

Influence of different complexity levels of road traffic models on air quality modelling at street scale

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Abstract

Urban mobility accounts for 38% and 19% of nitrogen oxide (NO_x) and particulate matter (PM) emissions at European urban areas, respectively. Despite of all the technological development around automobile industry, urban areas are still facing problems related to exposure to high levels of air pollutants. Increase the accuracy of both emissions and air quality modelling from road traffic is a key-issue for the management of air pollution in road transport sector. This study assessed the influence of using different road traffic emission models on the accuracy of air quality modelling with street level resolution, having as case study an urban area located on the centre region of Portugal. Two emission models, with different complexity levels regarding the ability to characterize the traffic dynamics were analysed, namely, TREM (Transport Emission Model for Line Sources) and VSP (Vehicle Specific Power), based on data obtained in an experimental campaign. To perform the air quality simulations the VADIS (pollutant DISpersion in the atmosphere under VAriable wind conditions) model was used and two pollutants were analysed: NO_x and PM₁₀. The results showed that the magnitude of PM₁₀ and NO_x concentrations were result of a conjoint influence of traffic dynamics and meteorological conditions. Comparison between measured and modelled data showed that the VADIS model could track the evolution of NO_x levels, for both emission models considered, displaying a high correlation (>0.8) between traffic-related NO_x emissions and NO_x concentrations. For PM₁₀, VADIS model is more sensitive to the differences in the emissions calculation; however, it was observed that the traffic-related PM₁₀ emissions accounts 1.3 – 8.4% to the PM₁₀ concentration levels at the study area.

Keywords: CFD modelling, experimental campaign, emissions modelling, street air quality, road traffic

1. Introduction

In the European Union (EU) 72% of the population lives in urban areas, i.e. 42% in cities and 30% in towns and suburban areas (Eurostat, 2015, EEA, 2016a). These numbers show a high demand on transport needs in urban areas; the tendency shows that transport needs tend to grow, increasing the pressure in this sector. Emissions due to road traffic sector are known to make a large contribution to air pollution on urban areas, especially to the particulate matter with an aerodynamic diameter less than or equal to 10 µm (PM₁₀) and nitrogen oxides (NO_x) concentrations (Masiol et al., 2012; Rissler et al., 2012; Pant and Harrison, 2013). In recent years, air quality patterns in Europe have improved due to the implementation of effective policies and

44 actions to reduce air pollutants emissions. At the transport sector a set control measures of road-
45 traffic emissions was implemented, such as the introduction of Euro emission standards and
46 consequently the installation of catalytic converters and diesel particulate filters in vehicles, have
47 decreased total emissions of NO_x, PM and carbon monoxide (CO) from road transport (EEA,
48 2015a). In fact, these reductions were more significant in CO emissions (70% between 2000 and
49 2013). Additionally, the introduction of fuel quality standards, namely limiting sulphur and banning
50 lead, contributed to a decrease of emissions, such as sulphur oxides (SO_x) (EEA, 2015a).

51 Despite of that, in 2014, passenger cars emissions of NO_x increased by 3.3% (EU-28) due to an
52 increase of transport activity and an increase in the number of diesel cars in Europe, being the
53 first annual increase since 1990 (EEA, 2016b). Currently, up to 30% of European citizens living
54 in cities are still exposed to air pollution levels exceeding European Union air quality standards
55 (EEA, 2014, 2015b). According with the European Environment Agency (EEA), in the EU-28, in
56 2013, the exposure levels has been estimated as causing 436k deaths due to PM_{2.5} (particulate
57 matter with an aerodynamic diameter less than or equal to 2.5 µm) exposure, 68k due to NO₂
58 exposure and 16k due to O₃ exposure, per year (EEA, 2016a). In Portugal, the impacts of road
59 traffic emissions on air quality are mostly noticeable in high and medium-sized urban areas. Air
60 Quality Plans (AQP) have been developed for these areas since 2001 for PM₁₀ and NO₂, and
61 more recently for ozone (O₃) (Miranda et al., 2015). Despite some improvements on air quality
62 levels after the AQP implementation, recent data still indicate exceedances to the legal limit
63 values, thus assessment of PM₁₀ and NO₂ concentrations at local scale is still required. Air
64 pollution is still a current issue alarmingly threatening human health and well-being in urban areas
65 (Costa et al., 2016).

66 Computational Fluid Dynamics (CFD) methods became widely used on air quality studies at local
67 scale due to their capability to deal with complex structure of air flows and turbulence (Tominaga
68 & Stathopoulos, 2013; Lateb et al., 2015). Despite the complexity behind the development of
69 these models, the accuracy and precision of their results are often low and usually associated
70 with the emission inventories used as input in those models (Taghavi et al., 2005). Urban emission
71 inventories with higher temporal and spatial resolution are needed for several applications, such
72 as urban air pollution modelling, population exposure modelling, definition of sustainable urban
73 development policies, etc. In the case of road traffic, the most commonly used technique to
74 quantify the emissions is based on the principle that the average emission factor for a certain
75 pollutant and a given type of vehicles vary according to the average speed during a trip (Thunis
76 et al., 2016). For urban applications, hourly emissions for each road link are usually required.
77 Uncertainty of these data, as well as uncertainty associated with the resulting emissions, is an
78 important scope of research. Atmospheric emission inventories are usually quantified using one
79 of the two approaches: i) top-down, based on the disaggregation process of total emissions from
80 a certain area to smaller administrative units or a regular grid with higher resolution (Eicker et al.,
81 2008); and ii) bottom-up, based on emission estimation using detailed data of each emission
82 source. The top-down approach is very useful when local detailed information about the emissions
83 of different activity sectors are scarce (Palacios et al., 2001). A study conducted by Coelho et al.
84 (2014) have used a combination of different road traffic emissions models based on a bottom-up
85 and a top-down approach to assess if the outputs of an air quality model can be improved in a
86 regional level. The study concluded that the bottom-up approach would be most suitable used at
87 an urban level, when PM₁₀ concentrations are a major concern (in terms of exceeding the air
88 quality standards established for this pollutant). The availability of input data in terms of quantity
89 and quality is pointed as a relevant issue when the bottom-up approach is applied.

90 The use of Computational Fluid Dynamics (CFD) models allied with the inclusion of reliable
91 emissions for road-traffic are preponderant to define and evaluate the impacts of different
92 measures and scenarios to enhance air quality at urban areas. The aim of the presented work is
93 to characterize the air quality of a typical medium-size city and to compare the influence of

94 different traffic emission models, based on the bottom-up emission approach, in the performance
95 of the CFD model VADIS. For that, two different pollutants were considered, the PM₁₀ and NO_x.
96 A neighborhood area located in Aveiro city (centre region of Portugal) was considered as case
97 study, which is characterized by a high traffic intensity. This work is distinguishable from previous
98 air quality studies conducted at the same region, due to the applied methodology that provides
99 an accurate and highly spatially resolved road traffic emission (by means of real measured traffic
100 data) and air quality data (at street scale). This feature allied to the evaluation of how different
101 complexity levels of road traffic emission data influence air quality model performance (given an
102 outlook regarding the uncertainties) at street level is quite novel. This work is a multidisciplinary
103 study that addresses different components of the atmosphere and its linkages with the
104 anthroposphere. Highly spatial data have been identified as a key component of a decision-
105 support tool for the analysis and evaluation of a variety of air quality and climate change policies,
106 which linked to the need of accomplish the sustainable development goal of make cities
107 sustainable and resilient, shows the pertinence and relevance of the followed work.

