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Comparison of microscale traffic emission models for urban networks

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Comparison of microscale traffic emission models for urban networks

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E-mail: c.quaassdorff@upm.es**Keywords:** road traffic emissions, microscale modelling, PΔP, PHEM-light, VERSIT+_{micro}, VISSIMSupplementary material for this article is available [online](#)

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**Abstract**

Traffic-related air quality issues remain in urban areas worldwide. For this reason, there is an increasing need to estimate the contribution of road traffic to atmospheric emissions at local level with high temporal and spatial resolution. Modal models compute emission rates as a function of specific engine or vehicle operating conditions at the highest resolution (seconds). They can be applied for microscale studies being a cost-effective tool to emulate differences in emissions levels in road networks. Two modal emission models, the Australian PΔP (Power-delta-Power) and the simplified version of the European PHEM (Passenger Car and Heavy-duty Emission Model), PHEM-light model, have been used. Also, a comparison to the cycle-variable emission model VERSIT+_{micro} (Netherlands organisation for applied scientific research state of the art traffic emission model) has been performed. For the comparison of both modal models, the main variables involved in traffic emission calculation were identified. 1 Hz speed-time profiles for individual vehicles were generated with the traffic microsimulation model VISSIM (Vehrkkehr in Statden SIMulation) for different traffic conditions. To understand the response of modal models, detailed estimations of NO_x emissions and fuel consumption were compared for different vehicle classes. Instantaneous emission profiles for individual driving patterns are highly sensitive to speed-acceleration profiles, vehicle mass, and road gradient, which are essential variables for the emission calculation. Although there are differences between European and Australian models, engine power and load were used to map vehicle classes for a more consistent comparison. It is essential to accurately define these parameters for each vehicle class in addition to detailed driving patterns to obtain high-resolution emissions estimates. In this sense, a larger number of vehicle classes included in the model provides more flexibility to develop representative emissions estimates. Emission predictions between modal models were reasonably consistent presenting larger differences with the cycle-variable model, despite both modal models being based on different on-road fleet measurements. In conclusion, analysing emission estimations for different traffic conditions demonstrates the importance of an accurate definition of the model parameters for a specific vehicle fleet.

1. Introduction

Over recent years, significant progress has been made in reducing emissions of greenhouse gases and urban air quality relevant air pollutants from the transport sector in high-income regions. However,

some traffic-related air quality issues remain in urban areas worldwide, including Europe and Australia.

In Europe, the transport sector is still the highest contributor to nitrogen oxides (NO_x) emissions, mainly due to road transport (responsible for 28% of total NO_x emissions considering all activity sectors)

and holds a significant share for other relevant pollutants, such as particulate matter (PM) (EEA 2020, 2021). Non-compliance with European air quality standards is often linked to highly polluted microenvironments (hot-spots) which are areas influenced by traffic emissions with high pollutant concentrations. Those require local intervention in addition to city-scale plans and measures (Miranda *et al* 2015, Thunis *et al* 2016, EEA 2021).

In Australia, passenger cars are responsible for roughly half of the transport greenhouse gas emissions (CC 2017). Similarly to Europe, air quality standards for criteria pollutants in Australia can be exceeded locally due to the contribution of road traffic emissions (Keywood *et al* 2017).

At the local scale, emissions need to be estimated for each vehicle, since they depend on individual acceleration–deceleration patterns (Int Panis *et al* 2006). Suitable assessment methods include direct measurements of exhaust emissions of single vehicles for a complete vehicle fleet by using for instance tunnel studies (Hausberger *et al* 2003, Smit *et al* 2017), or remote sensing detectors (Pujadas *et al* 2004, Smit and Bluett 2011, Chen and Borken-Kleefeld 2014, Smit *et al* 2021).

However, modelling techniques are needed to anticipate the outcome of traffic-related emission abatement measures (Perez-Prada and Monzon 2017, Borge *et al* 2018). Methods used to produce mobile source emission inventories usually address the national or regional scale and are based on a set of emission factors from standard driving cycles (Barth *et al* 1996) and aggregated vehicle activity data (EEA 2019 for Europe, NPI 2015 for Australia) This approach does not capture actual driving behaviour needed to estimate high-resolution emissions.

Studies for hot-spots require high-resolution (microscopic) emission models that can capture vehicle emission processes at microscale (Borge *et al* 2014), known as type A models according to the classification of Smit *et al* (2008). This type of models explicitly consider congestion through a detailed representation of actual driving behaviour (Smit *et al* 2010). This is estimated for each single vehicle based on second by second speed information (speed-time profile) obtained from direct measurements or from microscale traffic simulation models. Type A models include cycle-variable models where the emission factors (emissions per travelled distance in g km^{-1}) are related to variables from the driving cycle (Smit *et al* 2010), being the driving cycle in this case a fixed and reproducible second by second speed-time profile used for emission analyses (Barlow *et al* 2009). An example of this type are the Netherlands organisation for applied scientific research state-of-the-art road traffic emission model—VERSIT+—(Smit *et al* 2007). Type A models also include modal models where the emission factors are calculated by engine or vehicle operating conditions (Smit *et al* 2010). Those

models are deterministic based on engine variables and vary in level of complexity and demand for input data (Smit 2013) providing the most detailed representation of traffic emissions. Examples of this type are the Passenger car and Heavy-duty Emission Model—PHEM—(Hausberger *et al* 2009) or the Power-delta-Power emission model—P Δ P—(Smit 2013). These are based on portable emission measurement systems (PEMS) and laboratory tests to sample vehicle emission information for model development.

Cycle-variable models, such as VERSIT+_{micro}, have been previously tested in urban hot-spots with satisfactory results in comparison to an extensively evaluated regional emission model (Quassdorff *et al* 2016). Scenario-averaged emission factors estimated with the VISSIM-VERSIT+_{micro} modelling system fitted well those from the average-speed model COPERT (COmputer Programme to calculate Emissions from Road Transport) (Ntziachristos *et al* 2009), reference model in Europe (EEA 2019) for inventory compilation and used for the estimation of city-scale (Madrid) traffic emissions in that particular application. In addition, emission results from VERSIT+_{micro} have been successfully incorporated in high-resolution air quality modelling studies based on computational fluid dynamics (CFD) (Sanchez *et al* 2017). Specifically, cycle-variable emissions have been found to perform well for stationary-state CFD simulations based on a Reynolds-Averaged Navier–Stokes approach (Santiago *et al* 2017). Nonetheless, emissions for non-stationary simulations with higher temporal resolution (seconds) require the integration of modal emission models.

Despite their complexity and input requirements, modal models have been applied to real traffic situations. For instance, the instantaneous emission model PHEM was coupled to the traffic simulation model SUMO (Simulation of Urban MOBility model) (Hausberger and Krajzewicz 2014) in the COLOMBO project. Also, the impact of urban driving behaviour on fuel consumption (FC) was analysed in an Australian urban context with the P Δ P emission model coupled to the AIMSUN traffic model (Smit *et al* 2013). However, the understanding of the applicability and performance of different modal models for emission estimation in real traffic scenarios is limited.

In this contribution, two modal emission models (PHEM-light and P Δ P) are applied to two urban networks (in Australia and Spain) under different congestion scenarios (peak and off-peak hours). The aim of this comparison is to contribute to the understanding of the main differences between these two modal models and their applicability to different road network configurations in different traffic scenarios. Those have been selected to determine the applicability of the models to different urban networks and identify similarities in the emission calculation and spatial distribution for those road configurations. The

results are also compared with those of VERSIT+_{micro} for the same networks and scenarios. This additional test helps understanding to what extent the increase of spatial and temporal resolution provided by modal models improves the emission estimates of simpler cycle-variable models. This work aims to (a) examine and clarify the practical implications associated with using different types of models, and (b) identify key variables for microscale emission calculation in urban areas for the development of local road traffic emission inventories.

