CO_2-Based Response Emission Modelling

Norbert E. Ligterink, Stephan van Zyl and Uilke Stelwagen*

Sustainable Transport and Logistics Group, TNO, PO Box 49, 2600 AX Delft, The Netherlands, norbert.ligterink@tno.nl

Introduction

With a shift to on-road emission testing, both for European legislation (RDE Real Driving Emissions) as in the TNO in-house test program, emission modelling demands for a PEMS-based approach. In comparison to NEDC-based emission modelling, the emission variations in PEMS test results depend on many more aspects, such as emission control strategy, varying ambient conditions, and varying road loads, road surface, tyre pressure, wind, etc.. The need for a development in emission modelling is dictated by the new emission data. In part this might also be due to complex engine control strategies, which result in some cases in different pollutant emissions for apparently similar vehicle operation. (Roocroft 2014) To disentangle external circumstances and the intrinsic variation data should be presented and used in the normalized variables. The most common variable are the specific emissions, i.e., NO_x:CO_2 [g/g] ratio. In the simplest approximations the ratio is assumed constant. (Ligterink, 2012) This principle is central in the response modelling approach (Wiener 1949, Polderman 1998) : the variations in the pollutant emissions over time is peeled off as deviations, in all manners, from the fixed ratio of pollutant emissions and $CO_{2.}$

In the Netherlands VERSIT+ is used as emission model for air quality assessments. The philosophy has always been to test the vehicle as a whole, and to ensure sufficient data is collected for the statistical assessment for the average emissions and the variations. It relies, unlike most other emission models, on very little technical vehicle information. Hence, the analysis of emission data is central without bias introduced from assumptions on the vehicle and engine operation. In the same spirit the CO_2 response emission modelling, presented in this paper, is developed. The emission data, and the lowest error in the prediction, should determine the final model.

Vehicle emission rates are strongly related to the power of the vehicle. In this project, a two-stage approach for on-road emission modelling is proposed and developed. First, the CO_2 emission rate which is directly related to the (internal) is linked to physical aspects of the total power. Next, pollutant emissions are related to the CO_2 rate using response modelling. This two-stage approach is validated on a set of PEMS emission measurements comprising data of 10 different LD Euro-6 vehicles and more than 200 different test cycles.

Methodology

The emission modelling approach proposed in this paper consists of two stages. From driving behavior to CO_2 emissions, and from CO_2 emissions to pollutant emissions. Unlike velocity, acceleration, engine speed, etc. the CO_2 time series is a single signal. It can therefore be analyzed in more detail, establishing the delay effects such as from the turbo. The two stage approach reduces the statistical variation in each of the separate steps.

Stage 1: Estimation of the CO2 emission rate

The number of assumptions are very limited: A functional model is developed in which the CO_2 emission rate is linked to the physical aspects of the total power demand. The actual emission measurements are used as input to the model in order to determine the model parameters. The CO_2 emission of a vehicle is roughly equivalent to its demanded instantaneous engine power and can be expressed as a relation between CO_2 rate and power, where power is decomposed in velocity v and force F:

$$CO2 = v \bullet F,$$

or more specifically as:

$$CO2 = v \bullet [M\ a + F0 + F1v + F2\ v^2 + \ldots].$$

In this study, the equation is further expanded to include several degrees of velocity v, acceleration a and engine speeds RPM. The RPM is expressed as the difference in RPM with respect to a general formula based on vehicle velocity. The effective values for x_i are determined within the equation

$$CO2 = a\ v\ x_1 + a\ v^2 x_2 + v\ x_3 + v^2 x_4 + v^3 x_5 + v^4 x_6 + v^5 x_7 + RPM\ x_8 + RPM^2 x_9.$$

where CO_2 is the CO_2 emission rate [in g/s]. When taking into account that there are n time samples and m parameters, the same equation can be written in matrix notation y = A x. The effective values for parameters x_i are determined using a least squares error fit:

$$x = (A^T A)^{-1} A^T y.$$

Using a small amount of parameters will make the fit inaccurate, while using many parameters will increase the risk of overfitting. Separate parameters lose their significance as certain effects may reappear in different parameters as well. In this project, it was chosen for a model with good accuracy and robustness.

