Errors in model predictions of NO_x traffic emissions at road level – impacts of input data quality

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Abstract

This study investigates the effects of three important input variables on the prediction accuracy of average speed emission models. These variables are average speed, basic traffic composition (proportion of heavy-duty vehicles) and model choice (COPERT, QGEPA). Sensitivity analysis (conditional NRSA) is used to determine to what extent the possible range in these input variables influences model outcomes (i.e. NO_x emissions for road links), and hence accuracy. It is shown that maximum errors can be large (up to a factor of about 3.5). Moreover, they are a function of the level of congestion with errors generally increasing with the level of congestion. Traffic composition is shown to most strongly affect NO_x emissions (29-241%), followed by average speed (2-168%) and model choice (0-177%). The results were similar for arterial roads and freeways. These results can be used to provide direction to the collection of model input data, further model development and model application. The external errors found in this study appear to be of the same order of magnitude as internal errors that have been reported from (partial) road validation studies. This implies that in terms of further improvements of traffic emission modeling, focus should be on both the quality of input data (application) and the quality of the actual emission models (model development). Given the relevance of these results, it would be worthwhile to extend and refine this work by including other air pollutant and greenhouse gas emissions, and to use more complex traffic and emission models.

Keywords: accuracy, error, road traffic emission, modeling, sensitivity analysis, NO_x, congestion.

WIT Transactions on Ecology and the Environment, Vol 116, © 2008 WIT Press
www.witpress.com, ISSN 1743-3541 (on-line)
doi:10.2495/AIR080271

1 Introduction

Road traffic is an important global source of air pollution and greenhouse gas emissions and its significance is increasing. As emissions are a complex function of many variables, impacts and solutions are commonly evaluated using multidisciplinary combinations of transport, emissions and dispersion models at different scales, ranging from local road projects to entire urban or regional transport networks and even national or global emission inventories. There is an increasing need for valid and accurate modeling results as many national and local authorities are faced with difficulties in meeting air quality standards and other environmental policy targets (e.g. National Emission Ceilings). There is however limited knowledge about the reliability of calculated emissions from road traffic. Testing the overall accuracy of road traffic emission models (model validation) is difficult as "true" emission values are unknown and cannot practically be determined by measurement.

A review of current literature showed that available validation studies are restricted to specific models (or model versions) and specific situations. Some studies report on modeling results that are close to observed values, but most studies indicate that errors in emission predictions can be quite substantial. Two types of validation studies can be distinguished, namely area and road level studies:

- Validation of traffic emission models at area level is possible by using ambient air pollutant concentration data collected downwind of these areas. In the US and Europe, a number of studies have compared ambient air sampling data or emission fluxes to the results from combined emission and dispersion modeling [1–4]. For NO_x, differences varying between a factor (predicted/observed) of 1.0 [1] to 2.2 [4] have been found.
- Validation at road level is possible for specific traffic situations during relatively short time periods and they include tunnel studies (e.g. [5–9]), near-road air quality monitoring (e.g. [10–14]) and remote-sensing studies (e.g. [15–18]). For NO_x, differences varying between a factor (predicted/observed) of 0.4 [19] to 4.2 [20] have been reported.

The accuracy of emission model predictions is affected by both internal and external errors. Internal errors are associated with the emission model itself (e.g. emission factors). External errors are associated with the errors in model input variables. Road level validation studies commonly use measured input data for key variables such as vehicle kilometers travelled (VKT, i.e. traffic volume multiplied with road length), travel speeds and traffic composition (e.g. [21–23]). As a result, these studies tend to quantify internal errors. In contrast, area level validation studies tend to quantify both internal and external emission modeling errors, since the model predictions are often based on the combination of traffic, emission and dispersion models. Similarly, the use of ambient concentration data in road level validation studies often requires the use of dispersion models (e.g. [24, 25]). As a consequence, these studies validate the model chain and do not directly assess the accuracy of emission modeling. This complicates explanation of the discrepancies between ambient and modeled data. For instance, errors due to dispersion modeling may have offset or amplified emission modeling errors, but the magnitude and direction of these errors in the validation studies are unknown.