108 The paper is structured as followed: section 2 describes the case study and the modelling setup
109 methodology, including a brief description of the applied models and their configuration for the
110 simulations. The air quality status of the study area is characterized in section 3. A comparative
111 analysis of the emission models approaches and its influence on the accuracy of the air quality
112 model results is also presented in section 3. Conclusions follow in section 4.

113

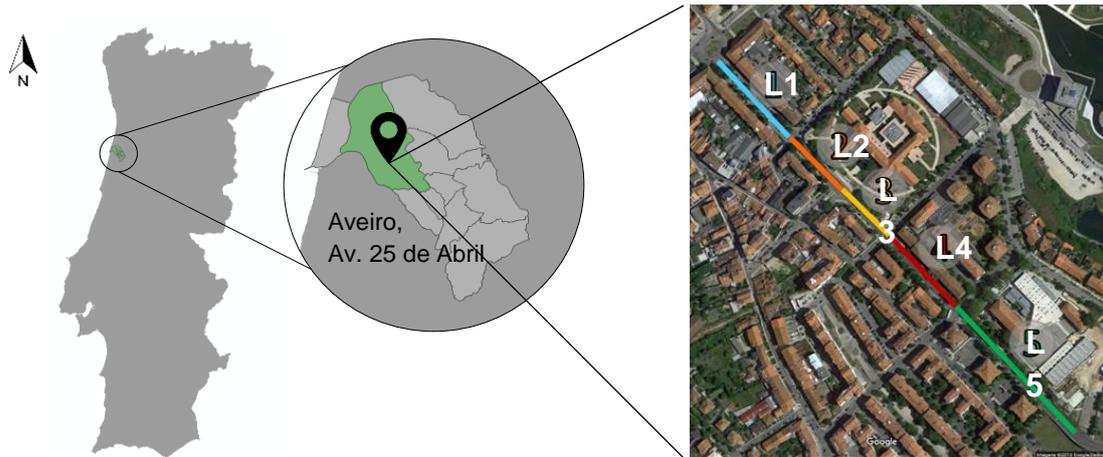
114 **2. Data and Method**

115 2.1. Case study description

116 A main avenue of the city of Aveiro, a medium-size city in Northwest Portugal, called *Avenida 25*
117 *de Abril* (Fig. 1) was selected as case study. This avenue is located near the city centre,
118 surrounded by residential buildings (building blocks of similar height) and two schools. The case
119 study is located in one of the most important thoroughfares of the city (responsible for the majority
120 of the road traffic emission of the neighbourhood – around 80%) which crosses several secondary
121 roads (with low road traffic volume). An Air Quality Station (AQS), classified as urban traffic
122 according to the type of emission source, is built-in in the middle of the avenue. The AQS is
123 monitoring the concentration of multiple pollutants, which makes the case study an ideal case,
124 since allows a comparison between the CFD model results and the real-world measurements.

125 Several studies have been performed through the years in this area. The most recently, performed
126 by Valente et al. (2014), assessed the individual exposure of a set of student's to carbon
127 monoxide concentrations, inside the classrooms, related to road traffic emissions. This study
128 shows, through a local scale computational approach, that the individual exposure of pedestrians
129 in an urban area is extremely spatially dependent, as a consequence of the wind flow and air
130 pollutant dispersion patterns and characteristics. Also, their exposure in the indoors varies along
131 with the outdoor concentration's. These results reinforce the need to perform studies on outdoor
132 air quality, particularly in urban areas where schools and hospitals take place and where
133 susceptible population groups spend a high amount of time, focused on road traffic as emission
134 source. Guarantee the accuracy of these emission estimations, at local scale, is crucial to reduce
135 the errors related to numerical models application. This will enable, for example, the assessment
136 of urban planning options to enhance air quality and to reduce population exposure.

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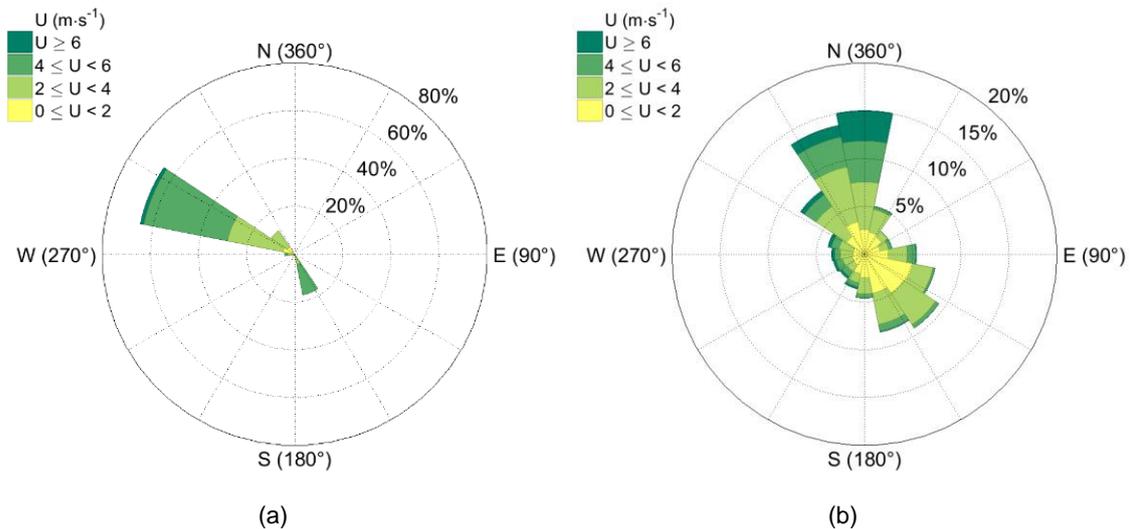


138

139 Fig. 1. Geographical location of Aveiro, Avenida 25 de Abril: Centre region of Portugal. Avenida 25 de Abril
 140 is located in the centre region of mainland Portugal, in the municipality of Aveiro at $40^{\circ}38'14.9''N$ $8^{\circ}38'54.5''W$
 141 (Google earth V10, SIO, NOAA, United States Navy, NGA, GEBCO, Image Landset, Image IBCAO,
 142 <http://www.earth.google.com> [November 20, 2017]). Five link numbers (left image) highlights the *Avenida*
 143 *25 de Abril* length. Each link is identified with a distinct colour: L1 with a blue colour, L2 with an orange
 144 colour, L3 with a yellow colour, L4 with a red colour and L5 with a green colour.

145

146 To accomplish the purposed goal, an experimental campaign (on 7th of February 2017) was
 147 performed in this avenue to characterize the traffic flow (speed, time and distance) and to count
 148 the number of vehicles which use this road in an hourly basis. This data was used as an input for
 149 the traffic emissions models (see section 2.2.1). Fig. 2a characterizes the meteorological
 150 conditions (wind velocity and wind direction) for the experimental campaign day, measured in a
 151 meteorological station located closed to the study area.