The variation in CO_2 can be explained for a large part in such a fit model. The unexplained variations can be investigated as the second-by-second difference between the post-diction and the measurement is available, which allows one to focus on part of the trip, such as road sections with deviations, and cold-start operation. The CO_2 emission rate is also used to obtain the typical load patterns of heavy-duty vehicles in the test program. Based on the road type, the engine power, and the total vehicle weight, the peak in the CO_2 rate, and the associated engine load, shifts forward or backward. Moreover, the high-load moments, for example of interest in PM emissions depends on all these factors in a complex combination.

Stage 2: Response modelling of pollutant emissions

The driving behaviour and conditions are less under control by on-road testing. The CO_2 rate is therefore a better proxy for the engine operation. Hence the modelling of pollutant emissions as a function of time-series CO_2 will provide a more robust emission model. The first part of the emission model is the instantaneous relation between CO_2 rate and the pollutant emission, e.g. NO_x:

$$NOx_{instananeous}[g/s] = X_1\ CO2[g/s] + X_2\ (CO2[g/s])^2 + \ldots$$

Where X_1 and X_2 are the parameters to be fitted, corresponding the proportional NOx and a disproportional increase in NO_x with CO_2 and engine power.

This provides already the global relation between fuel consumption and pollutant emissions, such as also measured in remote emission sensing programs, using the concentrations of gaseous components.

The second part of the emission response model is a generic response model, to account for delays, such as turbo, shifts in engine loads, etc.. It uses the signal op previous seconds to improve the relation between CO_2 and NO_x. Two standard parts to the response are a typical decrease with a linear rise and an increase in the NOx emission with the second-order variations:

$$NOx[g/s] = NOx^{instantaneous} + X^{response}*(CO2(t) - CO2(t-1)) + X^{transient}*(CO2(t) - 2\ CO2(t-1) + CO2(t-2))$$

Where $NOx^{instantaneous}$ is the nonlinear fit of the second-by-second signals. This is typically the only part covered in a standard emission model, like based on an engine map. In that case the load and RPM yield, via a look-up table, a value for both the CO_2 emission and the NO_x emission, fixing a direct link. The parameter of the response $X^{response}$ is typically negative, the parameter of the transient $X^{transient}$ also negative, indicating a more than proportional increase in NO_x emissions with a peak in the CO_2 emissions.

The options to generate such a response model for pollutant emissions of the basis of the CO_2 times series is manifold. The different terms in such a model are typically correlated. Hence, it is important to select terms in the pollutant response model which span as much of the relevant dependencies, without much correlation between the variables.

The two stages of the complete emission model: from driving behavior to pollutant emissions is visualized in Figure 1. In different stages of modelling the emission data is used to determine the model parameters.