Natural variation in traffic emissions may also complicate emission model validation. For instance, emissions from a traffic stream may vary substantially due to random fluctuations in the number of high-emitters, the number of cold-start vehicles, etc. [26]. These factors cannot be controlled and their proportion in the traffic stream is often unknown. Moreover, fleet characteristics continuously change in time and this significantly affects emissions observations [27]. Thus, a model may have performed well a number of years ago, but this may no longer be the case for the current situation. Finally, model validation is not possible for situations for which there is a lack of empirical data (e.g. future years).

In conclusion, validation of road traffic emission models is difficult and only limited information is available. Further work to increase our understanding in model accuracy is thus required. The quality of emission model input data is obviously an important factor for the accuracy of emission predictions. In particular the impact of input data accuracy on emission predictions seems to be an area where further work would be valuable. Identification of the most important input data can be used to provide guidance and direction to data acquisition (e.g. new emission testing focused on critical aspects), further emission model development (e.g. focus efforts on critical aspects) and model application (e.g. focus efforts on collecting input data that are most relevant).

This study seeks to quantify maximum errors due to changes in selected important input variables on prediction accuracy of two selected models, and to assess its relevance. Although more complex emission models and input data can be used, as will be discussed later, this study presents a first-order assessment of possible emission prediction errors to assess the relevance of input data accuracy in relation to reported results from validation studies.

2 Methodology

In addition to model verification and model validation, a model itself can be used to examine uncertainty in the predictions of traffic emissions. Sensitivity analysis (SA) can be used for this purpose, as it is able to apportion prediction variability to specific inputs [28]. There are various SA methods [29], but mathematical SA is well-suited to quantitatively assess the sensitivity of a model output to the (possible) range of variation of an input. An important limitation of traditional SA is that only a small portion of the possible space of (combined) input values is investigated. To address this limitation, conditional one-at-a-time (OAT) nominal range sensitivity analysis (NRSA) will be used. In addition, graphical methods will be used to clarify the results where useful.

NRSA is applicable to deterministic models and evaluates the effect of model outputs exerted by individually varying only one of the model inputs (OAT), while holding all other inputs at constant values. Conditional NRSA conditions the sensitivity on specific sets of input values (scenarios). These inputs are varied across their entire range of plausible values (two extreme values), which are derived from either test data, expert judgment or literature review. For each scenario the impact on the model output is then evaluated. The sensitivity of the model to a scenario is represented as a positive or negative percentage change compared to the nominal situation:

$$S_{i,alt} = \frac{E_{alt,i} - E_{nom,i}}{E_{nom,i}} \times 100\%. \quad (1)$$

$E_{nom,i}$ and $E_{alt,i}$ are the predicted total traffic emissions (kg/h) for the nominal and alternative scenarios (minimum, maximum) for traffic situation *i*, respectively. Here traffic situation is defined in terms of road type (arterial, freeway) and level of congestion (V/C ratio). As will be discussed below, $E_{nom,i}$ and $E_{alt,i}$ are determined from computation of 21 different speed-congestion relationships and associated emission factors for two models (COPERT, QGEPA) and three basic traffic compositions (defined as proportion heavy duty vehicles). The maximum absolute error for traffic situation *i* (e_i) is then computed as:

$$e_i = MAX\left(\left| S_{i,\min} \right|, \left| S_{i,\max} \right| \right). \quad (2)$$

$S_{i,min}$ and $S_{i,max}$ represent the sensitivity for the predicted minimum and maximum scenarios.

2.1 Emission model selection

Many road traffic emission models exist around the world. Of these models, so-called average speed models are most commonly applied in practice [35]. Although these models are complex with respect to the number of model categories (e.g. vehicle classes, number of pollutants, emission types), the overall computation process is straight forward. Road link emissions are computed by multiplying a composite emission factor for a pollutant (g/km) with total vehicle kilometers of travel (VKT). The composite emission factor for a link presents the "mean traffic stream emission factor" and it is equal to the sum of the emission factors for all vehicle classes and the VKT-weighted proportion of these classes in the traffic stream. These emission factors are computed as a function of average link speed, but can also be corrected for other factors such as road gradient, air conditioning and ambient temperature. As a consequence, total link (and thus network) emissions, are determined by three basic variables, namely VKT, traffic composition and traffic conditions (congestion, road gradient, etc.).