152 Fig. 2. a) Wind rose with meteorological data for 7th of February of 2017. b) Wind rose obtained from the
 153 meteorological measured data at the station located near the study area, for the period between 2012 and
 154 2016.

155

156 The wind velocity and direction values were acquired at 10 m high, by a meteorological station
 157 which is located nearby the computational domain. These data describe the average hourly wind
 158 flow conditions that were used as inflow boundary conditions for the simulations (see section 2.2).

159 It can be observed that the wind direction was approximately constant from west-northwest
 160 (WNW) (Fig. 2a), indicating that the main street canyon is in line with the incoming flow.
 161 Noteworthy oscillations in the wind velocity were observed during the study period, with a
 162 maximum variation between 2 and 6 m·s⁻¹. The data acquired on the last five-years (2012-2016)
 163 in the meteorological station were also analysed (Fig. 2b), showing that the wind blows from the
 164 north-westerly quadrant with a frequency of more than 40%, with the majority of the wind speed
 165 comprised in a range of 2 – 6 m·s⁻¹. The period of the experimental campaign is therefore
 166 representative of the typical meteorological conditions of the study area, corresponding also to
 167 neutral stability conditions, in agreement with the numerical approach adopted in this study.

168

169 2.2. Modelling setup

170 2.2.1. Emission approaches

171 The experimental campaign was performed with the application of emissions models based on a
 172 bottom-up approaches. For vehicle dynamic monitoring three different light-duty vehicles (Table
 173 1) were equipped with Global Navigation Satellite System (GNSS) data loggers to collect second-
 174 by-second trajectory data and covering a total of 128 km and 160 runs in each direction. For traffic
 175 flow monitoring, two static video cameras were used, one located at the beginning and another
 176 located at the end of the road segment.

177

178 Table 1. Data Collection Vehicles Characterization.

Vehicle Name	Type of fuel	Year	Engine Size (L)	Horsepower
<i>Opel Astra</i>	Gasoline	2006	1.3	90
<i>Renault Scenic</i>	Gasoline	2004	1.5	100
<i>Toyota Yaris</i>	Diesel	2016	1.0	75

179

180 The avenue with 0.7 km was divided in five different links based on the intersections connections
 181 (Fig. 1) and the total emissions were calculated for each link. Two intersections are controlled by
 182 traffic lights. Hourly averaged PM10 and NOx emissions for the main avenue of the study area
 183 were estimated by applying the Vehicle Specific Power (VSP) model and the Transport Emission
 184 Model for Line Sources (TREM).

185

186 VSP

187 The VSP model is based on vehicle specific power concept for estimating vehicular emissions
 188 (USEPA, 2002). This model represents the sum of the loads resulting from aerodynamic drag,
 189 acceleration, rolling resistance, and road grade, all divided by the mass of the vehicle (Palacios,
 190 1999). VSP values are categorized in 14 modes. Modes 1 and 2 represents deceleration modes,
 191 mode 3 includes the idle mode, while VSP modes 4 to 14 represent combinations of positive
 192 accelerations and growing speeds. Equation (1) provides the VSP calculation for passenger
 193 vehicle (USEPA, 2002). Then for each mode a specific emission factor is assigned to estimate
 194 NOx and PM emissions.

$$195 \quad VSP = v \times [1.1 \times a + 9.81 \times \sin(\arctan(\text{grade})) + 0.132] + 0.00032 \times v^3 \quad (1)$$

196 where *VSP* is the Vehicle Specific Power (kW·ton⁻¹), *v* is the vehicle instantaneous speed (m·s⁻¹),
 197 *a* is the vehicle instantaneous acceleration or deceleration (m·s⁻²) and the *grade* is the terrain

198 gradient (decimal fraction). The VSP methodology was applied based on the national fleet sample
199 based on COPERT software (Computer Programme to calculate Emissions from Road Transport)
200 related with national fleet (23% - diesel vehicle with more than 2500 cm³, 34% - diesel vehicle
201 until 1900 cm³, 36% - gasoline vehicle until 1400 cm³, 6% - gasoline vehicle until 1800 cm³. and
202 0,6% gasoline vehicles with more than 2000 cm³) (Emisia SA, 2017).

203

204 **TREM**

205 TREM was firstly developed on the basis of COST319/MEET approach and focused on CO, NO_x,
206 Volatile Organic Compounds including methane, carbon dioxide, sulphur dioxide and PM10
207 (Borrego et al. 2000, 2003, 2004; Tchepel et al., 2012). The prime objective of TREM is the
208 estimation of road traffic emissions with high temporal and spatial resolution to be used in air
209 quality modelling. Although the average-speed approach for the emission factors implemented in
210 the model follows the European guidelines (EMEP/EEA 2010) the way how transport activity data
211 are considered for the emission inventorying is conceptually different. Roads are considered as
212 line sources and emissions induced by vehicles are estimated individually for each road segment
213 considering detailed information on traffic flow, in this case, obtained in the experimental
214 campaign.

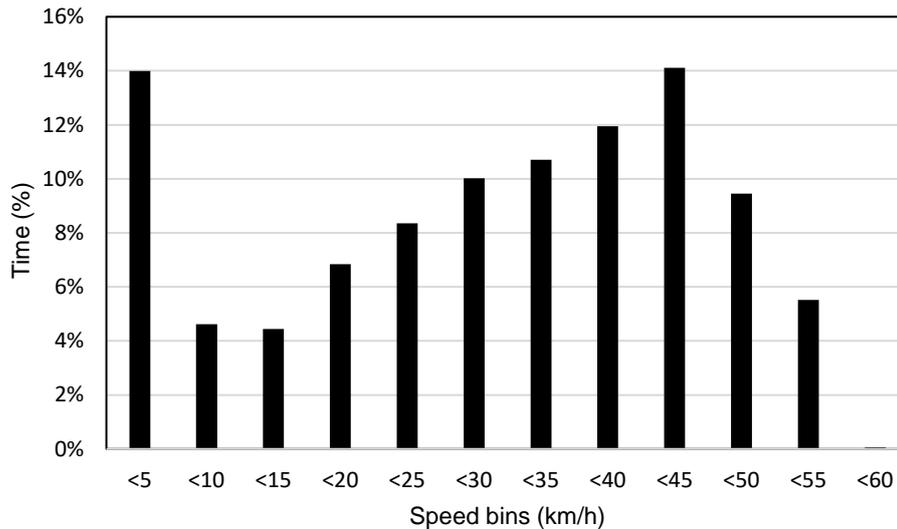
215 The emission of the pollutant p (E_p [g]) for each road segment is estimated by the model as
216 following:

$$217 \quad E_p = \sum (e_{ip}(v) \cdot N_i) \cdot L \quad (2)$$

218 where: $e_{ip}(v)$ is the emission factor ($\text{g} \cdot \text{km}^{-1}$) for pollutant p and vehicle class i defined as a function
219 of average speed v ($\text{km} \cdot \text{h}^{-1}$); N_i is the number of vehicles of class i and L is the road segment
220 length (km). The emission factors were derived from the average speed (approximately $30 \text{ km} \cdot \text{h}^{-1}$
221 in the considered road), fuel type (gasoline, diesel and liquefied petroleum gas), engine capacity
222 and emission technology (emission standards implementation associated to vehicle age).
223 Different vehicles categories are taking into account by TREM: passenger cars, light duty
224 vehicles, heavy duty vehicles and urban buses. The national vehicle fleet composition was
225 obtained from the COPERT database. Also, and since the TREM model needs a detailed
226 discretization regarding the vehicle categories (a total of 350 classes are considered in the
227 model), national and regional statistical information were used for this purpose (ACAP, 2015).