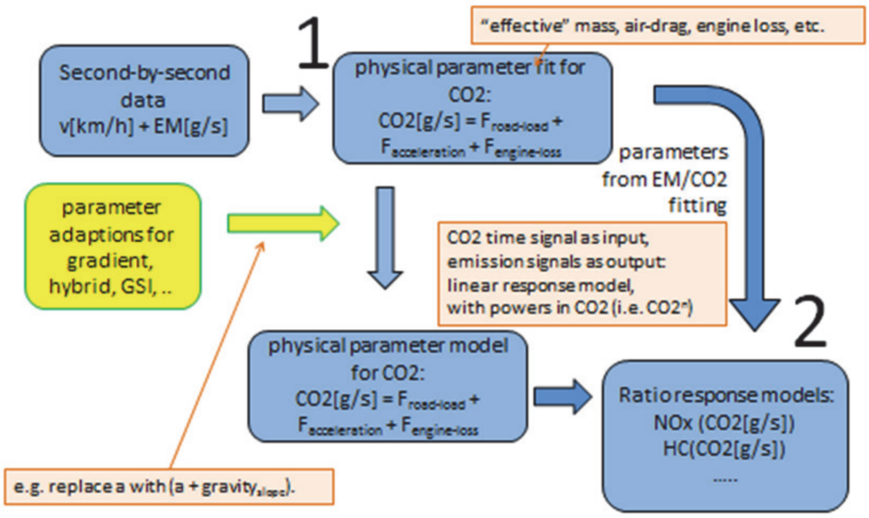

Figure 1: The general set-up of the RDE (Real Driving Emissions) CO_2-based response modelling of pollutant emissions. It allows for the study of the effects of road slopes, weight changes, and GSI as well.

Selecting the best CO_2 emission model

In order to optimize the model postdiction of CO_2, the number and size of model parameters were varied and tested for their performance. The performance of the models were tested on 218 independent PEMS measurements. The results yields a choice of model parameters in with good performance in terms of accuracy and robustness. In the following section, the estimation error between measured and modelled CO_2 rate, also referred to as QC_{err}, was taken as a measure for accuracy. The number of parameters were taken as a measure for robustness. The estimation error was defined as follows:

$$QCerr = \frac{\sqrt{\frac{\sum_1^n e^2}{n}}}{\frac{\sum_1^n CO_{2,meas}}{n}}$$

In test 1, the number of parameters were step-wise increased from 1 to 9 (see Table 1).

Table 1: Model configuration – Test 1: Model size choice

	av x_1	av^2 x_2	v x_3	v^2 x_4	v^3 x_5	v^4 x_6	v^5 x_7	RPM x_8	RPM^2 x_9
Model 1	1	0	0	0	0	0	0	0	0
Model 2	1	1	0	0	0	0	0	0	0
Model 3	1	1	1	0	0	0	0	0	0
Model 4	1	1	1	1	0	0	0	0	0
Model 5	1	1	1	1	1	0	0	0	0
Model 6	1	1	1	1	1	1	0	0	0
Model 7	1	1	1	1	1	1	1	0	0
Model 8	1	1	1	1	1	1	1	1	0
Model 9	1	1	1	1	1	1	1	1	1

The estimation error obtained for the different models and different PEMS measurements are shown in Figure 3. The estimation error has been normalized to the largest model, in order to see what the relative difference is in performance. The red striped line shows the average normalized estimation error The lower figure shows an enlarged view of the figure above.

As can be seen the estimation error reduces with the introduction of every parameter. For some parameters this reduction is only small. For example, adding parameters with higher degree orders has only marginal effect on the estimation error. This applies to the terms a*v, v and RPM alike. For other parameters, the reduction of the estimation error is more significant. A clear decrease in the slope is seen with the introduction of RPM and v^3.

The model results show that four parameters can achieve an estimation that is only 10% worse than the estimation with nine parameters. It seems that at least one of the terms a*v, v and RPM have to be included in the model to achieve this estimation, however the question remains which exponent of these terms achieves the best results.

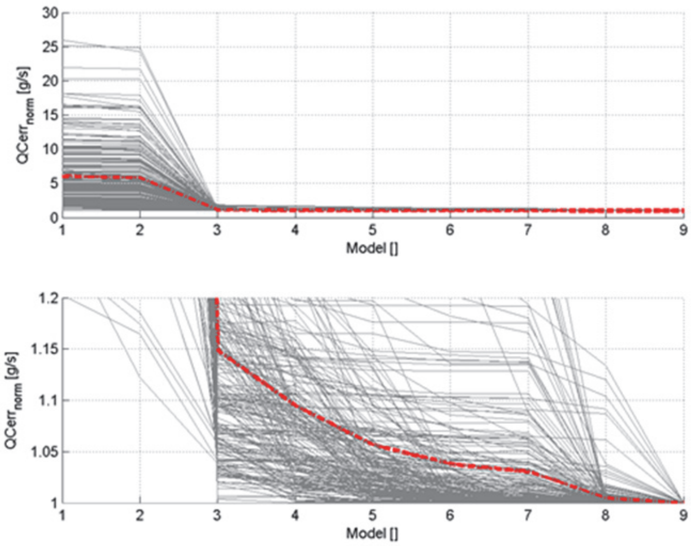

Figure 2: Test 1 – Normalized estimation error of different PEMS measurements and different models (grey) and average of normalized estimation error (red)