2. Materials

2.1. Traffic modelling

The traffic microsimulation model VISSIM has been used to generate the information about speed-time profiles for individual vehicles that are required by the three emission models used in this study. VISSIM is able to obtain individual vehicle speed-time profiles considering traffic lights configuration, traffic composition and public transport taking into account the interaction between private vehicles traffic and public transport (Fellendorf and Vortisch 2010). Moreover, as explained in Fellendorf and Vortisch (2010), VISSIM does not follow the traditional link-node approach based on centroids in the road network to distribute traffic fluxes across links (understanding a link as a road segment with constant properties). Instead, it uses a link-connector system where links are joined on a lane basis facilitating the creation of complex geometries. This software, widely used for traffic research at microscale (Fontes *et al* 2015), is designed to reproduce realistic traffic flow under different real-world conditions (Fellendorf and Vortisch 2001) providing vehicle speed-time profiles (Hirschmann *et al* 2010) and improved for emission estimations (Song *et al* 2015). The model was calibrated to reproduce local traffic conditions according to the US Department of Transportation procedures (U.S. DOT 2019).

The main VISSIM output consists of a vehicle record file that includes 1 Hz resolution information of vehicle type, speed (km h^{-1}), XY coordinate (coordinates of rear end position of vehicle) and road gradient (%) for each vehicle. Speed-time profiles for the individual vehicles are obtained from this file. Considering technical characteristics and typical driving behaviour, VISSIM uses three main vehicle classes: (a) heavy goods vehicles (HGV), (b) cars and (c) buses.

2.2. Emission modelling

P Δ P (Smit 2013) is a modal emission model that uses engine power and the change in engine power as main variables to simulate vehicle fuel consumption (FC) and carbon dioxide (CO_2) and NO_x emissions for the Australian fleet. The model requires information on vehicle speed (1 Hz), road gradient, vehicle loading and use of air conditioning. The P Δ P model is based

on a mathematical relationship between emission measurements during tests and the engine power of the vehicle. This model uses a 73-categories vehicle classification scheme based on COPERT-Australia (Smit and Ntziachristos 2013) that takes into account fuel type (petrol and diesel) and Australian emission standards (Australian Design Rule—ADR—, i.e. pre-EURO and EURO1-6/I–VI equivalent emission standards). The main input file contains the information regarding vehicle type (Passenger Car – PC –, Sport Utility Vehicle – SUV –, Light Commercial Vehicle – LCV –, Medium Commercial Vehicle – MCV –, Articulated Truck – AT –, Light bus – BUS-L – and Heavy bus – BUS-H –), cycle (user defined name), time (s), speed (1 Hz in km h^{-1}), vehicle loading (% of full load), road gradient (%) and other relevant parameters for the emission and FC computation (Smit 2013).

PHEM-light (Hausberger and Krajzewicz 2014), is a simplification of the European modal emission model PHEM (Hausberger *et al* 2009). PHEM-light retains relevant information of vehicle parameters and emission behaviour in Characteristic Emission curves over Power (CEP) for European vehicles. These CEP curves define the emission amount (g h^{-1}) as function of the actual engine power. As a result, PHEM-light compute instantaneous FC along with CO_2 , NO_x , CO, Hydrocarbons (HC) and Particulate Matter (PM) emissions for a given speed and acceleration combination. The model requires an input file containing all vehicle speeds (1 Hz in km h^{-1}) and road gradient (%) information for one driving cycle. Vehicle parameters such as vehicle mass, loading or engine rated power among others are divided into 131 classes that combines vehicle type (PC, LCV, HDV), vehicle size class (LCV I, II, III and HDV I and II) vehicle category (Rigid truck, Trailer Truck, Coach, City Bus), fuel (Diesel, Petrol, Battery Electric Vehicle – BEV –, Compressed Natural Gas – CNG –) and Euro standard (EURO0 to EURO6c). This information is then combined for the 1 Hz engine power computation of each individual vehicle over one driving cycle.

VERSIT+ is a Dutch multivariate regression cycle- and vehicle-variable emission model, which requires speed time profiles to obtain various traffic flow variables that are used to predict representative emission factors (g km^{-1}) for a set of 246 emission model classes (specific emission algorithms for each combination of vehicle category and air pollutant, Smit *et al* 2007). This model is used in this study to contrast the results of modal models with the simpler and more aggregated approach followed by cycle-variable models.

3. Methods

3.1. Comparison methodology

A comparison is made through all calculation steps between both modal models by using scatter analysis

