A coupled macroscopic traffic and pollutant emission modelling system for Barcelona

Daniel Rodriguez-Rey a, Marc Guevara a,∗, M Paz Linares b, Josep Casanovas b,c, Juan Salmerón b, Albert Soret a, Oriol Jorba a, Carles Tena a, Carlos Pérez García-Pando a,d

a Barcelona Supercomputing Center, Barcelona, 08034, Spain
b Universitat Politècnica de Catalunya-Barcelona Tech UPC, Carrer Jordi Girona 1-3, 08034, Barcelona, Spain
c Computer Sciences Department, Barcelona Supercomputing Center, Barcelona, 08034, Spain
d ICREA, Catalan Institution for Research and Advanced Studies, Barcelona, 08010, Spain

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A B S T R A C T

We present a coupled macroscopic traffic and emission modelling system tailored to the Barcelona metropolitan area that allows estimating hourly road transport emissions at road link level. We use the developed system to perform an emission sensitivity analysis of typically high uncertainty emission features and assess their impact. We also explore the uncertainties of our system compared to a microscopic approach in a representative area of Barcelona. The developed macroscopic system shows a high sensitivity to spatially-resolved vehicle fleet composition inputs, meteorological effects on diesel engines (+19% in NOx) and non-exhaust sources (80% of total PM emissions). The comparison with the microscopic system shows that discrepancies grow as a function of the congestion level, up to +65% in NOx. The resulting coupled system will be used in further steps of the research to evaluate the impact of traffic management strategies upon urban emissions and air quality levels in Barcelona.

1. Introduction

Air pollution is a public health threat in most urban environments, where road transport is often the main contributor (EEA, 2019). Nitrogen oxides (NOx) and particulate matter (PM) are of special concern as they are strongly associated with respiratory and cardiovascular morbidity and premature mortality (Lelieveld et al., 2015). To prevent air pollution, the European Union (EU) established the 2008/50/EC EU Ambient Air Quality Directive (AQD), which sets maximum concentration limit values for specific air pollutants. Yet, most of the largest European urban conurbations struggle to meet the AQD for NO2 and especially PM (EEA, 2019). In the city of Barcelona (Spain), chronic nitrogen dioxides (NOx) and fine particular matter (PM2.5) concentrations exceed both the AQD limit values and the World Health Organization air quality guidelines (ASPB, 2018). Consequently, Barcelona and other large urban conurbations have been forced to apply action plans to improve their air quality by reducing traffic activity and emissions.

The AQD encourages the use of numerical models in the evaluation of air quality plans. In this context, the combination of traffic and emission factor models has become an extended practice to generate emission modelling inputs and derive traffic emissions at different scales (i.e macroscopic, mesoscopic and microscopic). While the precise definition of scales differs for traffic and emission

∗ Corresponding author.
E-mail address: marc.guevara@bsc.es (M. Guevara).

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factor models, in both cases they are related to the resolution of the vehicle dynamics, rather than to the spatial or temporal resolution. For emission factor models, resolution is related to the level of aggregation of vehicle dynamics (Smit et al., 2008), which ranges from using average speed and total flow per segment in macroscopic models (e.g. COPERT (EMEP/EEA, 2017)), to instantaneous speed per vehicle for microscopic models (e.g. PHEM (Hausberger et al., 2009)). The scale of traffic simulators is related to the traffic assignment method, either Static Traffic Assignment (STA) or Dynamic Traffic Assignment (DTA) – the latter resolving travel demand time-dependent flow conditions in a more realistic way (Zhou et al., 2015) – and to the level of aggregation of the demand that is used to resolve vehicle-to-vehicle interactions.

There is an extensive literature with case studies of coupled traffic simulators and traffic emission models at different scales (Fontes et al., 2015; Osorio and Nanduri, 2015). It is generally accepted that traffic emissions derived from microscopic approaches using DTA are more accurate than those estimated with a macroscopic system, due to a better vehicle dynamics estimation, small time-step and ability to capture congestion behaviour. Some examples of the better performance of microscopic approaches compared to macroscopic can be found in Quaasddorff et al. (2016), Tu et al. (2018), Zhang et al. (2011) and Lejri et al. (2018). However, in contrast to the macroscopic approach, the microscopic one is typically limited to very localised sites due to the detailed data needed by the traffic model and the high computational load (Fallah Shorshani et al., 2015; Tu et al., 2018; Lejri et al., 2018), which hampers its applicability for evaluating traffic emissions at city or metropolitan level.

Despite some of the inherent limitations of a macroscopic system, recent studies have shown that large improvements can still be achieved by focusing on a better representation of critical components such as the vehicle emission rates, vehicle activity patterns and vehicle fleet distribution. In the Île-de-France André et al. (2018) found as much as 14% and 11% more NO\textsubscript{x} and VOC emissions when using the observed vehicle fleet composition compared to the registered one due to a higher presence of diesel vehicles. In Madrid, Pérez et al. (2019) also found a large difference between the fraction of observed (70%) and registered (47%) diesel powered vehicles. Grange et al. (2019) reported a large previously unaccounted temperature effect on emissions, with an estimated 38% average increase in NO\textsubscript{x} diesel emissions in Europe. Results from this study are independent from the cold-start effect, which can additionally increase NO\textsubscript{x} emissions by up to 39% and 166% for diesel and gasoline vehicles respectively (Faria et al., 2018). Amato et al. (2014) showed that resuspension alone can contribute as much PM as tailpipe emissions, that with the addition of other non-exhaust sources (e.g. road, tyre and brake wear) increase the total weight of non-exhaust over PM totals, as reported by Martini and Grigoratos (2014) and Rexeis and Hausberger (2009). However, in other studies the estimated emissions are often limited to exhaust (Chen et al., 2017; Fontes et al., 2015), or non-exhaust wear emissions (Pérez et al., 2019), but few of them include also resuspension.

The coupling of traffic and emission models also allows to estimate the emission impact that different mobility policies could imply, since the traffic flow response to modifications on the network is also simulated. In Barcelona, traffic emissions are currently calculated with regional and local data inventories. The followed methodology is based on static traffic flow data and therefore it is unable to quantify the changes in mobility patterns induced by the application of traffic management strategies.