Based on the results shown above, another test was performed in order to determine the best parameter choice in terms of parameter exponents. For this purpose, the three terms a v, v and RPM were separately varied with higher exponent parameters such as a*v^{2}, v^2, v^3, v^4, v^5, RPM^2. The parameters of this model were varied independently in order to observe the effect on the estimation error, see Table 2.

Table 2: Model configuration – Test 2: Parameter choice

	av x_1	av^2 x_2	v x_3	v^2 x_4	v^3 x_5	v^4 x_6	v^5 x_7	RPM x_8	RPM^2 x_9
Model 1	1	0	1	0	0	0	0	1	0
Model 2	0	1	1	0	0	0	0	1	0
Model 3	1	0	0	1	0	0	0	1	0
Model 4	1	0	0	0	1	0	0	1	0
Model 5	1	0	0	0	0	1	0	1	0
Model 6	1	0	0	0	0	0	1	1	0
Model 7	1	0	1	0	0	0	0	0	1
Model 8	1	0	1	0	1	0	0	1	0
Model 9	1	1	1	1	1	1	1	1	1

The resulting average normalized estimation error of test 2 is shown in Figure 3. As shown, model 2 achieves on average a slightly lower estimation error than model 1. Effectively, a*v^2 x_2 therefore seems a better parameter choice than a v x_1, Also, model 7 achieves better results than model 1. This would imply that RPM^2 x_9 achieves better results than RPM x_8. With three parameters alone, the 10% barrier for the estimation error (as discussed above) cannot be penetrated. Only by adding another parameter, such as v^3 x_5 the estimation error is in the range of 10% of the 9 parameter model.

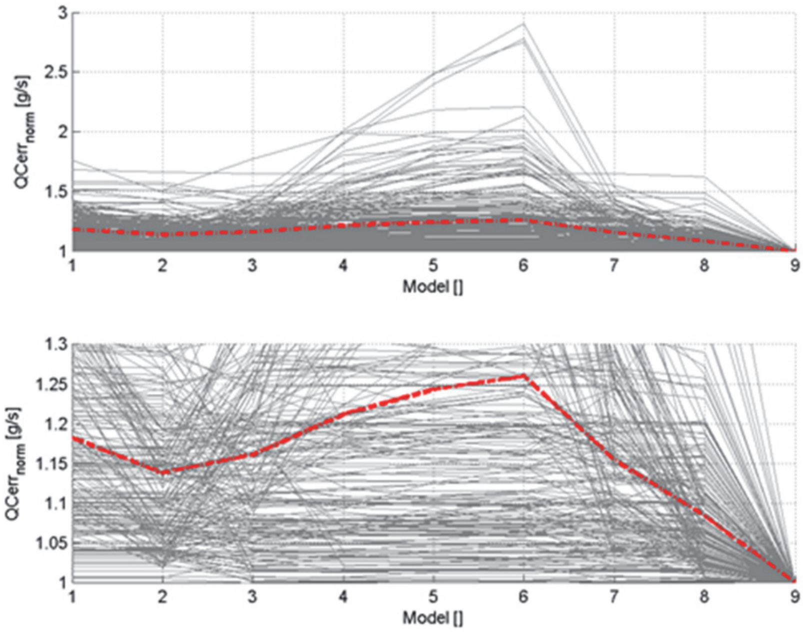

Figure 3: Test 2 – Normalized estimation error of different PEMS measurements and different models (grey) and average of normalized estimation error (red)

Since model 8 accounts for all physical measures tested and achieves good estimation accuracy with only four parameters, this model was selected for further modelling: CO2 = a v x_1 + v x_3 + v^3 x_5 + RPM x_8. (also see Table 3). Though parameters 2 (a*v^2 x_2) and 9 (RPM^2 x_9) achieve somewhat lower estimation errors, on average the difference is only low in comparison to parameters 1 (a v x_1) and 8 (RPM x_8).