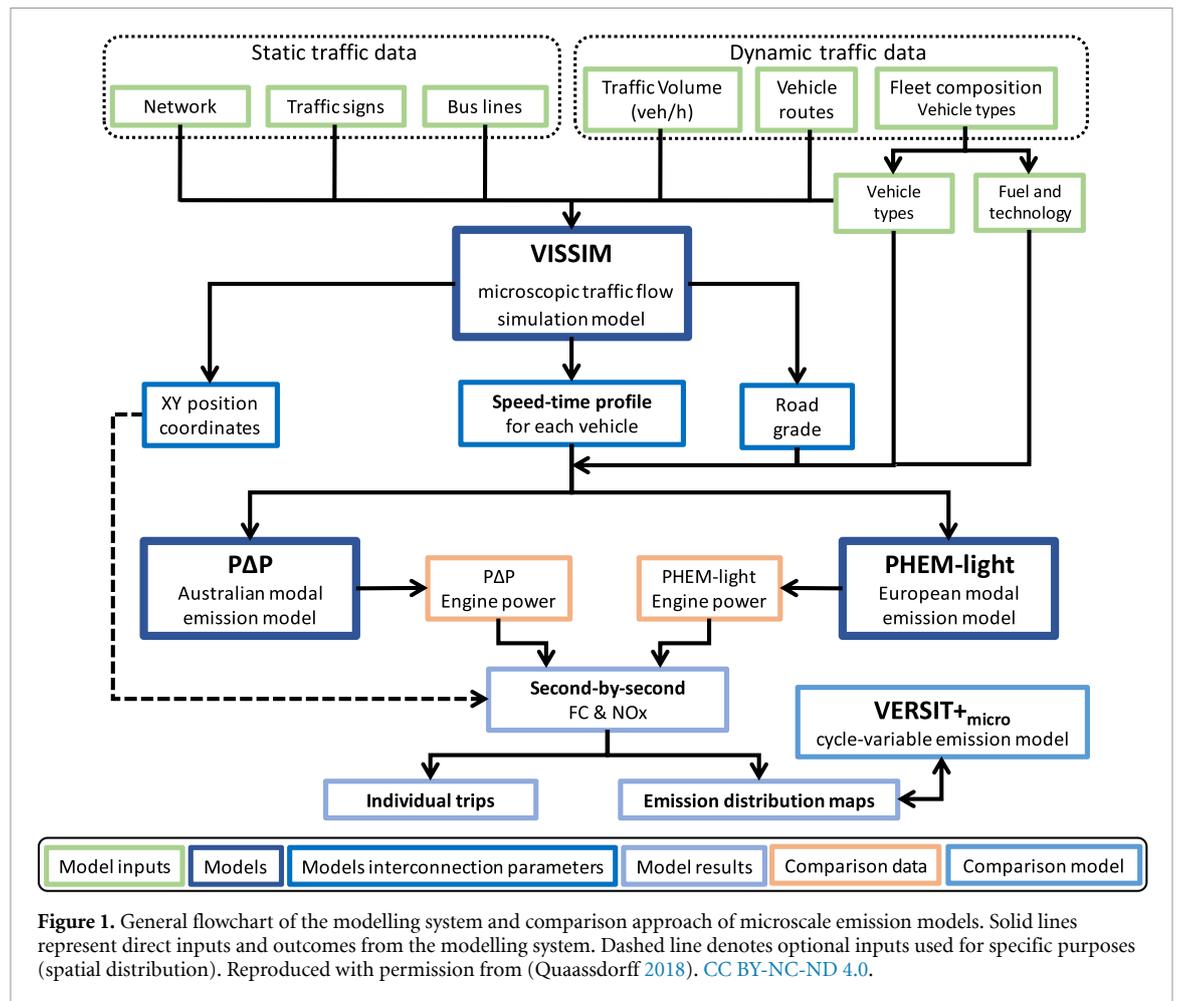


Figure 1. General flowchart of the modelling system and comparison approach of microscale emission models. Solid lines represent direct inputs and outcomes from the modelling system. Dashed line denotes optional inputs used for specific purposes (spatial distribution). Reproduced with permission from (Quaassdorff 2018). CC BY-NC-ND 4.0.

to obtain the relationship between the emission rates and FC results of the models. In order to be able to perform this analysis, first, vehicle classes are matched to a common classification. Then, engine power has been computed for selected individual trips (driving cycles) and analysed to understand the reason for differences between P Δ P and PHEM-light for the same driving cycle and similar vehicle classes (included in Supplementary Material—SM—). Finally, both models have been applied to two real network case studies and results of NO_x emissions and FC have been analysed (outputs in common in both modal models). All computations are based on the exact same traffic simulations provided by VISSIM. In this case, VISSIM relies on a set of static and dynamic traffic data that are used to obtain 1 Hz speed-time profiles, road grade and vehicle position. Speed-time profiles are used to feed the three microscale emission models, and road grade for the modal models. Based on these information, modal models provide engine power results that are used to estimate the second by second FC and emissions for individual vehicle trips that have been compared for modal models using scatter analysis. Emission distribution maps are generated by combining the second by second information on emissions and vehicle position. Those emission maps results have been compared between modal

models and to the cycle-variable emission model (figure 1).

3.2. Vehicle class mapping between models

First, in order to compare both modal models and minimize differences among models due to the different vehicle fleets they rely on, vehicles classes with similar characteristics have been matched. To obtain an accurate mapping between models for this study, vehicle rated engine power and average mass for each combination of vehicle class and emission standard has been examined. Since Australian emission standards are based on European regulations, equivalent EURO and ADR classes based on the gross vehicle mass (GVM) can be determined (details can be found in SM table A1).

Main vehicle classes were attributed and matched using rated engine power, average weight and mean engine capacity parameters so that a representative power-to-mass (PtM) ratio could be computed for each vehicle category. Differences in PtM were minimized by changing the vehicle loading variable defined in the input file for P Δ P vehicles (for each ADR category) to match the ratios assumed by PHEM-light, eventually obtaining a consistent 14-category classification scheme for both models (table 1). This match is helpful to explain differences

Table 1. Mapping between P Δ P and PHEM-light vehicle categories and relation to those of VISSIM.

Main vehicle		P Δ P				PHEM-light			
Category	VISSIM Category	Vehicle class	Description ^{a,b}	RPow ^c (kW)	VM + load ^d (T)	Vehicle class	Description ^e	RPow ^c (kW)	VM + load ^d (T)
Light-duty	Car	PC-S-petrol	Small passenger car E.cap.<2.1	80.4	1.51	PC-Otto-Conv	Passenger cars Petrol-Conv. 1.18 T < VM < 1.25 T	71.4	1.27
		PC-M-petrol	Medium passenger car E.cap.2–3.1	105.1	1.79	LCV-Otto-Conv_SI	Light commercial Petrol-Conv. vehicle SI: VM \leq 1.305 T	52.3	1.29
		PC-L-petrol	Large passenger car E.cap.>3.1	180.0	2.23	LCV-Otto-Conv_SII	Light commercial Petrol-Conv. vehicle SII: 1.305 T < VM \leq 1.76 T	68.3	1.57
Heavy-duty	HGV	PC-ML-diesel	Large and medium passenger car E.cap.>2.1	82.3	2.42	LCV-Diesel-Conv_SII	Light commercial Diesel-Conv. vehicle SII: 1.305 T < VM \leq 1.76 T	68.0	1.79
		LCV-petrol	Light commercial vehicles GVM \leq 3.5 T	120.7	2.48	LCV-Otto-Conv_SIII	Light commercial Petrol-Conv. vehicle SIII: 1.76 T < VM \leq 3.5 T	91.4	2.18
		LCV-diesel	Light commercial vehicles GVM \leq 3.5 T	72.7	2.63	LCV-Diesel-Conv_SIII	Light commercial Diesel-Conv. vehicle SIII: 1.76 T < VM \leq 3.5 T	80.3	2.42
Heavy-duty	HGV	SUV-diesel	Sport utility vehicle 4-wheel drives	95.3	2.65	LCV-Diesel-Conv_SII	Light commercial Diesel-Conv. vehicle SII: 1.305 T < VM \leq 1.76 T	68.0	1.79
		SUV-C-petrol	Compact sport utility vehicle 4-wheel drives, E.cap. \leq 2.5 T	118.3	2.15	PC-Otto-Conv	Passenger cars Petrol-Conv. 1.18 T < VM < 1.25 T	71.4	1.27
		SUV-L-petrol	Large sport utility vehicle 4-wheel drives, E.cap.>2.5 T	146.8	2.48	PC-Otto-Conv	Passenger cars Petrol-Conv. 1.18 T < VM < 1.25 T	71.4	1.27
		MCV-diesel	Rigid medium commercial vehicle GVM 3.5–12.0 T	165.5	9.28	HDV_RT-Diesel-Conv_SI	Heavy-duty vehicle-Rigid Truck Diesel-Conv. SI: 6.821 T VM + 1.577 T Load	166.2	8.40
		HCV-diesel	Rigid heavy commercial vehicle GVM 12.0–25.0 T	184.0	13.92	HDV_RT-Diesel-Conv_SII	Heavy-duty vehicle-Rigid Truck Diesel-Conv. SII: 12.143 T VM + 6.559 T Load	274.6	18.70

(Continued.)

Table 1. (Continued.)

Main vehicle Category	VISSIM Category	PΔP			PHEM-light			
Category	Vehicle class	Description ^{a,b}	RPow ^c (kW)	VM + load ^d (T)	Vehicle class	Description ^e	RPow ^c (kW)	VM + load ^d (T)
	AT-diesel	Articulated truck GVM >25 T	382.9	43.71	HDV_TT-Diesel-Conv	Heavy-duty vehicle-Tractor, trailer, articulated truck	291.2	29,95
Bus	BUS-H-diesel	Heavy bus GVM >8.5 T	253.3	17.45	HDV_CO-Diesel-Conv	Diesel-Conv. GVM >3.5 T Heavy-duty vehicle-Coaches	318.5	19,89
	BUS-L-diesel	Light bus GVM ≤8.5 T	103.4	5.95	HDV_CB-Diesel-Conv	Diesel-Conv. GVM >3.5 T Heavy-duty vehicle-City Bus Diesel-Conv. GVM >3.5 T	179.5	11,39

^a E. cap.: Engine capacity.^b GVM: Gross Vehicle Mass.^c RPow: Engine Rated Power.^d VM + load: Loaded vehicle weight.^e VM: Vehicle mass



Figure 2. Traffic microsimulation domain of 1250 m \times 600 m (black rectangle) for Woolloongabba area with red lines for traffic lights. Reproduced with permission from (Quaassdorff 2018). CC BY-NC-ND 4.0.

between the models and to identify the most relevant parameters to estimate emissions at microscale.