In this study, we present the development of a macroscopic traffic-emission coupled system tailored and tested for Barcelona using multiple sources of local data (e.g. GPS based measurements, traffic loop detectors or a remote sensing device campaign). The coupled system estimates high resolution traffic emissions for the first crown of the Metropolitan Area of Barcelona, an area with more than two million inhabitants, a vehicle density of approximately 6,000 vehicles km\textsuperscript{-2} and 26% of the daily trips done by private transport (Ajuntament de Barcelona, 2017). The developed system is used to: (i) quantify hourly and street-level NO\textsubscript{x} and PM\textsubscript{10} emissions for the year 2017 and (ii) provide an extensive analysis of some key features implemented upon the emission calculation, including spatially-constrained vehicle fleet composition, meteorological influences, non-exhaust PM sources and public bus transport routing. We further evaluate and discuss the expected uncertainties of our macroscopic system in comparison to a microscopic approach in a specific area of the city.
Section 2 provides a description of the study domain, the traffic and emission models used, the input data and the calibration and coupling processes. In Section 3, we (i) show the annual emission modelling results, (ii) evaluate the impact upon emissions of some of the key inputs implemented and (iii) analyse the uncertainties of our system in comparison to a microscopic approach. Section 4 presents the conclusions.

2. Methodology

In this section, we describe the macroscopic traffic and emission models along with their calibration and coupling. We also describe the microscopic system used for comparison. A schematic representation of the macroscopic and microscopic coupling approaches is shown in Fig. 1.

2.1. BCN-VML: Macroscopic traffic modelling

The traffic model is based on the detailed multimodal transport model Barcelona Virtual Mobility Lab (BCN-VML), which uses the PTV Visum platform (Montero et al., 2018). BCN-VML was developed within the framework of the Cooperative Automotive Research Network (CARNET) initiative (CARNET, 2017), a knowledge hub for automotive science and technology, and in collaboration with SEAT, PTV IBERIA, Volkswagen Group Research and the Universitat Politècnica de Catalunya (UPC).

The BCN-VML working domain comprises the First Crown of the Metropolitan Area of Barcelona plus a large extension including its access highways. The demand of BCN-VML is composed of almost 4 million trips, distributed in 265,000 links and 625 zones. For computational time optimisation, two working domains with different levels of detail are used. The first one covers a large area of around 6,000 km². This domain is less detailed and mostly focuses on highways and national roads. The second domain, which is the focus of the present study, comprises a detailed build of Barcelona and 17 municipalities surrounding the city, gathering a population of more than two million inhabitants (Institut d’Estadística de Catalunya, 2019) (Fig. 2a). The wider domain allows the BCN-VML to properly diverge the traffic into the different accesses of the city. In this way we avoid forcing the entrance through a particular city access according to its adjacent outflow zone, without adding an excessive load to the simulation.

The road network was built based on geographical maps from HERE (Here, 2020), with manual edition for specific areas. It has a hierarchy of 12 different link types which hold different road capacities, speed limit and Volume Delay Functions which penalise total travel time through a link (Kucharski Rafal and Drabicki, 2017).

Finally, the traffic demand data needed to perform the private transport traffic assignment between pairs of transport zones, the origin–destination matrices, were obtained from mobile phone KINEO (Kineo, 2017) from March 2017. Public transport (bus line routes, stops and frequencies) were built according to the public transport data of the Metropolitan Area of Barcelona (TMB, 2019). Since buses cannot circulate through all of the available network, the public bus transport is associated with a different simulation process than the private transport. More details are provided in Section 2.3.

2.1.1. Calibration of the BCN-VML

The calibration of the BCN-VML model requires adjusting the estimated traffic flow and vehicle speed. The calibration of the BCN-VML estimated traffic flow for the city of Barcelona and its access roads was performed using observed hourly business-as-usual daily traffic flow data from 138 local automatic loop detectors from the Barcelona network (Ajuntament de Barcelona, 2019)
Fig. 2. (a) Representation of the BCN-VML road network and associated business as usual daily traffic used in the present study, which comprises the city of Barcelona and its surrounding municipalities. Dark green squares indicate the 138 permanent loop detectors used to calibrate the vehicle flow. (b) Regression plot showing observed vs modelled flow (10^3 number of vehicles) from a 24 h simulation with BCN-VML. 138 observations, RMSE = 35%, $R^2 = 0.77$, mean relative error = 27%.

Some network properties such as road lane capacity and allowed turnings had to be manually adjusted along with the demand to further minimise discrepancies with observations. The comparison between simulated and observed traffic flows shows a $R^2$ of 0.77 (Fig. 2b).

The calibration of the BCN-VML estimated vehicle speed was done based on three different sources of information: (I) TomTom GPS-based historical hourly average speeds (TomTom, 2019), (II) average speed circulation statistics reported by the Barcelona city council (Ajuntament de Barcelona, 2017) and (III) measured hourly speed values reported from permanent detectors located in the suburban ring-roads (Barcelona city council, Mobility and transport department, personal communication, 2017). The comparison between simulated and observed speed values (hourly maximum and daily average) is summarised in Fig. 3a. The results are provided separately for the inner city, where the speed limit varies between 30 and 50 km/h, and the ring-roads, where the speed limit varies between 60 and 80 km/h depending on the road section. The BCN-VML vehicle speed overestimated the average speed values at the inner city area by a 65%. Additionally, the hourly speed profiles were neither matching the TomTom speed profiles nor the measured hourly speed values (Fig. 3b). The overestimated speed values at the inner city from the BCN-VML output are a consequence of the lack of intersection stopping time. BCN-VML’s speeds are at link level, without considering what happens at nodes (i.e. intersections), hence there is no stopping time for each route, leading to unrealistic high speed values, close to the speed limit. On the other hand, the wrong speed profiling from BCN-VML is related to the traffic assignment methodology. STA estimates speeds by the volume delay functions, which depends directly on the traffic flow of the simulated hour, generating an artificial speed profile which does not represent correctly the speed behaviour. In reality, traffic speed is not directly proportional to traffic flow. Instead, it has a steady value near to maximum until congestion is achieved, which happens at a certain point of traffic density, as reported in Thomson and Bull (2002). This behaviour is characteristic of STA and will be explained in Section 3.3 when compared with a microscopic DTA approach. To overcome this, the substitution of the BCN-VML estimated speeds by the TomTom speed values would only partially solve the issue. As seen by Fig. 3b TomTom speeds underestimate the observed values at the city ring-roads. This bias in TomTom speed values has already been seen in other studies (Gwara, 2017) and a possible reason could reside in that most of the people using these devices in the city are unfamiliar with the route they are following and therefore their speed is lower than the average of other vehicles. The solution applied to correct the estimated vehicle speeds goes through two steps: (1) the BCN-VML speed profile was replaced by the TomTom-based speed profiles, and (2) the estimated speeds by the BCN-VML at the inner city were reduced with a scalability factor obtained from the observed average urban speed. The corrections to the estimated speed profile and maximum speed are shown in Fig. 3.