Table 3: Choice of the final model

	a v x_1	av^2 x_2	v x_3	v^2 x_4	v^3 x_5	v^4 x_6	v^5 x_7	RPM x_8	RPM^2 x_9
Final Model	1	0	1	0	1	0	0	1	0

Below, two figures are shown with the results achieved with the final model. Both figures contain four subplots. From the top down, Figure 2 shows in the velocity profile of the PEMS driving cycle, the related CO_2 emission rate (measured and modelled), the estimation error rate and the estimated values for X_i. From the top down, Figure 4 shows the estimation error rate as well as the error biases dependent on the velocity, the acceleration and the CO_2 emission rate.

Figure 3 shows that the emission rate can be well modelled using a LSE fit and the model parameters chosen above. The respective error does not show specific systematic dependencies, however it can be seen that large CO_2 emission peaks are predicted less accurately. The lowest plot in Figure 2 shows the level of contribution of the single parameters to the model. As can be seen, RPM has a very important contribution to the model, whereas the contribution of a*v and v^3 are lower.

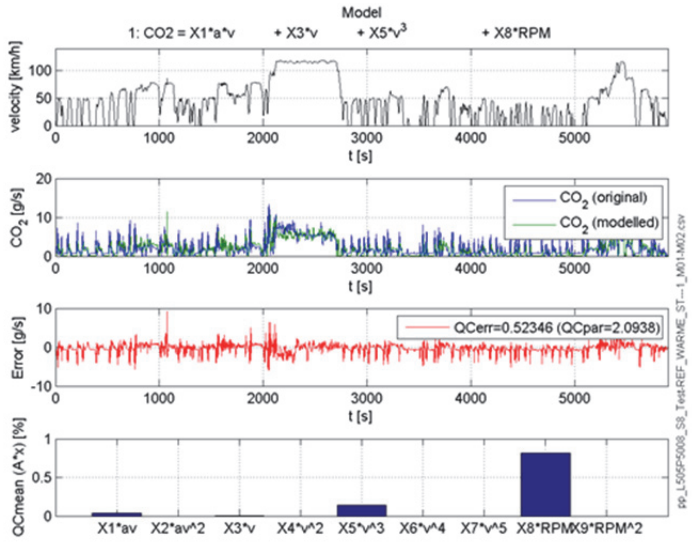

Figure 4: PEMS measurement: velocity profile (top), CO_2 emission rate (second), estimation error (third), parameter size (bottom).

Figure 3 and specifically the subplots 2 to 4 show that the bias of the error in dependency to model inputs like velocity, acceleration and CO_2 are low.

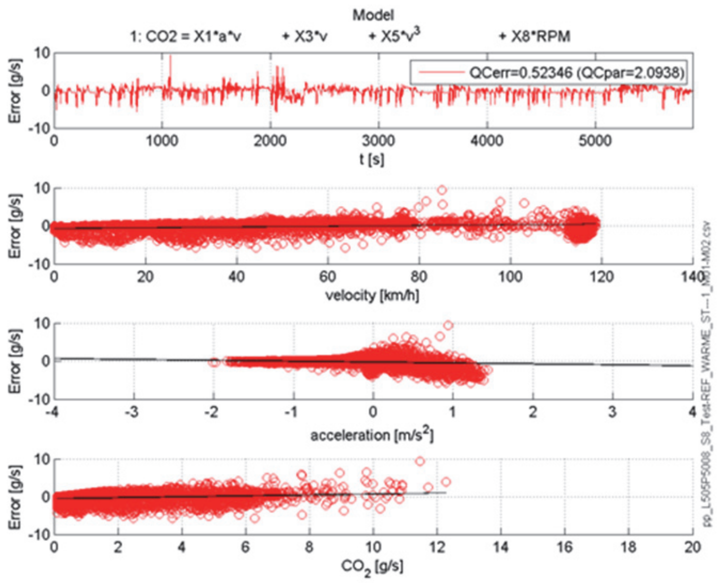

Figure 5: Estimation error: over time (top), with reference to velocity (second), acceleration (third) and CO2 emission rate (bottom)