Given their common use and their relative simplicity of application, two average speed emission models were selected for this study, namely COPERT III [30] and QGEPA 2002 [31]. COPERT is (and has been) extensively used for emission modeling in Europe and other parts of the world. QGEPA is an Australian model that has been developed using Australian test data in combination with information from other models such as MOBILE6 [32]. Using these two models, speed-dependent composite NO_x emission factors were computed for three basic traffic composition scenarios (0, 5 and 20% heavy duty vehicles). The results are shown in Figure 1.

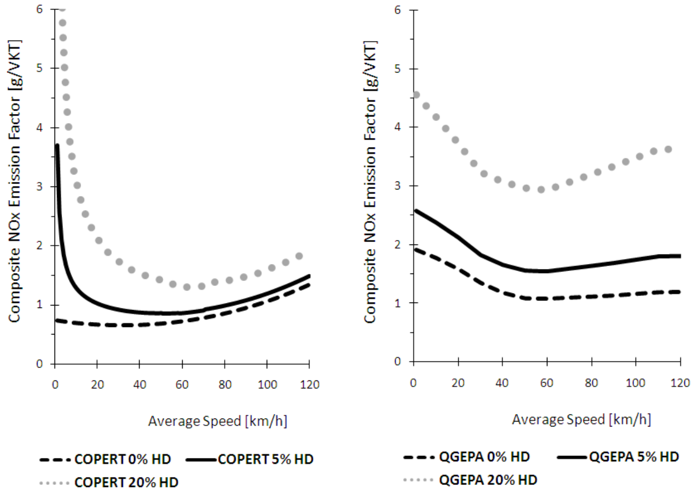

Figure 1: Composite emission factor curves for two emission models.

The composite emission factors were developed in different steps. Firstly, speed-dependent emission factors were computed for 32 vehicle classes, which are defined in terms of vehicle type (car, articulated truck, bus, etc.), fuel type (petrol, diesel, LPG) and technology type (legislative emission standards, type of catalyst, etc.). Secondly, these detailed emission factors were weighted using 2003 Brisbane fleet composition data that was taken from Smit [33]. Thirdly, the three basic traffic composition scenarios were developed by weighting the proportion of light-duty and heavy-duty vehicles accordingly.

2.2 Variable selection for simulation

This study will focus on three basic emission model variables, namely VKT, basic traffic composition (proportion of light-duty and heavy duty vehicles) and traffic conditions (level of congestion, expressed as volume-to-capacity ratio). It will also include, to some extent, internal errors by using two different emission models. The two models will reflect differences in emissions test data (e.g. due to country-specific differences in emission control technology and calibration of the engine and emission control systems), modeling approach and development (e.g. choice of driving cycles, statistical modeling), presence (or absence) of national inspection and maintenance programs and possibly systematic differences in measurement results between laboratories.

The use of traffic field data as input has a clear advantage in terms of accuracy when compared to modeled data. Moreover, data from traffic models may be the only source that can be (feasibly) used. In the simulations, the focus will be on variables for which field data are relatively scarce, i.e. traffic composition and average speed, but not VKT as will be discussed below.

2.2.1 Vehicle kilometers travelled

Efforts to improve the quality of emission model input data should focus on variables that have been shown to have a large effect on emission predictions. In this respect, the amount of travel (VKT) is a particularly important input variable as errors in VKT are proportionally propagated into emission predictions [33]. Therefore, particular attention should be directed at obtaining accurate information on traffic volumes. Compared to other input variables such as average speed and traffic composition, accurate VKT estimates for roads are relatively easy to obtain as traffic count data are commonly measured at various points (e.g. automatic detection, manual counting surveys) in road networks. Errors in VKT input, and thus emission prediction, are relatively small compared to traffic composition and average speed (as will be shown later), and this variable is therefore not included in the simulations.