228 Fig. 3 shows the histogram of time spent under different speed ranges. It should be highlighted
229 the high percentage of time spent in stop and go situations ($0-5 \text{ km} \cdot \text{h}^{-1}$) and a high variability of
230 the time spent operating on the remaining speed bins. The main difference between VSP and
231 TREM methodologies is related to vehicle speed. VSP considers the instantaneous speed and
232 acceleration, allowing the characterization of vehicles dynamics, particularly important in the case
233 study, due to presence of traffic lights and the existence of pick up and drop off points related to
234 the schools. TREM considers the average speed, and so, reflects a homogeneous vehicle
235 behaviour, which implies a limited capacity to reflect traffic behaviour and speed variations in an
236 urban arterial. On the other hand emissions factors for VSP estimations are based on a limited
237 number of vehicles' categories, which represents a limitation in terms of the representativeness
238 of local fleet characteristics, whereas TREM model emissions factors arise from the linkages
239 between four categories of data sub-divided according to the fuel used, and by engine size, weight
240 or technology level of the vehicle, allowing a higher degree of detail in the characterization of fleet
241 composition. These distinct methods will be traduced in different levels of emission estimation
242 accuracy.

243



244

245 Fig. 3. Histogram of Speed data frequency (relative time spent over different speed bins).

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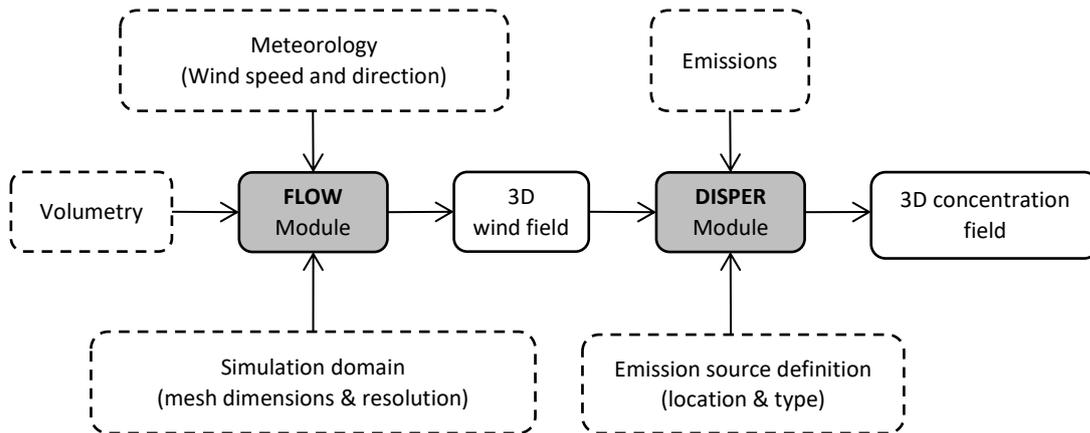
247 2.2.2. Air quality modelling

248 The CFD model VADIS (pollutant DISpersion in the atmosphere under VArable wind conditions)
 249 was applied to the case study to assess local scale air pollutants dispersion. VADIS performance
 250 has been improved through the years, based on the comparison of modelled data with wind tunnel
 251 measurements and data from air quality stations (Borrego et al., 2003, 2004; Richards et al.,
 252 2006; Amorim et al., 2013; Rodrigues et al., 2018; Rafael et al., 2018). Currently, VADIS has the
 253 capability to support multi-obstacle (e.g. buildings and trees) and multi-source description as well
 254 as, time varying flow fields and time varying emissions, allowing the evaluation of maximum short-
 255 term local concentrations in urban geometries (Amorim et al., 2013).

256 The VADIS structure is based on a bi-modular approach: the FLOW and the DISPER modules
 257 (Fig. 4). The FLOW module uses the numerical solution of the three-dimensional (3D) Reynolds
 258 averaged Navier-Stokes equations applying the $k - \epsilon$ turbulence closure scheme to calculate the
 259 wind, turbulent viscosity, pressure, turbulence kinetic energy and temperature 3D fields. In this
 260 module two different grids are used: the wind and the cartographic grids. The information related
 261 to the obstacles (buildings or vegetation) and to the emission sources position (e.g. roads) and
 262 dimensions is defined on the cartographic grid. The wind field is calculated over an Eulerian
 263 Cartesian 3D grid, which is overlaid to the cartographic one and rotates according to the wind
 264 direction. The grids dimensions and number of cells in each axis must be defined as a
 265 compromise between the required resolution, accuracy and the computational demand. The
 266 DISPER module applies the Lagrangian approach to the computation of the 3D pollutant
 267 concentration field using the wind field previously estimated by the FLOW. The Lagrangian
 268 approach assumes that the spatial and temporal dispersion of the mass of pollutant emitted is
 269 represented by a large number of numerical particles arbitrarily released in the flow. In each time
 270 step, each particle displacement is calculated by the sum of a deterministic component obtained
 271 from the velocity field, the stochastic component related with the local turbulence translated by
 272 the Langevin stochastic theory and the influence of the fluctuation forces, represent by the
 273 Langevin equation (Lee and Naesslund, 1998). Initially, the wind field is calculated considering
 274 the stationary conditions (FLOW module) and then the model calculated the displacement of
 275 these numerical particles over the cartographic grid (DISPER module). Integrated in the DISPER
 276 module, the Urban Vegetation (URVE) module, accounts for the aerodynamic effects of trees over

277 the 3D wind field. Consequently, the dispersion of the emitted air pollutants is conditioned by
 278 vegetation through this disturbed wind flow, allowing a better understanding of the flow and
 279 dispersion of air pollutants in urban environments. The magnitude of this perturbation depends
 280 most of all on the characteristics of the vegetation itself (e.g., location, size) and of the incoming
 281 air flow (e.g., velocity, direction, turbulence).

282 The output provided by VADIS includes the three wind velocity components, the turbulent
 283 viscosity, the turbulent kinetic energy, the turbulent dissipation and the pollutant concentration in
 284 each grid cell for the entire cartographic grid. A more complete description of VADIS can be found
 285 on Borrego et al. (2003, 2004) and Amorim et al. (2013).



286
 287 Fig. 4. Representative scheme of VADIS model.