Selecting the best pollutant emissions model

Currently, the most important pollutant emission is the NO_x from diesel passenger cars. Since the introduction of emission regulation it has not been under control. There is, despite even decreasing limits in the type approval, a very limited reduction of real-world NO_x emission since 1992. Hence, the focus is on this vehicle category. However, the approach is generic.

The CO_2 emissions, with its underlying physical principles, leads to similar emission dependencies over a wide range of vehicles and technologies. For pollutant emissions the situation is very different. The optimal choice of an emission model for pollutant emissions of certain vehicles and gaseous components may not fit other vehicles or pollutants. Hence the strategy, although based on extensive testing, must be more generic and based on first principles. These principles are designed to cover different aspects observed in pollutant emissions:

1. nonlinear effects (e.g. $NO_x[g/s] \sim (CO_2[g/s])^2$)
2. constant load effects (RPM increases but load remains the same)
3. delay effects (for example turbo speeding up and heating effects)
4. transient operation (variations outside optimization region of the engine)

In the response modelling these aspects are covered by different terms. The nonlinear terms are essential to yield a proper emission prediction. A linear-response emission model can only yield a prediction proportional with the CO_2 emission:

$$NOx_t = x_0\ CO2_t + x_1\ CO2_{t-1} + x_2\ CO2_{t-2} + x_3\ CO2_{t-3} + x_4\ CO2_{t-4} + \dots$$

This linear model yields a prediction of the NO_x emission over the total trip equal to the sum of x_i's times the sum CO_2. From the emission data, it is clear that with higher engine powers and CO_2 rates, the NO_x emissions increases disproportional in most cases, and the linear response is insufficient. (Ligterink, 2012)

With nonlinear terms the number of possibilities of a model increases exponentially. In many cases it generates a situation too complex to handle efficiently. Three aspects ensure appropriate control:

1. Linearity of the fitting procedure: the model is a sum of nonlinear terms, which can be fitted with least square error method.
2. Terms with some physical meaning, as the aspect mentioned above.
3. Orthogonal terms with limited correlations among them.

The first and second conditions have also been used the stage 1: the CO_2 emission model. Again the risk of overfitting is present here. The number of terms must be limited, to allow for a stable fitting process. A robust and complete model covering the different aspects is a fit with the following five terms:

- $CO2 = CO2_t$, to be used in the nonlinear fit of the instantaneous response: CO2 and $(CO2)^2$
- $\Delta CO2 = CO2_t - CO2_{t-1}$, the fast change orthogonal to the average (does not affect the sum emission, but shifts the emission in time)
- $CO2^2_{transient} = (CO2_t - 2\ CO2_{t-1} + CO2_{t-2})^2$ the rapid fluctuations in CO_2 rates, the second type of nonlinear term, which generates a deviation from the proportional result.
- $CO2_{delay} = CO2\ (CO2_\tau - CO2)$ the additional nonlinear term orthogonal to the instantaneous part $(CO2_{average})^2$.

The $CO2_\tau$ is the buffered CO_2 signal, with a response time τ:

$$CO2_\tau = ((\tau - 1)\ CO2_\tau + CO2)/\tau$$

It expresses the time-invariant average CO_2 rate over a time τ. Depending on the technology the appropriate response time τ will change. However, from driving behavior the typical transients will not take longer than 20 seconds. Hence τ=30 is an appropriate value to determine the average CO_2 rate and engine operation. This separates, for example, accelerations in urban and motorway driving, which are both associated with peaks in the CO_2 emission, but against different average CO_2 emissions. The complete five-parameter model to be fitted with the emission data is therefore:

$$NOx_t = x_1\ CO2 + x_2\ (CO2)^2 + x_3\ \Delta CO2 + x_4\ CO2^2_{transient} + x_5\ CO2\ (CO2_{30} - CO2)$$