2.2.2 Basic traffic composition

Basic vehicle classification data (e.g. light vehicle, heavy vehicle, perhaps a few heavy vehicle sub classes) is usually available for major roads. However, more comprehensive classification data, needed for emission estimation, is more difficult to obtain since they are usually collected by less common manual classified counting surveys or video image surveys [34]. For a detailed breakdown of (mean) traffic composition, additional data is commonly derived from other sources such as the National Bureau of Statistics and fleet turnover modeling. Following analysis of the Brisbane road network [32], a minimum, nominal and maximum value for the proportion of heavy-duty vehicles in the traffic stream of 0%, 5% and 20%, respectively, was determined for use in the sensitivity analysis.

2.2.3 Level of congestion

Average speed is needed as input to the selected emission models. Average speed, however, is not an adequate congestion indicator in certain speed intervals (between about 15 and 60 km/h) as the relationship between average speed and level of congestion is road-type specific [35]. As average speed models are based on emissions tests using driving cycles that typically run for about 10 minutes, the definition of average speed needs to be carefully considered when input speed data are collected. For instance, speed data measured at certain points in the network (e.g. by dual-loop detectors) can only be used when they represent average speeds for traffic conditions that are relatively homogeneous and stable over some distance of road (e.g. free-flow freeway driving away from on- and off ramps). On the other hand, average speeds measured on specific segments of road or entire routes using travel time studies [36] would align with the spatial resolution of driving cycles, but are only available to a limited extent.

There are several indicators for congestion but volume-to-capacity ratio (V/C) is a good one, since it combines the two principal causes of congestion (traffic demand and capacity) into one variable. Because of the availability of volume and capacity figures for network links and widespread acceptance by most transport agencies, V/C has been widely used as a fundamental congestion indicator [33]. To assess the relationship between prediction errors and congestion, a mathematical relationship between average speed and traffic conditions is needed and congestion functions can be used for this purpose. Congestion functions are used extensively in (macroscopic) traffic modeling and they are often calibrated using experimental data. They have evolved from relatively simple functions to more complex (sets of) equations by incorporating, for instance, traffic flow theory (e.g. queuing theory). The variables of traffic volume, road capacity and (mean) free-flow speed are fundamental to all congestion functions. The Akçelik function [37] is given as an example:

$$\bar{T}^* = \bar{T}^*_{ff} + 0.25\tau \left\{ \left({V}/{C} - 1 \right) + \sqrt{\left({V}/{C} - 1 \right)^2 + \frac{8 J_A {V}/{C}}{\tau C}} \right\} \tag{3}$$

where $\bar{T}^*$ represents mean unit travel time (min/km), which is (approximately) the reciprocal of average speed, $\bar{T}^*_{ff}$ represents free-flow unit travel time (min/km), V/C represents volume-to-capacity ratio, τ represents the time period over which traffic flow exceeds capacity (min), C is the road capacity (veh/h) and J_A is a delay parameter which is a function of road characteristics (e.g. signal density, signal coordination).

The posted speed limit on a road is often assumed to approximate the free-flow speed. Drivers tend to comply, on average, within certain margins above and below the speed limit in free-flowing traffic conditions. Therefore, the maximum mean speed in free-flow conditions is set to the speed limit plus 15 km/h for arterial roads and to the speed limit plus 25 km/h for freeways [38]. The minimum mean speed is set to 5 km/h below the speed limit for both arterials and freeways, and this can occur in specific conditions such as roads with strict radar control [35]. Using seven different congestion functions from a literature review [33] in combination with the three possible free-flow speeds (speed limit, minimum, maximum), an envelope of plausible mean speeds by level of congestion, including nominal speeds, has been computed for two basic road types (arterial, freeway).

The results are presented in figure 2 (next page). It shows that congestion has a large effect on average speed, and that congestion functions exhibit an inverted S-shape relationship between volume-to-capacity ratio and mean speed. The largest difference between congestion functions (50 km/h) occurs when traffic demand is near road capacity (V/C about unity).

For the sensitivity analysis is has been assumed that the range of average speed predictions by the different congestion functions represent the range of plausible values. The Akçelik function (eqn. 3) is the most complex function and its parameters have been calibrated using the aaSIDRA model, which is commonly used by traffic engineers around the world. Therefore this congestion function was taken to present the nominal situation as it provides probably the most accurate prediction of mean speed when the various functions are compared.