2.2. HERMESv3: Macroscopic emission modelling

The emission model used is the High-Electic Resolution Modelling Emission System version 3 (HERMESv3) developed at the Barcelona Supercomputing Center (Guevara et al., 2020). HERMESv3 estimates anthropogenic emissions at high spatial- (e.g. road link level) and temporal- (hourly) resolution using state-of-the-art and bottom-up calculation methods that combine local activity and emission factors along with meteorological data.
For road transport, HERMESv3 computes hourly exhaust (hot and cold-start), and non-exhaust emissions (tyre, road and brake wear and resuspension) per vehicle category and road link for all criteria pollutants (NO\textsubscript{x}; CO; non-methane volatile organic compounds, NMVOC; SO\textsubscript{2}; NH\textsubscript{3}) and particulate (PM\textsubscript{10}; PM\textsubscript{2.5}; black carbon, BC; organic carbon, OC). A total of 491 vehicle categories are considered, discriminated by vehicle and fuel type, EURO category, engine power and gross weight class.

Exhaust and wear emissions are computed using the vehicle and speed dependent emission factors reported by the Computer Programme to calculate Emissions from Road Transport version V (COPERT V) (EMISIA, 2016), which are included in the tier 3 approach of the European emission inventory guidelines EMEP/EEA (EMEP/EEA, 2017). Emissions from resuspension processes are estimated using vehicle type dependent emission factors (i.e. motorcycles, passenger cars, light duty vehicles, heavy duty vehicles), which were derived from a measurement campaign performed in Barcelona (Amato et al., 2012). The temperature effect on emissions considered by the cold-start is based on the hourly temperature data from the CopernicusERA5 dataset (C3S, 2017).

With the objective of assessing the performance of the emission model, we compared the COPERT V emission factors used in HERMESv3 against measured-based emission factors derived from a Remote Sensing Device campaign performed in Barcelona in 2017 (AMB and RACC, 2017). The results of this comparison can be found in (Rodriguez-Rey et al., 2018) and show a good agreement between the modelled and measured emission factors for all cases.

Most of the activity input data needed by HERMESv3 (e.g. mean vehicle speed, annual average daily traffic) is provided in a multilane shapefile, for which each row contains the information of a specific road link. Specific vehicle fleet composition profiles, business-as-usual daily traffic flow and speed temporal profiles are also assigned to each road link. The fleet composition profiles used by HERMESv3 are derived from the remote-sensing campaign mentioned above and information provided by the Barcelona’s Port Authority (Port de Barcelona, 2017). A total of five different fleet composition profiles were generated and assigned to different regions of the city (Fig. 4), which were classified as follows: (I) Inner city, with a large presence of motorbikes and mopeds, used in all urban links, (II) eastern ring road, since it is the main in route and out route for the port, heavy duty vehicles have a higher presence than in other areas, (III) port, links on the harbour area are massively dominated by heavy duty vehicles, (IV) western ring road, its composition is dominated by passenger cars, with a low presence of two-wheelers and heavy duty vehicles and (V) highway, motorbikes are practically nonexistent and is dominated by passenger cars and some heavy duty vehicles.

2.3. Coupling BCN-VML and HERMESv3

Fig. 5 shows the schematic workflow of the BCN-VML and HERMESv3 coupling (further referred as VML-HERMESv3). BCN-VML simulates private vehicle and public bus transport using independent approaches the results of which are then combined into a multilane shapefile read by HERMESv3. The upper part of the Figure describes the private transport process and the bottom part the public bus transport one.

Private transport demand is defined by an aggregated 24 h OD matrix for a business-as-usual day, which is disaggregated into hourly OD matrices by applying hourly traffic flow profiles derived from the local traffic loop detectors. Traffic assignment is done by an iterative user’s optimum static equilibrium assignment (STA) for each hour, which results in a shapefile of the whole domain that includes the simulated hourly traffic speed and volume per link. Emissions from public buses are differentiated from the rest of the fleet as they cannot circulate through all the network and have a different vehicle share composition. To reduce computational time, the public bus transport flow is calculated using the bus frequency and the number of bus lines going through each link while its speed is estimated with a proxy using the private transport speed, as described below.

The following processes are script-based. The code combines the private and public bus transport data and generates the vehicle flow profiles required by HERMESv3. Speed profiles are substituted with the TomTom data, as described in Section 2.1.1. Bus speed on each section is estimated with the section’s private transport speed and adapted with a factor obtained from the observed average urban bus speed in the city (TMB, 2020). Then, according to different specific network properties, each segment is tagged with its
Fig. 4. BCN-VML domain showing the road types classification used. The grey area shows the limits of the municipality of Barcelona, black segments represent all urban links, inside and outside Barcelona municipality, red and green links indicate eastern and western ring-road respectively, clear brown links represent the port and clear blue links highways. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 5. Schematic representation of the VML-HERMESv3 coupling, including: Input data, main and intermediate processes and output data. The upper part of the workflow describes the steps associated with private transport while the bottom part describes the public bus transport.

respective zone (e.g. inner city, western ring road, port...). The zone tag will be later read by HERMESv3 to assign the respective fleet composition, prepared aside.