It should be noted that a perfect match is not possible due to differences between the European and Australian fleets. For instance, Australian vehicles have higher average engine capacity than European counterparts. Fleet-specific vehicle parameters that influence the model classification, i.e. Gross Vehicle Mass, tare weight, rolling resistance and aerodynamic coefficients, were also compared. Both PHEM-light and P Δ P allow for adjustment of these vehicle parameters that are used to compare power demand in a cycle to better reflect local fleet distributions on demand. In this study the predefined vehicle parameters provided by the models were used, thus differences in the results are related to the different model approaches but also to different vehicle characteristics included in those models. This reflects the real-world differences between vehicle samples used for emissions testing and subsequent model development and calibration (sample from European fleet for PHEM-light, sample from Australian fleet for P Δ P) and will provide an insight on the practical implications associated with using different models in different parts of the world.

3.3. Hot-spot networks

Two traffic-hotspots with different urban networks configurations (in Australia and Spain) have been used in this study for comparison purposes. Those have been selected to determine the applicability of the models to different urban networks and identify similarities in the emission calculation and emission spatial distribution for those road configurations and vehicle fleets.

3.3.1. Urban streets combination in Woolloongabba (Brisbane)

Brisbane is the third biggest city in Australia with a metropolitan population of roughly 2.3 million. Figure 2 shows the selected area of 1250 m \times 600 m

around the South Brisbane Air Quality monitoring station in Woolloongabba (Coordinates: -27.484775 , 153.032061). Located adjacent to the Pacific Motorway, the urban streets of Woolloongabba present a complex interaction of different road types and traffic conditions. The domain includes part of a highway that redistributes the traffic to urban collectors and from there to urban roads.

3.3.2. Plaza Elíptica signalized roundabout (Madrid)

Madrid is the capital city of Spain and has around 3.2 million inhabitants (up to 6.5 million in the whole Madrid metropolitan area). The selected area (300 m \times 300 m domain) (figure 3), is a signalized roundabout—Plaza Elíptica—(Coordinates: 40.385251 , -3.717599) that presents high vehicle activity and a complex network configuration. Stop-and-go traffic conditions are frequent in the area (Quaassdorff *et al* 2016) and often result in high pollution levels and strong concentration gradients (Borge *et al* 2016).

3.3.3. Scenarios and fleet composition

Daily traffic patterns were analysed for both locations in order to select two 1 h scenarios representative of typical traffic conditions for weekday peak and off-peak hours (Quaassdorff 2018). These are contrasting scenarios that present different traffic flow (congestion conditions) that have an effect on the breaking-acceleration patterns of the vehicles and though on the emissions of each vehicle trip (Quaassdorff *et al* 2016). Peak hour traffic conditions (saturated) with more acceleration-deceleration patterns with an effect on the vehicle speed-time profiles are represented by the 16:30–17:30 p.m. period in Brisbane and 8:00–9:00 a.m. period for Madrid (local time in all cases). Low intensity traffic typical of off-peak hours (free-flow conditions) are studied through the 4:30–5:30 a.m. and the 4:00–5:00 a.m. periods in Brisbane and Madrid respectively. For those scenarios traffic

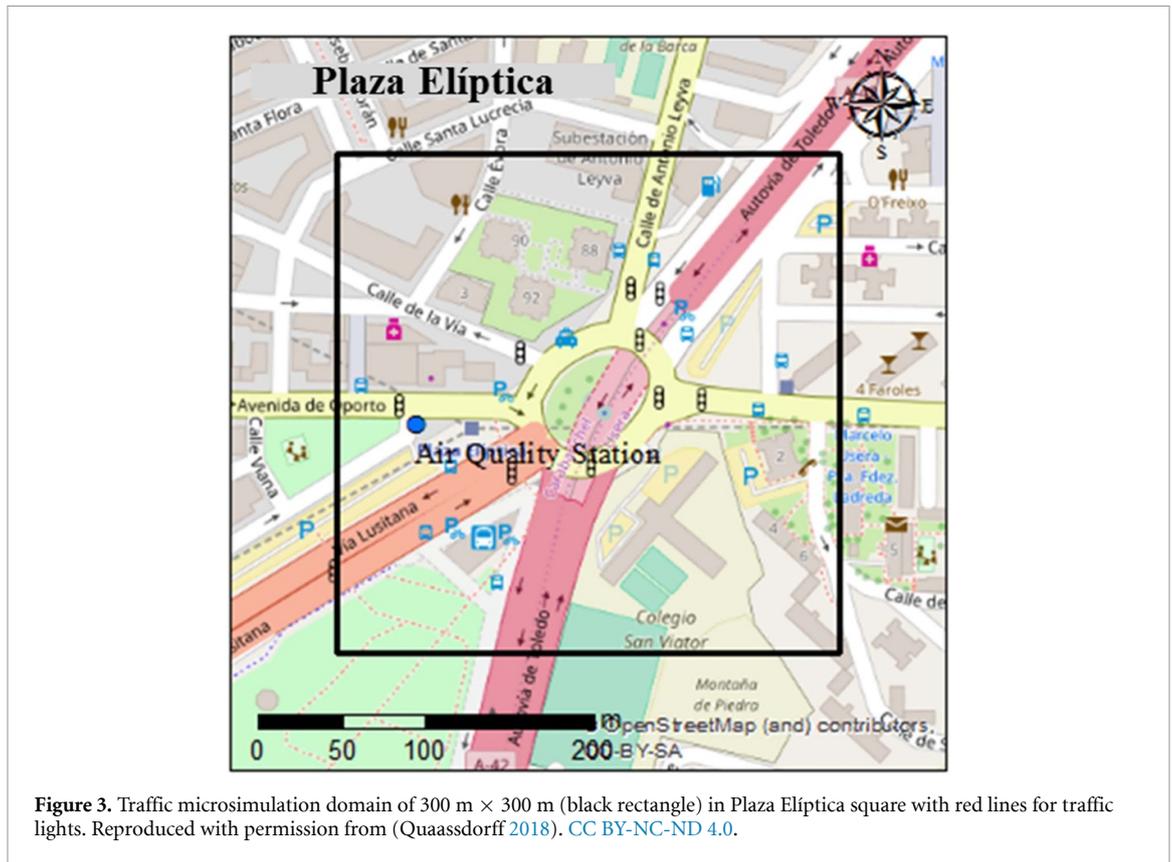


Figure 3. Traffic microsimulation domain of 300 m × 300 m (black rectangle) in Plaza Elíptica square with red lines for traffic lights. Reproduced with permission from (Quaassdorff 2018). CC BY-NC-ND 4.0.

