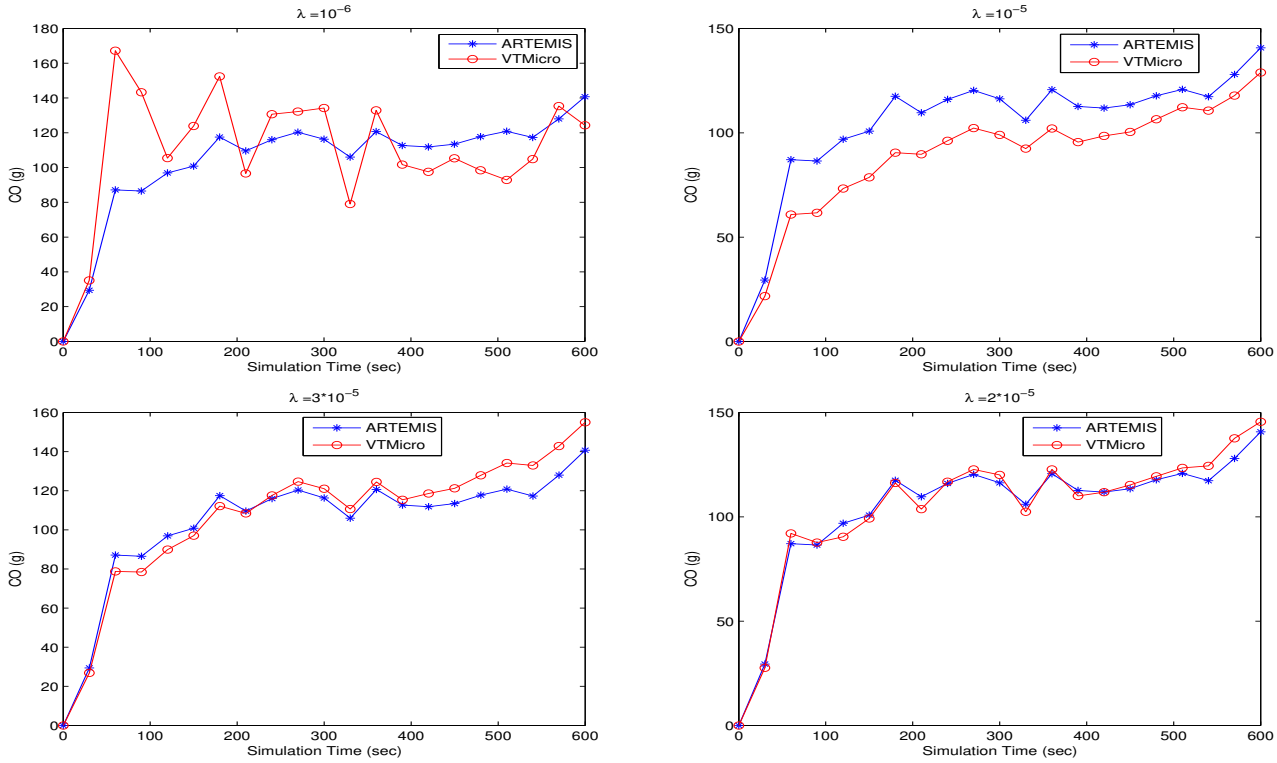

Fig. 4: Validation of dynamic emissions against ARTEMIS under different λ (30 seconds aggregate time)

with a commercial micro-simulation model. In addition, to apply the estimated microscopic emission model in real traffic impact management, parameters of different categories of vehicles have to be estimated by replicating the procedure proposed in this paper.

V. ACKNOWLEDGMENTS

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