HERMESv3 uses the resulting private and public bus transport multiline shapefile to estimate total hourly emissions per link according to the traffic flow, average link speed and vehicle fleet composition information associated to each section along with the COPERT V emission factors and meteorological information.

2.4. Aimsun–PHEMLight: Microscopic coupled system

We compare our macroscopic coupled system to a microscopic coupled system composed of the traffic simulator Aimsun Next (Barceló, 2011) and the instantaneous emission model PHEMLight (Reixis et al., 2014) over a small area of the city. Aimsun Next allows estimating the position and speed of every vehicle in the network based on its car-following model. PHEMLight is a simplified version of PHEM (Passenger car and Heavy duty Emission Model) that works with instantaneous vehicle specific power developed to work with a traffic simulator. A schematic workflow of the coupling is shown in Fig. 1.
The study domain is localised in an area of 0.4 km$^2$ (Fig. 6) and includes three main urban corridors in Barcelona representative of free flow, normal flow and heavy congestion conditions, respectively: (I) Aragó St., a six-lane street with a daily traffic flow of 80,000 veh/day and a green wave traffic light synchronisation that allows a fluent flow throughout, (II) Aribau St., a four-lane street with a daily traffic flow of 23,000 vehicles per day and (III) Balmes St., a four-lane street with a daily traffic flow of 35,000 vehicles per day.

The Aimsun road network was built based on Open Street Map (OpenStreetMap contributors, 2019), which was manually modified to fulfil all the model requirements. Traffic signalisation, reserved bus lanes and permitted turnings were applied according to on-site observations.

Since our goal is to assess the behaviour of VML-HERMESv3, the traffic flow was calibrated according to BCN-VML results for each street, rather than with the observed traffic counts of the area. The fleet composition used to estimate vehicle emissions with PHEMLight is the same as the “inner city” fleet composition used in the HERMESv3 emission model, described in Section 2.2.

3. Results and discussion

In this section the annual emission results from the VML-HERMESv3 system are shown and compared against other available studies along with a discussion of their temporal and spatial distribution. Section 3.2 introduces and discusses the impact on emissions of different key features of the macroscopic coupling system. Finally, in Section 3.3 we use the microscopic system described in Section 2.4 to quantify and understand the inherent limitations of the macroscopic approach under multiple traffic congestion conditions.

3.1. Annual emission modelling results

The VML-HERMESv3 was used to perform an annual simulation of 2017 for the domain represented in Fig. 2.

The NO$_x$ simulation results, at 30mx30 m resolution are shown in Fig. 7a. Major urban corridors are the ones with higher emissions together with the sub-urban ring-roads and main city accesses. This distribution in emissions is in agreement with the business-as-usual daily traffic flow shown in Fig. 2a. Due to the high proportion of HDV the port area also presents a relative high emission level despite its low vehicle flow. A representation of the temporal and spatial variation of emissions simulated by the VML-HERMESv3 system at the municipality of Barcelona can be seen in the upper and lower images of Fig. 8, respectively. The monthly profile clearly shows a strong emission decrease occurring during the month of August (approximately $-26\%$), which is mainly due to summer holidays. At the weekly level, emissions remain almost constant during the weekday and are followed by a strong weekend decrease ($-41\%)$. The hourly time profile shows how emissions reach a maximum level of activity at morning (between 07:00 and 08:00 h) and remain at or around this level for the rest of the day-time period (i.e. until 18:00 h).

In terms of spatial distribution, it is observed that the district of Eixample is the area of Barcelona with the largest amount of NO$_x$ emissions per square kilometre (291 kg day$^{-1}$ km$^{-2}$). Despite its relative small size (7.47 km$^2$), this district includes some of the main arterial and high-capacity roads connecting multiple areas of the city and therefore concentrates a large amount of traffic activity. On the contrary, two neighbouring districts of Eixample (Ciutat Vella and Gràcia) have around half of Eixample's
emissions (144 and 150 kg day\(^{-1}\) km\(^{-2}\), respectively). These two districts are the ones with the largest fractions of traffic-calming and pedestrian areas. In Section 3.2.1 the spatial variations of NO\(_x\) emissions in Barcelona are further discussed.

The total annual NO\(_x\) and PM\(_{10}\) emissions for the municipality of Barcelona were compared against two datasets that also rely on the COPERT emission factors to estimate vehicle emissions: (I) A local emission inventory done by Barcelona Regional (BR) (Regional, 2019), which corresponds to the year 2017 and (II) A report from the City Hall of Barcelona corresponding to the year 2013 (Ajuntament de Barcelona, 2015) (Fig. 7b). The VML-HERMESv3 model estimates a \(-5\%\) and a \(+9\%\) NO\(_x\) than the City Hall and the BR reports, respectively. For the first, the difference could be due to the older fleet composition of 2013, associated with higher emission factors. For the second, the difference might be caused by the applied mileage correction used in HERMESv3 for all petrol and diesel vehicles. On the other hand, the discrepancies for PM\(_{10}\) are higher. The VML-HERMESv3 model estimates are \(+18\%\) and \(+105\%\) larger than the ones provided in the City Hall and BR reports, respectively. These differences may be at least partly due to the inclusion of resuspension in VML-HERMESv3. Exhaust PM emissions have been progressively reduced with the introduction of new vehicle technologies (Guevara, 2016). Therefore, the 2013 City Hall report exhaust PM estimates should be higher than those provided by VML-HERMESv3 and the BR report. However, when adding the non-exhaust (resuspension) PM emissions on top of exhaust PM emissions, we end up with the values shown in Fig. 7b. A detailed explanation regarding non-exhaust emissions can be found in Section 3.2.4.

3.2. Sensitivity to key implemented features

This section provides a thorough emission sensitivity analysis of some of the key input parameters of the VML-HERMESv3 macroscopic coupling system, including: Vehicle fleet composition, public bus transport distribution, meteorology and non-exhaust sources. Unless otherwise stated, for each case the VLM-HERMESv3 coupled system was run using two different versions of the input dataset for a complete working day. The resulting emission results are then compared and discussed.