In the sensitivity analysis the three speed-congestion curves (minimum, nominal, maximum) for each road type, as depicted in figure 2, are used.

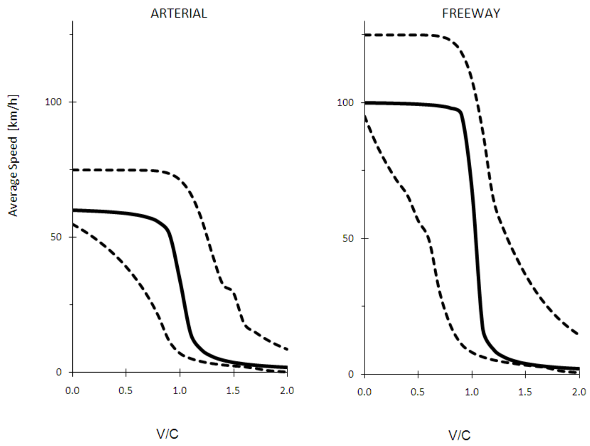

Figure 2: Plausible mean speed range and nominal speed by road type.

3 Results

Figure 3 (next page) presents the envelope of computed maximum absolute errors for average speed as a function of level of congestion and road type. It can be seen that errors can be quite substantial with a factor of up to 2.7 higher NO_x emissions compared to the nominal emissions value in freeway conditions, which was computed using the Akçelik function (eqn. 3). Errors are also dependent on congestion level, where relatively low errors (< about 30%) are computed for uncongested traffic conditions (V/C < 0.7). Errors peak when traffic flow approaches road capacity (V/C about 1), after which they are reduced but can still be substantial (< 60%). Although there are some differences (e.g. in maximum error value), road type does not seem to be an important factor in the relationship between prediction error and congestion level. The maximum values are consistently computed for one scenario, i.e. the COPERT model with 20% HDVs (denoted as COPERT/20%). However, the minimum values are computed for various scenarios depending on road type and congestion level, but include COPERT/0%, QGEPA/0% and QGEPA/20%. Interactions with traffic composition and model choice were observed in the simulations (not shown). For COPERT, errors generally increased with proportion HDVs; whereas, for QGEPA, errors generally decreased with proportion HDVs.

The extent of prediction error is dependent on two factors, i.e. the shape of the composite emissions curve and the difference in predicted average speeds. The location of the minimum value and the degree of non-linearity of both legs (left and right of the minimum value) of the parabolic curve are most relevant in this respect. For instance, figure 2 showed that for congested freeway conditions (V/C = 1) predicted average speeds can vary between 8 and 109 km/h with a nominal value of 68 km/h. Table 1 presents computed NO_x emission factors, sensitivities and maximum absolute errors for all scenarios (model, basic traffic composition). The strongly increasing and non-linear shape of the COPERT/20% composite emission factor curve at lower speeds, as was shown in Figure 1, results in a large increase in the emission factor for the nominal situation, and subsequently in a large sensitivity and error. In contrast, QGEPA/20% has substantially less non-linearity and also relatively large emission factors, which results in lower sensitivity and the lowest (maximum) error for this traffic situation.

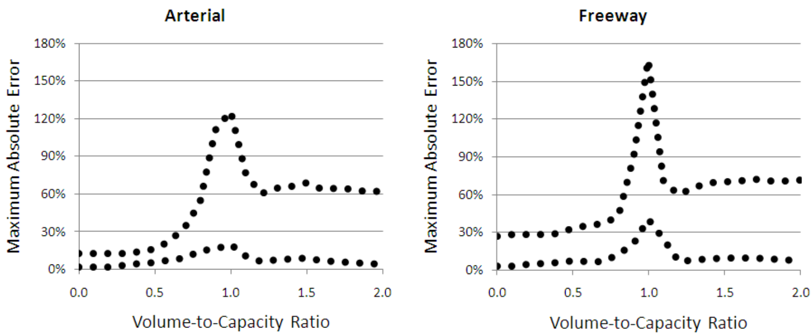

Figure 3: Envelope of maximum absolute errors for mean speed.