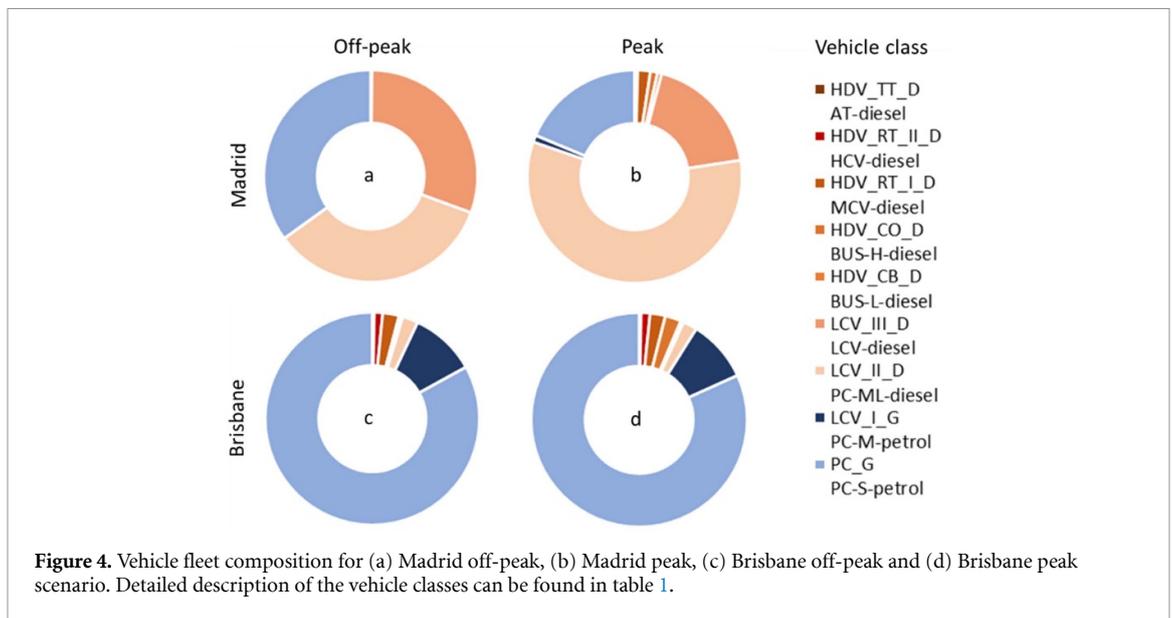


Figure 4. Vehicle fleet composition for (a) Madrid off-peak, (b) Madrid peak, (c) Brisbane off-peak and (d) Brisbane peak scenario. Detailed description of the vehicle classes can be found in table 1.

intensity estimated by the VISSIM model where compared to field counts. For that kind of data, one of the best statistics to assess the model performance is the Geoffrey E. Havers statistic (GEH). This statistic compare field data and simulations outputs for traffic flows. Calibration acceptance target of $GEH < 5$ for all links of a simulation is deemed as benchmark of good performance. In this study, the GEH statistic falls well below that calibration target for all the scenarios (Quaassdorff 2018).

Regarding fleet composition, the corresponding vehicle fleets for each of the selected scenarios are shown in figure 4. In the case of Madrid, the information is taken from the 2013 Madrid vehicle fleet study (Parque circulante 2014, Pérez et al 2019) and from experimental campaigns data obtained *in situ*. In the case of Brisbane, these data correspond to the default vehicle fleet input data for the PΔP model, i.e. representative of the Queensland vehicle fleet in 2010 and from information provided by the traffic information

system from Brisbane's city. There are significant differences between vehicle fleets, mainly regarding to the diesel share in Madrid City (in brown colours in figure 4). Additionally, the vehicle emission standard distribution for each of the scenarios can be found in SM table A2.

4. Results and discussion

4.1. Individual trip analysis for real-world networks

To perform a comparison between vehicle classes for real applications, in figure 5 1 h average NO_x and FC emission factors (g km^{-1}) and the corresponding NO_x/FC ratio (fuel based emission factor) have been calculated for each scenario and vehicle class and compared for both modal models (PHEM-light and P Δ P). The comparison is done by using scatter plot analysis and statistics that provide a measure on the strength of the relationship between both models and main differences.

Resulting NO_x/FC ratios are rather consistent for all scenarios and all vehicle classes, with an R^2 value of 0.833. This suggest that both modal models provide a consistent response under the whole range of conditions tested. Nevertheless, as shown in figure 5, significant differences appear on the calculation of FC and NO_x emissions factors in saturated conditions (peak-hour) for some vehicle classes. This is the case for Heavy-duty vehicles HDV-TT-D—AT-diesel and Buses HDV-CO-D—BUS-H-diesel, which present main differences of up to 40% for NO_x and 60% for FC. This is in agreement with the comparison of mesoscale traffic models performed by Borge *et al* (2012). A good agreement is obtained overall both for FC ($R^2 = 0.602$) and NO_x emission factors ($R^2 = 0.689$) as well as reasonable mean fractional biases (12.0% and 6.4% respectively). This analysis suggests that similar results can be achieved with any of the two models, if consistent input information on the vehicle fleet composition and vehicle characteristics is provided. Nevertheless, future studies should consider road load parameters to accurately include country-specific fleet characteristics in the models. Additionally, analyses over specific driving cycles are included in SM section 2.

Instantaneous emissions are sensitive to speed-time and acceleration profiles and thus, traffic congestion conditions (included in section 3 from the SM). As shown in figure 6, higher emission factors (g km^{-1}) are related to lower average speeds, following the typical distribution considered in average-speed mesoscale models such as COPERT (Ntziachristos *et al* 2009). High traffic intensity produces congestion conditions associated to braking-acceleration (stop-and-go) patterns. These stop-and-go situations result in lower average speeds for a