288

289 **Computational domain**

290 The computational domain was designed following the guidelines proposed by COST Action 732
 291 (Frank et al., 2007). Thus, for the simulation of urban flows with multiple buildings, the vertical,
 292 lateral and downwind extensions of the computational domain were defined with a minimum of
 293 $5H_{max}$, where H_{max} represents the height of the tallest building. The CFD simulations were
 294 performed for a domain of $1248 \times 1248 \times 120 \text{ m}^3$ (L x W x H), with a grid resolution of $3 \times 3 \times 3$
 295 m^3 , which totalize a number of 6 922 240 cells. The domain obstacles (urban design) was
 296 characterized according to a geographic information system (GIS), which allows the creation of a
 297 virtual configuration of the study area, and so, considering the influence of artificial and natural
 298 structures (buildings and trees) to the flow dynamics. The complexity of the urban objects
 299 (buildings and trees) within the computational domain was simplified by assembling adjacent
 300 individual volumes with similar characteristics. Specifically in the case of trees, the grouped
 301 elements were defined as parallelepipeds positioned at a given distance above ground,
 302 representing the average trunk height. The generation of the urban objects (3D buildings, trees
 303 and roads) have been virtually defined in VADIS using the geometry pre-processors developed,
 304 based on the coordinates of the objects (Fig. 5). This case study complies a total number of 297
 305 buildings with a height which varies between 3 and 24 m, and a number of 310 trees with a height
 306 varying between 3 m and 15 m (total height).

307 Inflow boundary conditions for the horizontal wind velocity components, u and v , were prescribed
 308 based on the meteorological data presented in section 2.1. Richards and Hoxey's (1993) vertical
 309 profile equations were used to specify the variation of velocity (U), k and ϵ with height at the inlet
 310 boundaries assuming neutral stability conditions. The remaining boundary conditions (upper,
 311 lower and wall boundaries, as well as tree boundaries conditions) were defined following the
 312 guidelines indicated by Amorim et al. (2013).

313 Numerical simulations for PM₁₀ and NO_x, for the entire experimental period (in an hourly basis),
314 for both emission models were carried out, in a total of 144 simulations.



315

316 Fig. 5. Computational domain considered for CFD simulations – *Avenida 25 de Abril* in Aveiro, Portugal. The
317 pink polygons represent the buildings, the green ones represent the trees, and the grey polygons represent
318 the roads. The black icon shows the location of the Air Quality Station.

319

320 2.3. Air quality measured data

321 Aiming to characterize the daily profile of NO_x and PM₁₀ concentrations and to assess the
322 accuracy of numerical simulations for the period of the experimental campaign, a monitoring
323 network consisting of two stations (an urban traffic station and a suburban background station)
324 was designed. Both stations belong to the national network QUALAR (<http://www.qualar.org>),
325 managed by the Portuguese Environmental Agency (APA). Air quality monitoring equipment with
326 similar technical specifications is used in both stations. The urban traffic [Urb.] station is located
327 within the study domain and so its concentrations are determined predominantly by the emissions
328 from nearby traffic. Data from a suburban background station [Back.], located southwest from the
329 study area at approximately 6.5 km, was included in the analysis. This station allows a
330 characterization of the concentrations levels that are not considerably influenced by single (local)
331 sources but by an integrated contribution from all sources. However, background concentration
332 are not a fixed value and vary in that it may be influenced by regional air quality and indirectly by
333 local sources, i.e. background concentration is likely to increase in response to peak traffic
334 emissions or decrease at night in response to minimal traffic emissions (Moreno et al., 2009).

335

336 3. Results and Discussion

337 Given the described methodology (section 2), the air quality status of the study area was
338 characterized, both in terms of road traffic emissions (section 3.1.1) and air quality, including the
339 assessment of the wind flow pattern and air pollutants concentration (section 3.1.2). Afterwards,
340 the influence of different emission approaches to the accuracy of VADIS performance was
341 evaluated (section 3.2), through a statistical analysis and evaluation of the temporal profiles.

342

343 3.1. Air quality status of study area

344 3.1.1. Road traffic emissions

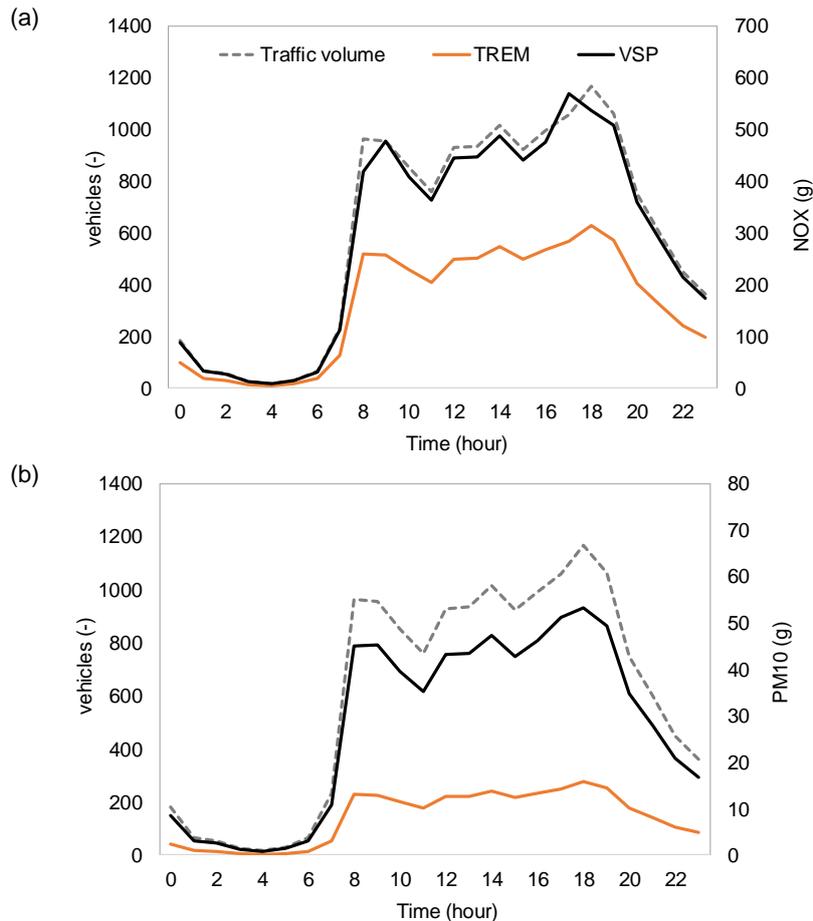
345 Based on the two emission models previously described, the hourly road traffic emissions were
346 estimated for the experimental campaign period conducted in the study area. Fig. 6 shows the
347 obtained results for both analysed pollutants, NO_x and PM₁₀, as well as the traffic flow data.

348 Since to perform the experimental campaign the avenue was divided in five links, it was possible
349 to assess the high emission hotspots through that road. High emission hotspots were achieved
350 in the link 2 and 3 (L2 and L3 in Fig. 1), with a daily average emission of 0.44 g·km⁻¹ and 0.22
351 g·km⁻¹ of NO_x, respectively for VSP and TREM models; average PM₁₀ emissions of 0.03 g·km⁻¹
352 [VSP] and 0.006 g·km⁻¹ [TREM] were obtained. These links are closely located to the school
353 placed in the study domain, where the daily average speed is low (<30 km·h⁻¹) related to the
354 presence of intersections, traffic lights and the existence of pick up and drop off points, which
355 increases stop-and-go situations. Consequently, these speed changes contribute to increased
356 total emission levels per vehicle. Analysing the daily traffic volume data (vehicles·h⁻¹), it is
357 observed a clear traffic dynamic behaviour, with distinct peak periods, 8-9 a.m. (with a traffic
358 volume of 965 vehicles, accounting for 6.7% of the total daily volume) and 6-7 p.m. (with a traffic
359 volume of 1166 vehicles, accounting for 8.1% of the total daily volume), and off-peak periods, 0-
360 7 a.m. (with an average traffic volume of 63 vehicles, which represents around 0.4% of the total
361 daily volume), which follows a typical daily traffic profile at urban environments (Coelho et al.,
362 2014). The work of Coelho et al. (2014) showed that in Portuguese urban roads the peak periods
363 occurs between 7-9 a.m. and 6-7 p.m., being conjointly responsible for around 16% of the total
364 daily volume; the off-peak periods occurs during the night-time (0-7 a.m.) and between 10 a.m.-
365 5 p.m.. In addition, the field campaign have shown that even during off-peak periods, a low
366 volume/capacity is maintained.