Table 1: Composite emissions factors, sensitivities and errors for traffic situation "Freeway, V/C = 1.0" for all six scenarios.

Average Speed	Composite NO_x Emission Factors QGEPA			Composite NO_x Emission Factors COPERT		
	0% HDV	5% HDV	20% HDV	0% HDV	5% HDV	20% HDV
(km/h)	(g/km)	(g/km)	(g/km)	(g/km)	(g/km)	(g/km)
8	1.80	2.42	4.26	0.70	1.40	3.49
68	1.09	1.58	3.04	0.76	0.90	1.31
109	1.19	1.79	3.61	1.18	1.32	1.72
$S_{i,min}$	65%	53%	40%	-9%	55%	167%
$S_{i,max}$	8%	13%	19%	55%	46%	32%
e_i	65%	53%	40%	55%	55%	167%

Figure 4 presents the envelope of computed maximum absolute errors for basic traffic composition as a function of level of congestion and road type. It can be seen that errors can be large with a factor of up to 3.4 higher NO_x emissions compared to the nominal emissions value (5% HDV) in both arterial freeway conditions. Errors are again dependent on congestion level, where smaller errors (50% to 100%) are computed for relatively uncongested traffic conditions (V/C < 0.7 for arterial, V/C < 1.0 for freeways). For more congested conditions, errors increase with congestion level. Road type does not seem to be an important factor in the relationship between prediction error and congestion level, although errors can be slightly higher in arterial driving conditions.

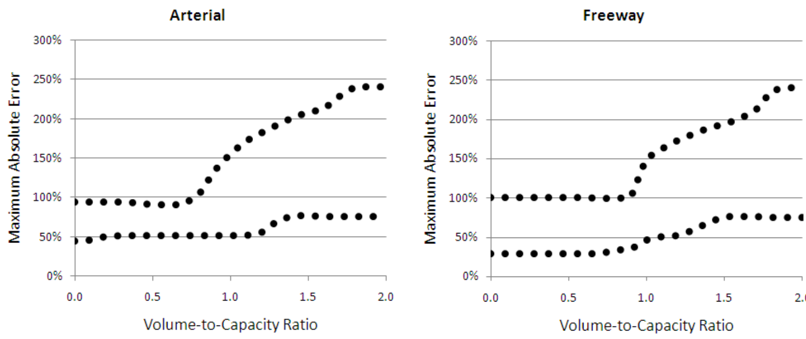

Figure 4: Envelope of maximum absolute errors for basic traffic composition.

Maximum error values are computed for QGEPA/max (maximum speed scenario) for V/C ratios less or equal to 0.8 (mean speeds higher than 55 km/h and 100 km/h for arterials and freeway, respectively) and for COPERT/max for V/C ratios larger than 0.8. In fact, error values computed for the QGEPA model are relatively stable and vary between 70% and 100%, where errors are reduced when congestion level increases. COPERT, on the other hand, is much more sensitive to congestion with errors starting from about 30-50% at free-flow conditions and then consistently increasing when V/C ratios exceed 0.5 (arterial) or 0.8 (freeway) up to errors between 120-240%.

As for average speed, the extent of prediction error is dependent on two factors, i.e. the shape of the composite emissions curve and the difference in predicted average speeds. In addition to the degree of non-linearity of the parabolic curve, the relative difference between composite emission factors for the nominal traffic composition and the minimum and maximum traffic compositions is relevant in this respect. Figure 1 shows that the relative difference between QGEPA/5% and QGEPA/20% is large and only varies slightly (75-100%) with congestion. In contrast, the relative difference between COPERT/5% and COPERT/20% is small at high speeds (30%) but consistently increases after that (up to 240%), having a larger difference than QGEPA at mean speeds below 35 km/h, which explains the increase in maximum error.

Figure 5 presents the envelope of computed maximum absolute errors for model choice as a function of level of congestion and road type. Although not an error in a strict scientific sense (we do not know which model is more accurate, so no baseline values were computed), this term is applied to be consistent with previous discussions. Nevertheless, model comparison provides a sense of possible internal errors that may arise from the arbitrary choices that were made and test data that were used in the development phase of the models.