3.2.1. Vehicle fleet composition

In this section we aim to highlight the importance of a spatially-distributed vehicle fleet composition on large domains. To do so, the estimated emissions using the observed vehicle fleet composition of the VML-HERMESv3 system described in Section 2.2 (further referred to as COMPO-OBSERVED) are compared against the emissions obtained using the censed vehicle fleet composition for Barcelona (further referred to as COMPO-CENSED). The COMPO-CENSED was derived from the official registration statistics provided by the Spain’s national traffic authority (Dirección General de Tráfico (DGT), 2019) and consist of a unique vehicle fleet composition profile that is applied homogeneously to all the road links of the working traffic network. Table 1 summarises the shares of the different vehicle categories (i.e. Passenger cars, light duty vehicles, motorcycles, mopeds and heavy duty vehicles) reported by each one of the profiles considered.

The emission results obtained using each one of the vehicle composition profile datasets are summarised in Table 2. Overall, total NO\(_x\) and PM\(_{10}\) emissions are slightly higher when using the COMPO-OBSERVED profiles (+5.8% and +7.4%, respectively). Nevertheless, important discrepancies appear when performing the comparison at the zone level.
1. The inner city presents a low discrepancy between emission results (−5.2% NO\textsubscript{x} and −7.5% PM\textsubscript{10} when using COMPO-OBSERVED), which is in line with the fact that both datasets present similar shares of general vehicle categories (Table 1). Discrepancies are mainly related to the different age and fuel distributions assumed in each case. For instance, in the case of passenger cars, the average age is of 8 years in the COMPO-OBSERVED dataset, whereas in the COMPO-CENSED is of 11 years.

2. At the port the predominance of HDV on the COMPO-OBSERVED (46% of the total vehicle share) enlarges NO\textsubscript{x} and PM\textsubscript{10} emissions by +788% and +279%, respectively.

3. The COMPO-OBSERVED eastern ring road NO\textsubscript{x} and PM\textsubscript{10} emissions are a +33.2% and a +60% higher than the COMPO-CENSED. This difference is due to the large amount of cargo vehicles (HDV and LDV) on the COMPO-OBSERVED. Note that the high difference in PM\textsubscript{10} is due to wear emissions, which increase with increasing speed, and resuspension which increase with vehicle weight.

4. For the bus fleet, the COMPO-OBSERVED has a 41.84% of CNG buses in contrast with the 5% from the COMPO-CENSED. This leads to NO\textsubscript{x} and PM\textsubscript{10} emission estimates a −17% and −7.4% lower for the COMPO-OBSERVED dataset in respect to the COMPO-CENSED. Note that the CNG-bus emission factor for NO\textsubscript{x} is approximately 60% lower than the diesel bus one.

Although differences in the overall emission estimates are minor, the vehicle share discriminated by zones has shown an important effect on the spatial distribution of the emission estimation.

3.2.2. Public transport bus service

In this section, the emissions from the specific public bus traffic network that was built using the BCN-VML traffic simulator (see Section 2.3) – referred to as BUS_SEP – are compared against an homogeneous distribution of this vehicle category (i.e. 4% of
the total traffic flow) across all the road links included in the domain of study – referred to as BUS_AG. The overall share of 4% is derived from the remote sensing campaign performed in the city. Fig. 9a shows the resulting public bus network and associated daily flow per link information from the BUS_SEP approach. As observed, major urban arterial roads are concentrating most of the bus routes and, subsequently, of the bus flow, while in tertiary and residential streets the number of bus lines is practically null. On the other hand, Fig. 9b shows the computed NO\textsubscript{x} emission difference (BUS_SEP–BUS_AG) at the road link level during the morning peak hour (i.e. 08:00 AM local time). Yellow and red colours indicate higher emissions from BUS_SEP, while blueish colours indicate higher emissions from BUS_AG. At the city level, total estimated emissions are practically equal. The BUS_SEP approach reports a +2% NO\textsubscript{x} and −1% PM\textsubscript{10} emissions when compared to the BUS_AG. Nevertheless, significant differences are observed when performing a comparison at the street level (Fig. 9b). The spatial pattern of the emission differences is in line with the bus flow information reported by BUS_SEP (Fig. 9a). Road links with higher bus flow values are the ones presenting larger NO\textsubscript{x} difference (up to +300%). On the other hand, heavy trafficked streets without bus lanes are highlighted with blueish colours, as a consequence of the higher emissions that the constant bus weight produces using the BUS_AG approach. This pattern is also observed in the port zone, in which the BUS_AG approach reports a 1.6% of buses. Maximum differences between the two approaches are up to +300% and −20%.

### 3.2.3. Temperature effect

For this sensitivity study, the temperature effect on emissions for the coldest day registered in the city of Barcelona during 2017 is simulated (17th February 2017). The observed average daily temperature at a weather station located in the city centre was 8.4 °C (AEMET, 2017). Vehicle emissions increase under cold temperatures due to several mechanical factors, which are represented by two corrections on vehicle hot exhaust emissions. The first, referred to as cold-start emissions, are caused by the extra emissions due to low performance of engine catalytic systems until they reach their optimum temperature, and affects both NO\textsubscript{x} and PM\textsubscript{10} emissions. Cold-start emissions are already considered in COPERT V and have been included in HERMESv3 following the Tier 3 methodology proposed by the EMEP/EEA guidelines as detailed in Guevara et al. (2020). We consider an average trip length of 6.47 km, which is based on the Barcelona mobility report of 2015 (ATM, 2015). The second correction affects NO\textsubscript{x} emission from diesel vehicles (Grange et al., 2019; Federal Office for the Environment, 2018) and it is not considered in COPERT V equations. This increase is associated with the Exhaust Gas Recirculation systems and Selective Catalytic Reduction systems operation at low temperatures. For diesel pre-Euro 6 vehicles NO\textsubscript{x} increase is due to the disconnection of the Exhaust Gas Recirculation system (EGR) at low temperatures to avoid moisture condensation issues. Diesel Euro 6 vehicles are also influenced by cold temperatures since the Selective Catalytic Reduction systems (SCR) they are mostly equipped with need NH\textsubscript{3} for NO\textsubscript{x} conversion, which comes from the AdBlue. AdBlue is converted into NH\textsubscript{3} in a reaction whose efficiency decreases at low temperatures, increasing NO\textsubscript{x} emissions.