367 The daily emissions of NO_x and PM₁₀ (g·h⁻¹) recorded for the study area, for all the emission
368 models applied, follows the hourly road traffic volume. As a result, high values of road traffic
369 emissions, varying according with the emission model used, with values of 286.2 g [TREM] and
370 477.3 g [VSP] for NO_x and in 14.5 g [TREM] and 49 g [VSP] for PM₁₀, were obtained for the peak
371 periods (hourly average of the morning and afternoon peaks). Therefore, the fluctuation of traffic
372 volumes over the day is one of the main factors determining the hourly total emissions. In addition,
373 two distinct inferences can be made: i) road traffic shows higher emission levels of NO_x (89.7%
374 [VSP] – 94% [TREM] higher than PM₁₀ emissions at peak periods) across the day; ii) different
375 emission models promotes different emission levels.

376 Regarding the first feature, it is observed that NO_x emissions are, in average, 95% higher [TREM]
377 than the PM₁₀ emission (a value of 90.3% was obtained for the case of VSP model). This is a
378 result of the emission factors considered in each model, higher for NO_x, which are in accordance
379 with European data. At European level for 2015, the road transport sector contribute around 30%
380 and 3.5% for the total of NO_x and PM₁₀ emissions (a ratio of around 8.6), respectively (EEA,
381 2017). Concerning the second feature, it is clear that the emissions estimated by the TREM
382 model, for both air pollutants, presents lower magnitude, -45.3% [NO_x] and -90.4% [PM₁₀] at
383 peak periods, when compared with the VSP model values. These differences can be explained
384 by the emission calculation method implemented at each model. As previously mentioned, VSP
385 is an instantaneous emission models based on second-by-second vehicle dynamics and clearly
386 include congestion in the modelling process, while the TREM model considers an average vehicle
387 speed where the emission rates are calculated based on standardized driving cycles (Smit et al.,
388 2008).

389



390 Fig. 6. Traffic emissions for 7th of February of 2017 for the two analysed pollutants, (a) NO_x and (b) PM₁₀,
 391 estimated according different emission approaches. The daily traffic volume is presented on the left axis
 392 (dashed line), while the emission rate is shown on the right axis.

393

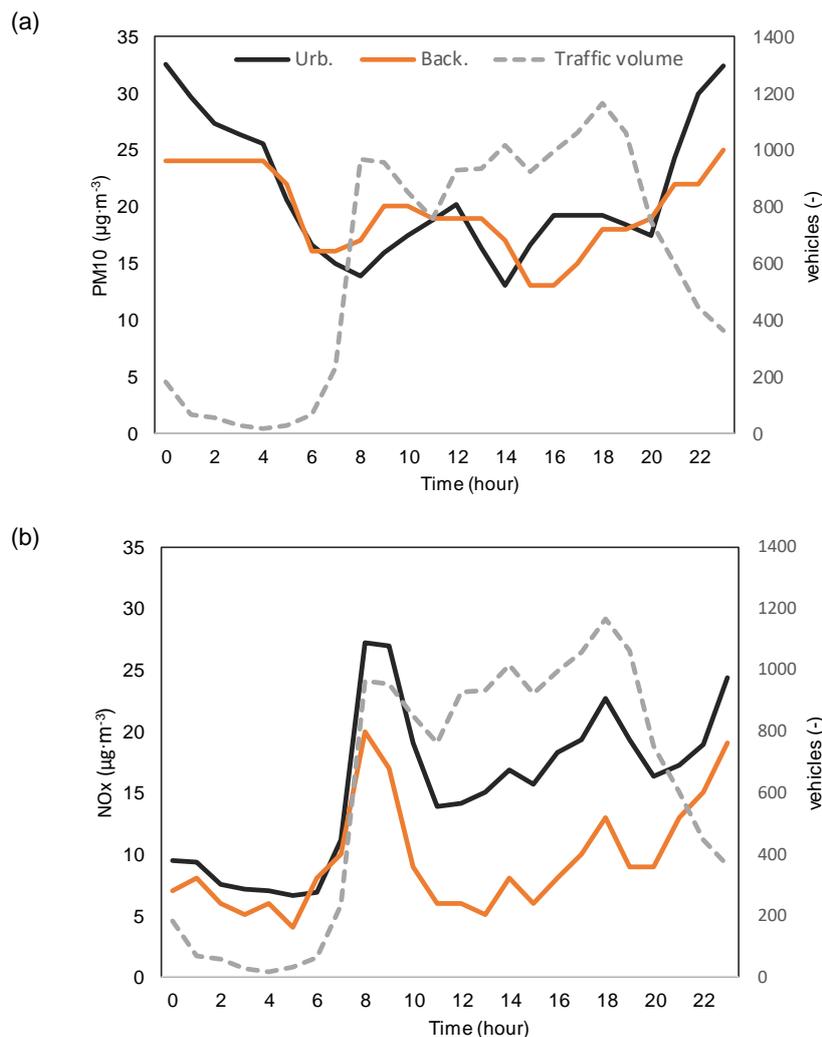
394 3.1.2. Air quality: local measurements and modelling

395 The air quality status of the study area was investigated following two distinct approaches: i)
 396 analysis of the NO_x and PM₁₀ concentrations daily profile, based on measured data acquired in
 397 two air quality monitoring stations, which allows a characterization of air pollutant concentrations
 398 time evolution (Fig. 7); ii) spatiotemporal analysis, through the mapping of PM₁₀ and NO_x hourly
 399 concentrations, based on the modelled data considering the emissions estimated by the different
 400 approaches under study, which allows an understanding of the spatial variability of the air
 401 pollutants concentration (Fig. 8).