The current model is under investigation with the emission data which is available. Hence, some fine-tuning. In the example below (Figure 6) the data of a CADC test is fitted with the five parameters. The first and second are given in the plot, while the remainder of the parameters shift the high NO_x at high CO_2 further upward, as the result of x_3 compensating this relation, and the NO_x at intermediate CO_2 rates somewhat downward, due to the effect of the transient yielding additional contributions. The parameters are all in the same range of magnitude, from 0.55 to 2.57. So they all contribute. In order of significance, the contributions are: $x_2 > x_1 > x_5 > x_4 > x_3$.

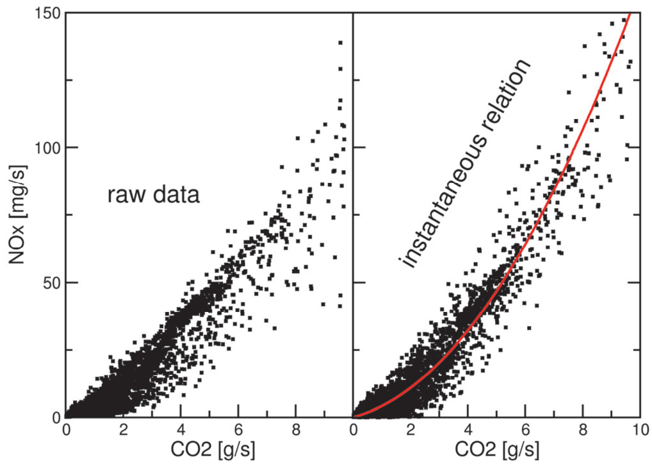

Figure 6: The raw data on the left of a single CADC test on a common Euro-5 diesel car, on the right the same data compensated for the terms for x_3, x_4, and x_5, together with relation (line) used for the instantaneous part described by x_1 and x_2.

The results seen in Figure 6 are observed for other Euro-5 diesel passenger cars as well. The instantaneous relation yields a higher NO_x emission at high load, but this in compensated somewhat by the limited load variations in these circumstances.

Conclusion and discussion

The emission modelling at TNO has always been a “small” step from representative emission measurements to standardized emission factors. The post-diction of the emission results is an important check, but also the study of the second-by-second residuals of the difference between measurements and model are an even more important check on the model quality. The RDE PEMS data, probably in combination with advanced emission reduction technology of the vehicles tested, shows the need for a new modelling approach, stable against variations in circumstances and trip variations. The two-stage approach with a limited number of nonlinear terms in a linear model allows for a proper fit of emission data in every stage. The right choice of terms ensures a robust model, which is applicable over a wide range of driving behavior and vehicle parameters.

The model is a simple set of terms and parameter values. This allows it to be used on large sets of streaming data, such as micro traffic simulations. It is fast and simple. The complexity lies in the derivation of the appropriate terms to be used. Furthermore, the parameters and the underlying linearity makes the emission model especially suitable for comparing vehicles and tests, factorizing effects, and attributing emissions to particular aspects of the influencing factors.

Aknowledgments

This study has benefitted from funding from the ecoDriver project (http://www.ecodriver-project.eu/) and extensive discussions with partners in this project: Isabel Wilmink (TNO), James Tate (Univ. Leeds), Andreas Tapani and Johan Olstam (VTI).

References

Ligterink, Norbert E., Kadijk, Gerrit, Van Mensch, Pim, Determination of Dutch NOx emission factors for Euro-5 diesel passenger cars, TNO report 2012 R11099.

Polderman, J.W., and Willems, J.C. Introduction to mathematical system theory, Springer, 1998.

Roocroft, A.J., Identifying and quantifying emission characteristics of modern passenger vehicles, TUDelft, Imperial College, student project report at TNO, 2014.

Wiener, N., Extrapolation, interpolation, and smoothing of stationary time series, Wiley, 1949.