To apply this temperature effect, the original COPERT V emission factors included in HERMESv3 were modified according to the temperature and vehicle dependent adjustment factors reported by Matzer et al. (2019).

Emissions for the coldest registered day in Barcelona were simulated under three different scenarios: (I) without considering any correction for cold temperature emissions (Temp_Raw), (II) considering cold-start emissions (Temp_CS), and (III) considering cold-start and NO\textsubscript{x} temperature effect (Temp_CS+CF). Table 3 summarises the NO\textsubscript{x} adjustment factors for diesel vehicles considered in the Temp_CS+CF scenario.

| Area               | PC   | LDV  | Motorcycles | Mopeds | HDV  | Temp_CS+CF | Temp_CS  | Temp_Raw |
|--------------------|------|------|-------------|--------|------|------------|----------|----------|
| Inner city         | 60%  | 15%  | 19%         | 4%     | 3%   | 62%        | 60%      | 62%      |
| Sub_East           | 66%  | 14%  | 8%          | 0%     | 12%  | 62%        | 60%      | 62%      |
| Sub_West           | 77%  | 9%   | 10%         | 0%     | 5%   | 62%        | 60%      | 62%      |
| Port               | 39%  | 9%   | 6%          | 0%     | 46%  | 62%        | 60%      | 62%      |
| Highway            | 74%  | 16%  | 2%          | 0%     | 9%   | 62%        | 60%      | 62%      |

| NO\textsubscript{x} | PM\textsubscript{10} | NO\textsubscript{x} Difference | PM\textsubscript{10} Difference |
|----------------------|-----------------------|--------------------------------|--------------------------------|
| Inner city           | 9,404                  | 9,915                          | −5.2%                          | −7.5%                          |
| Sub_East             | 1,577                  | 1,184                          | 246                            | 153                            | 33.3%                          | 60%                          |
| Sub_West             | 1,120                  | 1,179                          | 166                            | 158                            | −5%                            | 4.8%                          |
| Highway              | 2,766                  | 2,252                          | 405                            | 287                            | 22.8%                          | 40.9%                         |
| Port                 | 1,289                  | 145                            | 57                             | 15                             | 788%                           | 278%                          |
| Bus                  | 2,312                  | 2,787                          | 161                            | 174                            | −17.0%                         | −7.4%                         |
| TOTAL                | 18,469                 | 17,462                         | 2,202                          | 2,050                          | 5.8%                           | 7.4%                          |
Fig. 9. Daily flow representation (n° buses day\(^{-1}\) link\(^{-1}\)) of the BUS_SEP network implemented in the BCN-VML traffic simulator (a) and NO\(_x\) (g h\(^{-1}\) link\(^{-1}\)) difference between the separated bus approach (BUS_SEP) and the aggregated one (BUS_AG) for the 8 AM local time (b). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

| Euro class | Diesel PC correction factor | Diesel LDV correction factor |
|------------|----------------------------|-----------------------------|
| Euro 3     | 1.20                       |                             |
| Euro 4     | 1.35                       | 1.35                        |
| Euro 5     | 1.40                       | 1.35                        |
| Euro 6a,b  | 1.45                       | 1.20                        |
| Euro 6d-temp | 1.00                       | 1.00                        |
| Euro 6d    | 1.00                       | 1.00                        |

Table 3 shows the NO\(_x\) and PM\(_{10}\) emission [kg day\(^{-1}\)] for the coldest day of 2017, without considering temperature effect (Temp_Raw), considering cold-start emissions (Temp_CS) and considering cold-start emissions and diesel NO\(_x\) temperature effect (Temp_CS+CF). Difference exposes the relative difference between Temp_Raw and Temp_CS+CF.

|          | Temp_Raw | Temp_CS | Temp_CS+CF | Relative difference Temp_Raw vs Temp_CS+CF |
|----------|----------|---------|------------|------------------------------------------|
| NO\(_x\) | 15,866   | 16,375  | 18,867     | 19%                                      |
| PM\(_{10}\)| 1,899    | 1,983   | 1,983      | 4%                                       |

Table 4 shows the NO\(_x\) and PM\(_{10}\) emission values simulated for the three scenarios. Estimated NO\(_x\) and PM\(_{10}\) emission for the TEMP_CS scenario are +3% and +4% higher than Temp_Raw, respectively. NO\(_x\) difference increases up to +19% when considering the Temp_CS+CF scenario.

The resulting increased NO\(_x\) emissions are slightly lower than the ones reported by Grange et al. (2019), who estimated an increase between 30% to 45% for the majority of Spain using wintertime air temperatures compared with emissions at 20 °C. It is reasonable a lower NO\(_x\) increase in Barcelona since the city has mild temperatures due to its coastal situation and the urban build provokes higher temperatures than the suburban and rural locations.

3.2.4. Non-exhaust PM\(_{10}\) emissions

In this section, the VML-HERMESv3 model was run with and without the consideration of non-exhaust PM\(_{10}\) emission sources (i.e. road, tyre and brake wear and resuspension). Table 5 shows the aggregated emission factors (EF) considered in HERMESv3 for non-exhaust and exhaust PM\(_{10}\) for the different vehicle groups. These are computed weighting the emission factors of each vehicle technology according to its fractional contribution to the fleet composition in that group and the average urban speed observed in the VLM-HERMESv3 coupled system (28 km/h). Non-exhaust EF for HDV are the largest, followed by LDV, PC and motorbikes. In all cases except motorbikes, EF for total non-exhaust are much larger than for exhaust (from four times more in case of PC to ten times more in the case of HDV).
A comparison between the two simulations shows an increase of PM$_{10}$ emissions of +410% when considering all the non-exhaust sources. Table 6 shows the resulting PM$_{10}$ emissions discriminated by process (exhaust, resuspension and wear). The contribution of non-exhaust sources to total PM$_{10}$ emissions was found to be of 80%, which is in line with the results found by other studies, such as Rexeis and Hausberger (2009) (estimated a contribution between 80 to 90% for 2020 in Europe) and Harrison et al. (2012) (measured a contribution of 77% in London). More specifically, the resuspension process is the one dominating total emissions, with a contribution of 52%. This result is very similar to the one found by de la Paz et al. (2015) for the city of Madrid (contribution of 53%) which is in line with the fact that both cities are influenced by similar dry weather conditions. The current large contribution of non-exhaust to total PM emissions is expected to keep growing on the following years. This is caused by the technological and legislative improvements in PM exhaust emissions combined with a lack of abatement measures for non-exhaust sources (Guevara, 2016).