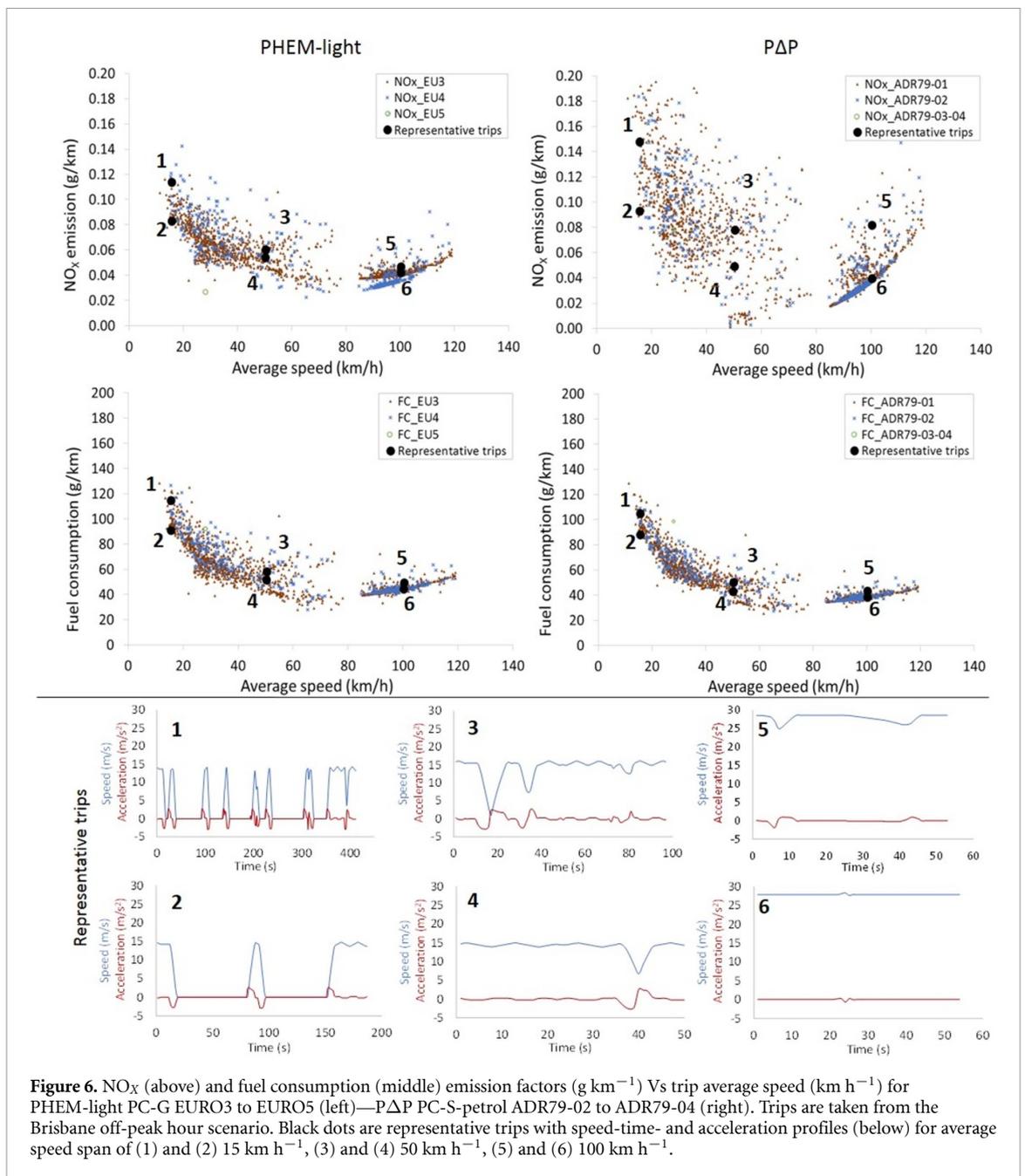
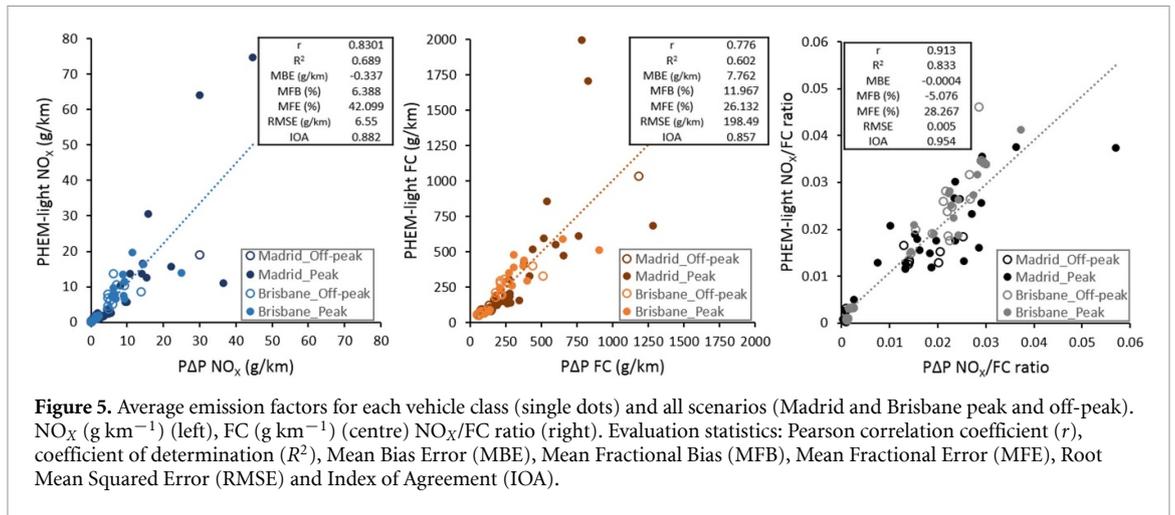
specific trip (in comparison to the same trip in free-flow conditions) and present higher values in emission predictions (g km^{-1}), particularly for P Δ P NO_x emissions which presents also larger spread. This suggests that P Δ P is more sensitive to variability in driving conditions. The variability of emissions factors is in general inversely proportional to average speed for both models. Nevertheless, maximum dispersion occurs around 25 km h^{-1} . Both emission models present a more stable response for free-flow high average speed, especially for FC (and consequently CO_2 emissions).

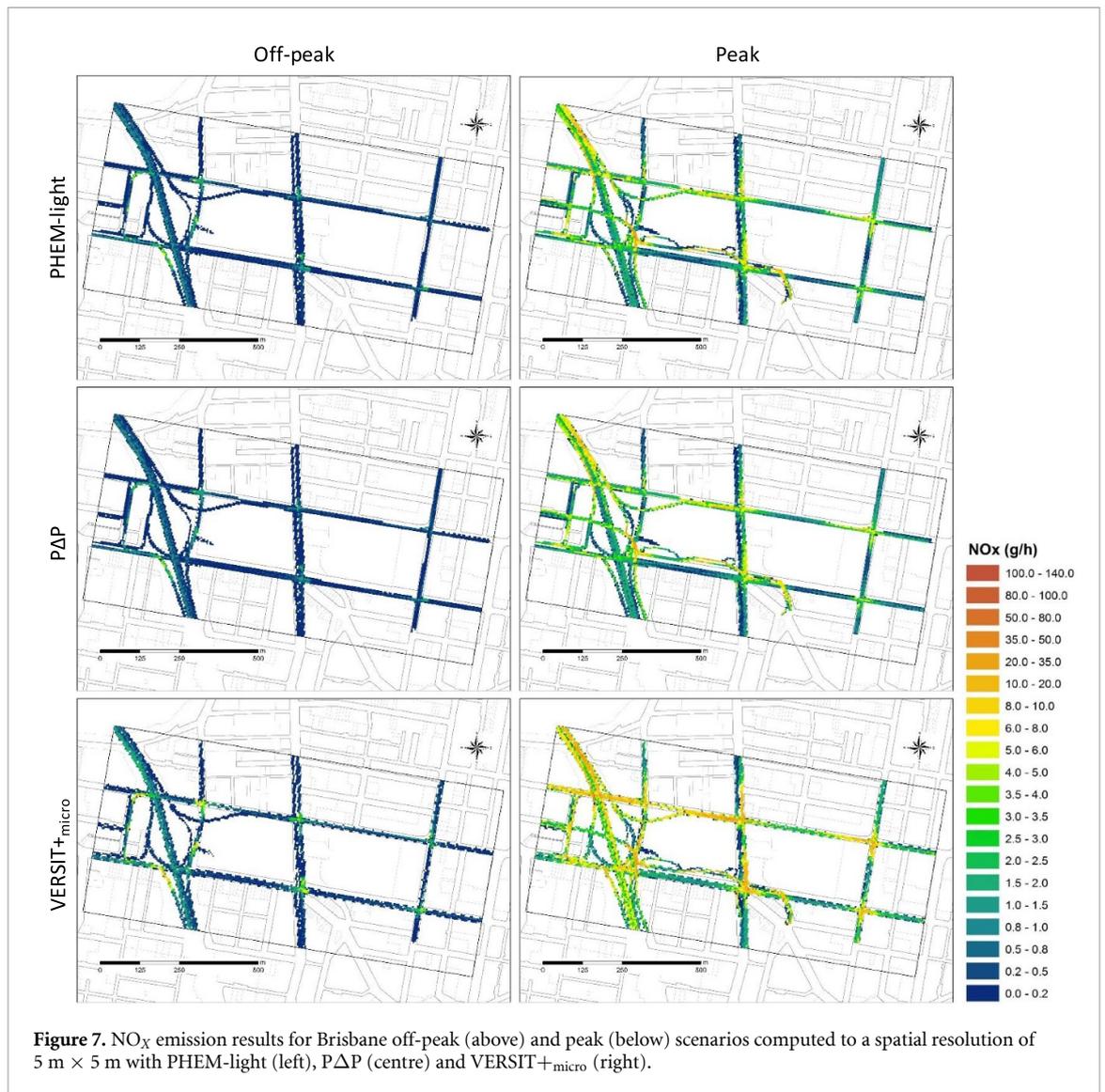
4.2. Emission distribution maps

Second by second P Δ P and PHEM-light emission results and instantaneous location reports provided by the traffic simulation model were used to produce high resolution emission maps. The maps were generated with ArcGIS® by aggregating the information on instantaneous NO_x emissions estimated by the modal models (1 s emission data are given with the corresponding coordinates) to the $5 \text{ m} \times 5 \text{ m}$ resolution mesh used by the cycle variable model. For comparison purposes with another type of model, the cycle variable model VERSIT+_{micro} through the ENVIVER interface (version Enterprise 4.0 released in 2016), emissions were represented on a $5 \text{ m} \times 5 \text{ m}$ resolution grid (figure 7 for Brisbane network and figure 8 for Madrid network).