402 Fig. 7 shows the measured PM₁₀ and NO_x concentrations daily profile, based on acquired data
 403 in two air quality stations (Urb. and Back. stations) for the period of the experimental campaign.
 404 In the case of PM₁₀ concentrations, for the reporting period, the maximum value at the urban
 405 station was 32.4 μg·m⁻³ at 11 p.m. (with a minimum value of 13 μg·m⁻³ at 2 p.m.); for the period
 406 of higher traffic volume (8 a.m. and 7 p.m.) the measured PM₁₀ concentration was 19 μg·m⁻³. All
 407 these values are below the daily limit-value established by Directive 2008/50/CE (50 μg·m⁻³) and
 408 closely to the average value registered in 2016, 20 μg·m⁻³. From the analysis of Fig.7, it is evident
 409 that the daily profile of PM₁₀ concentrations at both stations does not shows a clear linkage with
 410 the daily road traffic volume. In fact, the PM₁₀ daily profile at both measured stations are in
 411 accordance with the expected daily profile for a winter period (Gama et al., 2018), when the non-
 412 road traffic emission can have a more important role in PM₁₀ concentrations. Concentrations

413 decrease during the day from mid-morning to early evening. At night, the decrease occurs
414 following the evening peak between midnight and roughly 5 a.m. The amplitude of variation is
415 higher at night than during the afternoon. Regarding NO_x, the maximum concentration value at
416 the urban station is obtained at 8-9 a.m. (peak period), 27.2 µg·m⁻³, followed by a value of 22.7
417 µg·m⁻³ at 6-7 p.m. (peak period); a minimum value of 6.6 µg·m⁻³ is obtained at 5-6 a.m. (of-peak
418 period). It is evident that the daily profile of NO_x concentrations follows the hourly road traffic
419 volume, at both stations (see Fig. 7), following the emissions profile. It is interesting to note that
420 different magnitudes of NO_x concentrations were obtained in the peak periods, despite the slight
421 difference in the road traffic volume, especially knowing that a high road traffic volume was
422 obtained at 6-7 p.m. These differences are a result of the meteorological conditions. In the
423 morning peak a wind velocity of 1.9 m·s⁻¹ was registered, while at the afternoon peak a wind
424 velocity of 3.7 m·s⁻¹ was obtained; for both periods the wind blows from north-northwest. This
425 means that for a similar emission rate, the air quality is highly dependent of the meteorological
426 conditions, with high values of wind velocity promoting the dispersion of air pollutants. The
427 measured NO_x concentrations are significantly lower than the limit-value (200 µg·m⁻³, in an hourly
428 basis), but higher than the average value registered in 2016, 22.7 µg·m⁻³. Despite both air
429 pollutant concentrations were below the limit-value, should be noticed that the proximity of a
430 school is a critical issue. The study of Valente et al. (2014), for the same area, shows that the
431 daily indoor PM₁₀ concentration during occupancy periods were 2 to 4 times higher than the
432 concentrations registered outdoors, which could mean that the resident population (students and
433 people who lives in this neighbourhood) could be exposure to high levels of PM₁₀ concentrations.

434 For the urban traffic station, the data of last 5-years (2012-2016) of PM₁₀ and NO_x concentrations
435 were also analysed to assess the trend lines (Fig. S1 and Fig. S2 in the Supporting Information).
436 The results shows a concentration reduction trend for both pollutants through the years; the
437 annual PM₁₀ concentration in 2016 (20 µg·m⁻³) was 43% less than the value registered in 2012
438 (35 µg·m⁻³), while for NO_x, the annual concentration in 2016 (29.5 µg·m⁻³) was 6% less than the
439 value registered in 2012 (31.4 µg·m⁻³) (see Table S1 in the Supporting Information). High PM₁₀
440 concentrations were always registered in the winter months (December-February). Since no
441 noteworthy changes occurs in the road traffic volume in these months (compared with the entire
442 year), these data highlights the influence of non-road emission sources to the air quality of the
443 study area. NO_x concentrations shows a systematic daily profile, with high concentrations at 8-9
444 a.m. and 6-7 p.m. periods, consistent with the high daily traffic volume. The statistical comparison
445 between the experimental campaign time-series acquired in background station shows a high
446 correlation ($r = 0.85$) for hourly average NO_x values. Although for PM₁₀ a lower agreement ($r =$
447 0.79) was obtained, the magnitude presented in the suburban background station measurements
448 is, for the majority of the time-series, lower than that from the urban station. This indicates that
449 Back. is representative of Aveiro's background in the period under analysis.

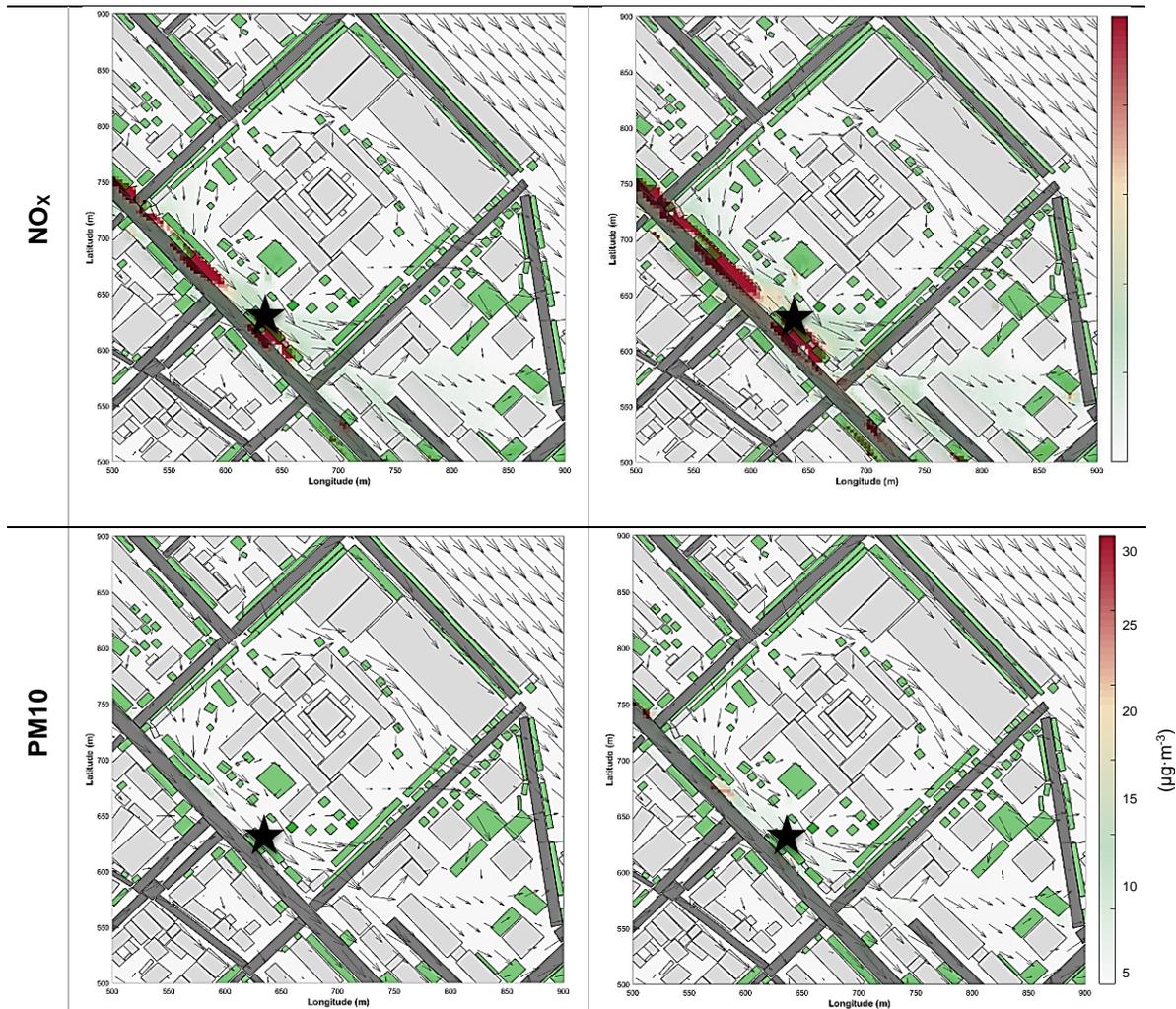


450 Fig. 7. Daily profile of (a) PM10 and (b) NOx concentration in the two air quality stations (urban traffic station
 451 [Urb.] and suburban background station [Back.]) for the 7th of February of 2017. The daily traffic volume
 452 (dashed line) is presented on the right axis.