### 3.3. Limited-area comparison with a microscopic system

This section uses the higher level of detail of the microscopic approach described in Section 2.4 to observe and discuss the possible emission discrepancies with the macroscopic system developed in this study. More precisely, we want to estimate the influence of traffic dynamics and vehicle-to-vehicle interaction on the emission results computed with AIMSUN–PHEMLight microscopic system. The discussion of the emission results is focused on the three urban corridors highlighted in Fig. 6.

A comparison of the hourly NO$_x$ and PM$_{10}$ exhaust emissions computed for each street and coupled system is shown in Fig. 10. Non-exhaust PM$_{10}$ sources were not considered because they are not estimated by the PHEMLight emission model. From the figure, it can be observed that the three streets present higher estimated emission discrepancies during the daytime hours when the traffic flow and congestion levels are higher. However, these modeling differences diverge between the different streets.

### Table 5
Comparison between average PM$_{10}$ non-exhaust and exhaust emission factors [g km$^{-1}$] as a function of the vehicle category and source type.

| PM$_{10}$ [g km$^{-1}$] | Road | Tyre | Brake | Resuspension | Total non-exhaust | Exhaust |
|------------------------|------|------|-------|--------------|------------------|---------|
| PC                     | 0.015| 0.011| 0.008 | 0.023        | 0.056            | 0.014   |
| LDV                    | 0.015| 0.017| 0.012 | 0.082        | 0.126            | 0.020   |
| HDV                    | 0.076| 0.027| 0.033 | 0.460        | 0.596            | 0.062   |
| Motorbikes             | 0.006| 0.005| 0.005 | 0.002        | 0.018            | 0.014   |

### Table 6
Simulated total exhaust and non-exhaust (resuspension, wear) daily PM$_{10}$ [kg] emissions.

|                       | Total PM$_{10}$ | Exhaust | Resuspension | Wear |
|-----------------------|-----------------|---------|--------------|------|
| VML-HERMESv3          | 2,145           | 412     | 1,127        | 606  |
| AIMSUN–PHEMLight      |                 |         |              |      |

### Table 7
Traffic and emission results obtained with the microscopic (AIMSUN–PHEMLight) and macroscopic (VML-HERMESv3) coupled systems for the three streets of study. The volume capacity ratio (V/C), the speed (km h$^{-1}$) and NO$_x$ emissions (kg day$^{-1}$) are presented, as well as the NO$_x$ relative difference between microscopic and macroscopic approach for each street.

|                       | V/C | Speed [km h$^{-1}$] | NO$_x$ [kg day$^{-1}$] | V/C | Speed [km h$^{-1}$] | NO$_x$ [kg day$^{-1}$] | NO$_x$ difference |
|-----------------------|-----|---------------------|------------------------|-----|---------------------|------------------------|-------------------|
| VML-HERMESv3          |     |                     |                        | AIMSUN–PHEMLight |                     |                        |                   |
| Aragó                 | 95% | 26.4                | 39                     | 70% | 38                  | 35                     | −11.7%            |
| Balme                 | 82% | 26.4                | 28                     | 50% | 18                  | 46                     | +65.4%            |
| Aribau                | 47% | 23.3                | 18                     | 25% | 24                  | 20                     | +15.5%            |

Two assumptions can probably explain the emission differences observed above. The first lies in the traffic assignment method used. STA, commonly used in macroscopic traffic models, is unable to propagate queues on the network where the links upstream a bottleneck remain unaffected. On the contrary, STA predicts congestion namely downstream the bottleneck and cannot model spillback. As a consequence, link flow may exceed capacity, there is no queue formation and the demand downstream the bottleneck cannot properly be adjusted. This situation becomes critical in very congested links like Balmes, and therefore can affect the level and location of emissions (Tsanakas et al., 2020). On the other hand, DTA used in microscopic traffic models can model spillback of the queues as traffic demand exceeds capacity. Traffic flow evolves over time and congestion dynamics are modelled in a more realistic way. Queues occur upstream the bottleneck and queue spillback may occur through the network. Under DTA congestion is better located, which has a significant effect on where peak emissions occur as proved by Wismans et al. (2013) and Tsanakas et al.
While Aimsun Next estimates the lowest of the average speeds for Balmes, the corrected BCN-VML speed estimates a similar value than in the other two streets. The second assumption is probably bound with the resolution of the simulation. A macroscopic model does not simulate individual vehicle dynamics, which are of special interest at stop-and-go situations. During these periods engines work consistently at high load provoking strong punctual emission peaks and the idling emissions due to the stopping time as also described by He et al. (2009). Therefore large emission differences are generated in comparison with an average speed emission model, which tends to sub-estimate emissions in stop-and-go conditions as reported by Khreis and Tate (2017) and Tu et al. (2018) among other studies. This pattern can be observed in Fig. 11, which shows the driving cycle (magenta dotted line) and associated NO\textsubscript{x} instantaneous emissions (blue line) of a diesel Euro 4 passenger car simulated by the AIMSUN–PHEMLight microscopic system for Arago St. (Fig. 11a) and Balmes St. (Fig. 11b). The associated emissions simulated by the VML-HERMESv3 macroscopic system are also included for comparison purposes. In Aragó St. the AIMSUN–PHEMLight driving cycle has gradual accelerations and a quasi constant speed during the whole cycle. On the contrary, in Balmes St. the simulated cycle is composed by multiple stop-and-go conditions, which generate high emission peaks. The associated constant NO\textsubscript{x} emissions for the VML-HERMESv3 system are within the range of the microscopic system. It is also important to mention that the associated driving time to cross the analysed street links differs from both approaches. For the congested street (Balmes), the VML model reports a driving time of 125 s, while AIMSUN's microscopic simulated car needs 660 s to cross the same link. This difference is a consequence of the stop-and-go driving behaviour and contributes to the absolute emission difference observed in Fig. 10. This high discrepancy between simulated driving times is not observed in Aragó St. (82 s with AIMSUN versus 86 s with VML) due to the free flow condition.