It can be seen that errors can be large in highly congested conditions with a factor of up to 2.8 higher NO_x emissions in both arterial freeway conditions. Errors are to some extent dependent on congestion level, where relatively stable errors for arterials (approximately 30-60%) and freeways (approximately 10-

60%) occur until traffic conditions reach capacity. After this point, errors remain stable except for arterials where errors can be close to zero. Only at very congested conditions (V/C > 1.7, mean speeds < 25 km/h), maximum errors increase further to a maximum value of about 180%.

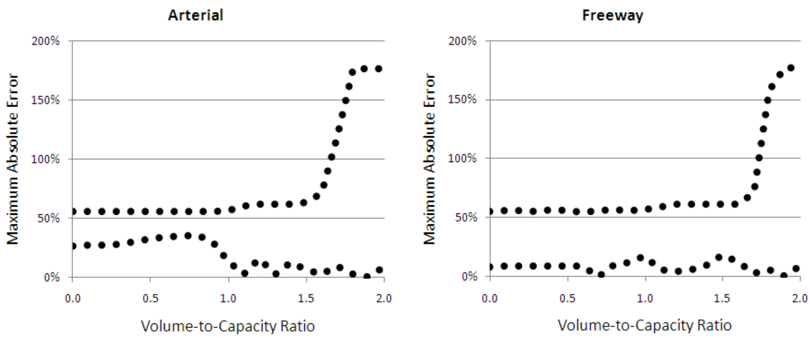

Figure 5: Envelope of maximum absolute errors for model choice.

The extent of prediction error is dependent on two factors, i.e. the shape of the two composite emissions curves for a particular basic traffic composition and the difference in predicted average speeds. The relative difference between composite emission factors for both models is clearly relevant in this respect. Comparison of COPERT and QGEPA composite emission factor curves (refer to figure 1) reveals that QGEPA generally predicts higher emission factors than COPERT and that for mean speeds smaller or larger than 36 km/h relative differences are largest for a basic traffic composition of 0% HDV or 20% HDV, respectively. For low speeds (< 25 km/h), where largest errors occur, the relative differences between QGEPA and COPERT composite emission factors vary between factors of 2.3 to 2.6, which explain the large error for these traffic situations.

4 Discussion and conclusions

This study has shown that emission predictions at road level are sensitive to possible errors in key input data consisting of traffic activity (VKT), mean speed and basic traffic composition, and model choice. The magnitude of possible errors for mean speed, traffic composition, and model choice were found to be dependent on level of congestion. It was also shown that interaction effects exist. The magnitude of these external errors can be substantial (up to a factor of 3.4). Importantly, they appear to be of the same order of magnitude as internal errors that have been reported from partial road validation studies. This implies that in terms of further improvements of traffic emission modeling, focus should be on both the quality of input data (application) and the quality of the actual emission models (model development).

One limitation of this study is its focus on NO_x. Given the results of this work, it seems valuable to examine the relationships between prediction errors and level of congestion for other air pollutants (e.g. PM_{10}, speciated hydrocarbons and greenhouse gas emissions).

There are some accuracy issues that have not been addressed in this work. A primary issue is that average speed models do not explicitly take driving dynamics into account [38]. This may introduce substantial errors in the emission predictions. For instance, NO_x emissions from an average Euro 3 petrol car could vary between about –80% to +200% around the COPERT estimate for an average speed of 60 km/h [39]. However, Smit *et al* [35] showed that driving dynamics are implicitly included as lower mean speeds in the real-world are naturally the result of, for example, more speed fluctuation and idle time.

Another issue is the use of a single (mean) speed for all vehicles on a section of road. In reality a distribution of average speeds would apply to a traffic stream. Smit *et al* [38] showed that this can potentially lead to substantial errors (up to 75%) in road link emissions. In order to address these issues, the work presented in this paper could be extended and refined by using more complex emissions models like VERSIT+ [39], PHEM [40] and DIVEM [41] and by using vehicle-specific driving behavior data in the simulation process, which could be sourced from microscopic simulation models [42].

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