The emission maps obtained with the three models present similar spatial distributions consistently identifying higher emissions around the main intersections where vehicles have to queue waiting for traffic signals to open. That increases acceleration time, and thus, emissions, especially at peak hours when more vehicles are in the network. Those very high resolution maps also provide detailed information on emission distributions that can be useful to understand spatio-temporal emission variations within a city and to feed microscale dispersion models to support air quality studies. Aggregated emission values for 1 h scenarios are shown in table 2.

At scenario level, PHEM-light predicts higher NO_x emissions for Brisbane simulations than P Δ P (13% and 10% for the off-peak hour and peak hour respectively). This is directly related to the dominance of ADR79-00 (EURO2) petrol passenger cars in these scenarios which present higher NO_x emission factor (SM section 4). This type of vehicle represents roughly 30% of the total vehicle fleet in Brisbane scenarios, whereas in Madrid scenarios the equivalent vehicles are only 4% to 10% of the fleet (SM section 1). On the other hand, for the signalized intersection in Madrid, P Δ P NO_x emissions are 39% higher than those predicted by PHEM for the off-peak hour scenario and 27% for the peak hour simulation. This is in agreement with the results obtained over the





individual trips presented in SM section 2. Comparing the modal models to the cycle variable model, differences are around 50% with the exception of the Madrid off-peak hour scenario where PΔP predicts higher total emissions for the domain. This scenario does not include Heavy-duty vehicles (figure 4), category where the main differences between modal and cycle-variable models appear (70% higher emissions for Heavy-duty vehicles in VERSIT+_{micro}, figure 9).

There is a good agreement between VERSIT+_{micro} and PΔP for the passenger car category (figure 9 left panel). This vehicle category represents the main percentage of the vehicle fleet in all scenarios (figure 4) and shows differences below 6% with a coefficient of determination (R^2) that reaches a value of 0.79 and a slope value of 1.06. The results suggest that modal models predict significant lower values than the cycle variable VERSIT+_{micro} model, despite the fact they reflect two different on-road fleets. Nevertheless, a good agreement between the car category with PΔP model has been found, which is interesting as both PHEM-light and VERSIT+ reflect European fleets.

Further validation is required to determine the accuracy of each approach for different applications in the EU.

In the case of road transport emission calculation, model validation is a key issue but the effectiveness/feasibility has to be taken into account. Specific validation studies are needed in order to obtain independent real-world emission measurements of sufficient sample size to verify emission factors and total emissions estimates. Comparison with independent and measured data is important for validation purposes and should be considered as a future work recommendation. For instance, in addition to e.g. tunnel studies and remote sensing, PEMS provide real-world emissions data for emission model updates and improvement (Franco *et al* 2013). The consideration and continuous update of measured emission factors from the new Worldwide Harmonized Light Vehicles Test Procedure (WLTP) and the Real-world exhaust emissions tests is important because it is widely accepted from the scientific community that emissions values and FC measured in laboratory were

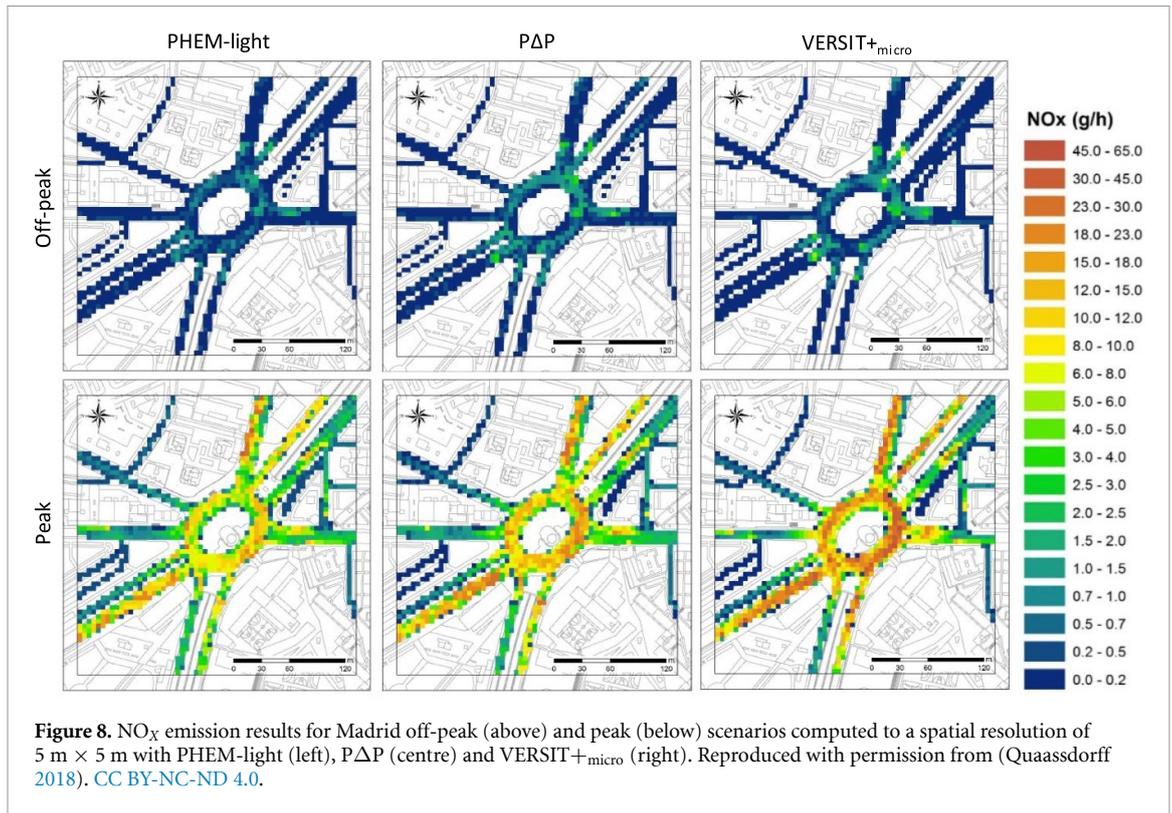


Figure 8. NO_x emission results for Madrid off-peak (above) and peak (below) scenarios computed to a spatial resolution of 5 m × 5 m with PHEM-light (left), PΔP (centre) and VERSIT+_{micro} (right). Reproduced with permission from (Quassdorff 2018). CC BY-NC-ND 4.0.

Table 2. Total NO_x emissions (g h⁻¹) for the four scenarios and the three emission models.