4. Conclusions

This paper presents the first coupled macroscopic traffic and emission modelling system tailored for Barcelona. This is done by using multiple sources of local measured data such as GPS based speed circulation statistics, automatic loop detectors or the circulating fleet composition and emission results from a remote sensing device campaign. The system is composed of the traffic simulator Barcelona Virtual Mobility Lab (BCN-VML) and the High-Elective Resolution Modelling Emission System version 3 (HERMESv3), which are based on Visum and COPERT V models, respectively.
An annual simulation showing total NO\textsubscript{x} and PM\textsubscript{10} emissions was performed with the developed coupled system. The computed annual emissions for the year 2017 were 3.800 tonnes for NO\textsubscript{x} and 427 tonnes for PM\textsubscript{10}. The computed annual NO\textsubscript{x} and PM\textsubscript{10} emission values were also compared against two local emission inventories. The VML-HERMESv3 NO\textsubscript{x} estimated emissions were in agreement with both inventories showing a discrepancy of −5% and +9%. On the other hand, the PM\textsubscript{10} differences were higher, up to +105%. This is believed to be caused by the high uncertainty of PM\textsubscript{10} estimates, and the consideration of all PM non-exhaust sources by the VML-HERMESv3 system.

A sensitivity analysis was performed to quantify the variability of NO\textsubscript{x} and PM\textsubscript{10} estimated emissions to different input parameters, including vehicle fleet composition, public bus transport implementation, temperature and non-exhaust PM sources. Moreover, a comparison of the VLM-HERMESv3 macroscopic coupled system with a microscopic coupled system composed by the Aimsun Next traffic simulator and the PHEMLight instantaneous emission model (AIMSUN–PHEMLight) was also performed in a hot spot of the city.

The main findings of the sensitivity analysis and intercomparison exercise are summarised below:

- Vehicle fleet composition: High emission differences were found when using the real circulating area-dependent fleet composition versus the homogeneous censed one. These were mostly influenced by the HDV presence from the port area, the fuel (gasoline or diesel) used and the vehicle age.
- Public bus network: The usage of real bus routes showed strong street gradient differences in several sections of more than +300% for NO\textsubscript{x} when compared with a constant bus share of 4% for the whole network. In contrast, reductions up to −20% in NO\textsubscript{x} emissions were found in sections without bus routes.
- Meteorological influence: An increase of +19% in NO\textsubscript{x} and +4% in PM\textsubscript{10} was found when considering the effect of cold-start and diesel NO\textsubscript{x} temperature-dependent processes. Although in Barcelona the temperature effect is reduced due to its mild weather, this can have a significant influence upon the overall emissions in colder regions.
- Non-exhaust PM sources: The inclusion of wear processes (i.e., tyre, brakes and road) and resuspension resulted in an increase of +410% of PM\textsubscript{10} emissions. Road resuspension, a process which is not considered in COPERT V, was found to be the largest contributor to non-exhaust emissions, representing a 50% of the total.
- Macroscopic versus microscopic approach: The congested traffic situation showed the highest discrepancies in NO\textsubscript{x} emissions (up to 65%) between the macroscopic and microscopic approached. In contrast, during free flow, differences were small, with +11% more NO\textsubscript{x} estimated by the macroscopic system. The DTA versus the STA and the individual vehicle dynamics characterisation of microscopic system versus the macroscopic traffic representation were found to be the reasons for such differences.

This research shows how the combination of several input parameters has a key role on the estimated overall and street level gradient emissions. Additionally, the usage of macroscopic or microscopic approaches influences emission estimation, specially in
high loaded streets where the macroscopic models show some limitations for which the modeller should be aware of. Although the estimated results of microscopic approach are more precise, its high data demand and computational load limits its application to very localised sites. Nowadays, the simulation of large urban areas can only be done by a macroscopic or mesoscopic approach, where several specific input parameters can be improved to better assess traffic emissions, as shown in this study. The applicability of the developed system to other areas is conditioned to the available local data. This is especially important for the build and calibration of the traffic model and the vehicle fleets used. Regarding the emission factors, the COPERT ones can be used as far as the domain is European. Otherwise, there should be a mapping between the COPERT vehicle categories and the local ones.

4.1. Future research

Additional improvements on the STA simulation could be considered in order to improve vehicle dynamics on congested situations. Tsanakas et al. (2020) applied the so called “quasidynamic” network loading on a STA simulation, which improved the simulated traffic dynamics during congestion. On another matter, the higher resolution of a microscopic traffic emission model was used by Rakha et al. (2011) using synthetic drive cycles generated with aggregated link traffic data from the mesoscopic traffic model (e.g. average speed, average stop duration or number of vehicle stops per unit distance).

On further steps of the research the capabilities of the presented macroscopic system will be used to evaluate the application of traffic management strategies in Barcelona. The generated response in emissions to the induced traffic changes allows to estimate the traffic emission impact that different mobility policies could have. The addition of a street dispersion model will also allow to quantify the air quality impact of the simulated mobility policies. The flexibility of the traffic-emission system combined with the performed refinement of the typically uncertain traffic emission parameters is expected to improve the simulated pollutant concentration values used for air quality assessments and health studies in Barcelona.

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CRediT authorship contribution statement

Daniel Rodriguez-Rey: Designed the research, Participated on the building and calibration of the BCN-VML model, Performed the model coupling process and ran the experiments, Prepared the paper. Marc Guevara: Designed the research, Supervision, Assisted the experiments. Mª Paz Linares: Designed the research, Participated on the building and calibration of the BCN-VML model. Josep Casanovas: Designed the research. Juan Salmerón: Participated on the building and calibration of the BCN-VML model. Albert Soret: Designed the research. Oriol Jorba: Supervision. Carles Tena: Assisted the experiments. Carlos Pérez García-Pando: Supervision.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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