Scenario	PHEM-light (g h ⁻¹)	PΔP (g h ⁻¹)	VERSIT+ _{micro} (g h ⁻¹)
Brisbane off-peak	1359	1183	2731
Brisbane peak	14 360	12 863	25 196
Madrid off-peak	197	322	293
Madrid peak	4148	5702	7818

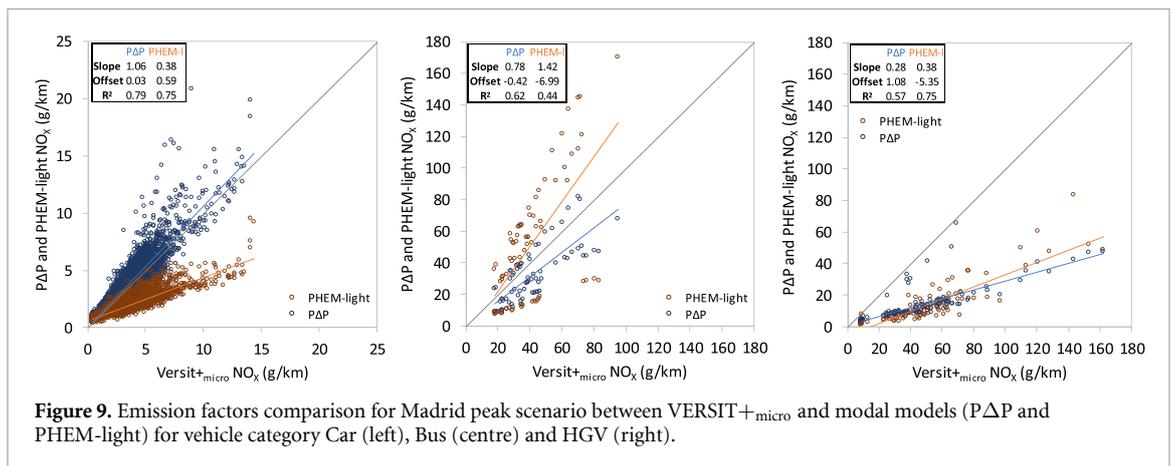


Figure 9. Emission factors comparison for Madrid peak scenario between VERSIT+_{micro} and modal models (PΔP and PHEM-light) for vehicle category Car (left), Bus (centre) and HGV (right).

underestimating emission levels obtained under real-world driving conditions (i.e. Kadijk et al 2017, Luján et al 2018). This validation process is an ongoing process.

4.2.1. CFD coupling possibilities

CFD air quality models provide the opportunity to estimate pollutant concentrations at very high spatial and temporal resolutions. Urban hot-spot require

specific analysis in order to undertake appropriate measures to reduce air pollution on those areas and CFD models can provide solutions for specific urban highly polluted areas when fed with detailed emission information.

Cycle-variable models are useful for applications where second by second resolution is not needed. However, the information generated by the modal emission models is suitable to generate emission maps

with temporal resolution up to one second and also high spatial resolution (1 m × 1 m grid resolution maps). The comparison of those models outcomes opens the opportunity to find a compromise between model complexity (and thus input information needs and computational burden) and accuracy, so a single modelling approach may be used for specific areas as well as for larger domains. That would provide a consistent view of traffic emissions across the scales.

At the high spatial resolution that modal models provide, traffic lanes with higher emissions rates can be simulated and are a promising option to analyse local emission abatement measures effects since they are suitable for high-resolution non-stationary air quality modelling with CFD models. Nevertheless, a CFD analysis would require various scenarios to reproduce the traffic fluctuations during a day and for a representative week. This method has provided good results in comparison to passive sampler's measurements by using cycle-variable emission outputs in stationary CFD simulations (Sanchez *et al* 2017). It is expected that instantaneous emissions provided by modal models could be useful to provide the highly detailed (spatially and temporally resolved) inputs for dynamic CFD simulations. Those can also be used for comparing emission predictions with independent measurements (road side air quality monitors) to quantify prediction errors in future data validation processes. This approach will provide continuously resolved evolution (in time and space) of pollutant concentrations with high resolution in future research steps.

5. Conclusions, study limitations and future research opportunities

Regarding key variables to consider for microscale emission calculation for the development of local road traffic emission inventories, both PΔP and PHEM-light use engine power algorithms to compute instantaneous emissions and fuel consumption. Our analysis suggests that vehicle classification is important. Differences in PtM ratio, rated engine power and road load coefficients are key variables for emission calculation for each vehicle category. It is essential to adjust them to a specific study case to obtain similar emission results when compiling road traffic emission inventories, regardless of the specific model being used. Furthermore, a larger number of vehicle classes allows more flexibility to provide representative emissions estimates. In this analysis hybrid and electric vehicles have not been considered as part of the fleet structure due to the low penetration in the analysed scenarios. Nevertheless, with the foreseeable increasing market penetration of these vehicles, their special emission behaviour should be depicted more precisely in future studies to include also other pollutants such as non-exhaust PM, which is still relevant for electric vehicles (TER 2020).

Regarding the practical implications associated with using different emission models, according to the results, reasonably consistent emission estimates can be achieved with any of the models, as long as reliable information on the vehicle fleet composition and vehicle characteristics is provided as input. Results show that NO_x to FC ratios are in reasonable agreement when comparing PΔP and PHEM-light for the individual vehicle categories. PΔP tends to predict higher emission factors than PHEM-light for the main light-duty vehicle categories. The main differences between models may relate to differences in engine and emission control technology in the on-road fleets, as well as other factors such as fuel quality, inspection and maintenance programs and so forth, which suggests that local calibration of vehicle emission models is essential for accurate modelling.

A larger spread in emission factors at low average speeds demonstrates the variability and the difficulty of accurately predicting emissions for stop-and-go conditions under saturated traffic situations. Congested conditions are usually the main cause for hot-spots and air quality non-compliance situations in urban areas. Modal models and cycle-variable models provide specific emission estimates for these conditions making them useful for a detailed analysis in urban hot-spots where stop-and-go conditions are more frequent. The VISSIM traffic model is useful to support a wide range of emission computation methodologies at microscale, and this similarly applies to other microscale traffic models such as AIMSUN. The analysis of emission estimations for driving patterns under different traffic conditions also reveals the importance of the congestion levels in a road network on the impacts on average speed and corresponding elevated emission factors. So that the accuracy of the traffic simulation model to reproduce real driving patterns is of special interest in future analysis.

The results from this study suggest that modal models predict significant lower values than the cycle-variable VERSIT+_{micro} model at road network level. Nevertheless, a good agreement between PΔP and VERSIT+_{micro} has been found for passenger vehicles (R^2 of 0.79). VERSIT+_{micro} predicts emissions twice as high as PHEM-light for this vehicle category, which represent more than 90% of the vehicle fleet in Madrid, resulting in substantial differences for total emissions. Further validation with independent data is required to determine the accuracy of each approach for different applications in the European Union and overseas.

Instantaneous emission information obtained with modal models is suitable to generate emission maps with high spatial and temporal resolution of up to 1 m × 1 m and 1 Hz. They provide cost-effective and fast emission estimates for different traffic scenarios for non-stationary CFD air quality modelling in urban areas. Nevertheless, real-world emission measurements are essential towards

the validation of emission factors and total emissions computed by these modelling techniques. Also continuous updates of measured emission factors from the new WLT Procedure and the Real-world exhaust emissions tests should be used to update emission algorithms in modal models. This validation process should be understood as an ongoing process to continue in the future and remain as a limitation of this study.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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Conflict of interest

The authors declare no competing interest.

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