453

454 Fig. 8 shows, by way of example, NOx and PM10 concentrations fields for the emission models
 455 under study for 3 m high horizontal streamlines, for the 8-9 a.m. period. The results shows that
 456 the analysed pollutants behave in a similar way across the domain (especially the concentration
 457 peaks distribution), independently of the emission model used to estimate the road traffic
 458 emissions. High concentrations were obtained nearby the school, which is a result of conjoint
 459 influence of high emissions (Links L2 and L3) and unfavourable conditions for air pollutants
 460 dispersion. This last feature is related to the characteristics of the urban morphology over the
 461 wind flow, that promotes the existence of recirculation areas between buildings and trees, zones
 462 characterised by a low wind velocity (average values of $0.9 \text{ m}\cdot\text{s}^{-1}$ for a wind inflow of $2 \text{ m}\cdot\text{s}^{-1}$ were
 463 obtained; for a maximum wind inflow of $5.4 \text{ m}\cdot\text{s}^{-1}$ [at 12 a.m.], a value of $3 \text{ m}\cdot\text{s}^{-1}$ was obtained),
 464 and so an accumulation of air pollutants concentration is endorsed. Analysing the study area as
 465 an all, for a spatial average, a wind velocity of $2.5 \text{ m}\cdot\text{s}^{-1}$ (daily average) was obtained; a maximum
 466 wind velocity of $12 \text{ m}\cdot\text{s}^{-1}$ (occurred at the beginning of the avenue) was obtained at 6 a.m. (for a
 467 wind flow of $3.7 \text{ m}\cdot\text{s}^{-1}$), when the domain is perfectly aligned with wind direction.

468



469 Fig. 8. NO_x and PM₁₀ concentrations fields for the emission models under study for 3 m high horizontal
 470 streamlines. Contours refer to the period of 8 a.m. (with an inflow wind velocity of 1.9 m·s⁻¹ and a wind
 471 direction of 308°). The arrows represent the wind flow behaviour (velocity and direction) within the
 472 computational domain. The black star shows the Air Quality Station's location.

473

474 Daily average PM₁₀ concentrations related to road-traffic emissions of 0.2 µg·m⁻³ [VSP] (ranging
 475 between 0.002 [at 4 a.m.] and 0.74 µg·m⁻³ [at 8-9 a.m.]) was obtained for a spatial average of the
 476 domain; an average value of 0.06 µg·m⁻³ was obtained when the TREM model was used to
 477 estimate the emissions. For this pollutant, a maximum value of 57 µg·m⁻³ [VSP] was obtained at
 478 8 a.m., in specific zones of the domain (near links L2 and L3); a maximum value of 17.1 was
 479 obtained considering TREM emissions, at the same time period. PM₁₀ levels higher than 5 µg·m⁻³
 480 were obtained at 7% of the domain cells, for both emission models. In the case of NO_x
 481 concentrations, a daily average values of 2.1 µg·m⁻³ [VSP] and 1.2 µg·m⁻³ [TREM] were obtained,
 482 considering a spatial average of the domain. Maximum NO_x levels were obtained for the same
 483 areas previously identified for PM₁₀ concentrations, with maximum values of 485 µg·m⁻³ [VSP]
 484 and 331.7 µg·m⁻³ [TREM], at 8-9 a.m. NO_x concentrations higher than the limit-value were
 485 obtained in around 0.1% of the domain cells, for all the analysed emission models; 2% of the
 486 domain displaced NO_x concentrations higher than 50 µg·m⁻³.

487 The dynamics of traffic (and related emissions, as already discussed in section 3.1.1.) and
 488 atmospheric conditions (wind velocity and wind direction) become evident in the magnitude of
 489 PM₁₀ and NO_x concentrations, at both measured and modelled data, as well as, in the location

490 of the NO_x and PM₁₀ hotspots (for modelled data). A correlation analysis was made to evaluate
491 the relative importance of the meteorological conditions and the traffic emissions to the modelled
492 air quality levels. Should be noted that due to complex interactions that occurs at the urban
493 environment, the correlation analysis cannot directly reflect the absolute influence of different
494 factors, but can provide important insights about its relative importance (Chen et al., 2017). For
495 both pollutants, a strong correlation was obtained between the traffic emissions and the air
496 pollutants concentrations. Traffic emissions explains 54% (when the VSP model is used) and 61%
497 (when the TREM model is used) of the NO_x concentrations, while the PM₁₀ concentrations are
498 explained in 62% (for both models). Regarding the meteorological conditions, the wind velocity
499 shows a more noteworthy role in the air quality levels than the wind direction; wind velocity
500 explains around 58% of PM₁₀ and NO_x concentrations. It was also concluded that the wind
501 velocity and air pollutants levels varies in an inverse way, which implies that the NO_x and PM₁₀
502 concentrations increase with a decrease of the wind velocity.

503

504 3.2 Comparative analysis of emission approaches

505 To assess the influence of different emission approaches in the accuracy of numerical
506 simulations, two analysis were carried out: i) a quantitative evaluation based on a set of statistical
507 metrics; and ii) a qualitative evaluation based on graphic visualization, through inter-modelling
508 time-series plots. Both analysis were performed considering only the effect of local emissions to
509 the air quality, and adding the contribution of background emission sources. This means that two
510 datasets were used to evaluate the accuracy of numerical simulations (both were compared with
511 the measured data acquired in the urban traffic station): i) modelled data only, and ii) modelled
512 data plus measured background concentrations; the background concentrations from the
513 suburban background station (see section 2.3), for the experimental period, were added hour-by-
514 hour to the modelled data. In the scope of this work, the background concentration is defined as
515 the concentration that would be measured in the absence of local emission sources that are
516 explicitly considered by the dispersion model. Therefore, the background air quality should
517 include a contribution of all other sources, natural and anthropogenic, except local traffic
518 emissions considered in the model inputs, giving an outlook of the relative contribution of non-
519 road emissions to the local air quality.

520 The statistical metric were calculated by applying model acceptance criteria proposed by Chang
521 and Hanna (2004) for air quality models assessment, which establishes performance measures
522 for the normalized mean square error (NMSE < 1.5), fraction of predictions within a factor of two
523 of observations (FAC2 > 0.5) and the mean bias (MBE < 0.3). Also the average value (MEAN),
524 the correlation coefficient (r) and the standard deviation (SIGMA) were considered in the analysis.
525 The performance measures were calculated applying the BOOT Statistical Model Evaluation
526 Software Package (Chang and Hanna, 2004).

527 Table 2 compiles the statistics for the comparison between model outputs and air quality
528 measurements of PM₁₀ and NO_x levels considering the hourly data. Aiming to distinguish the
529 effect of the background concentration on VADIS performance, both the direct modelled output
530 and with background are shown.

531 As can be seen, for NO_x, model acceptance criteria were fulfilled for the different emission models
532 used, with a similar performance; main differences were obtained for the MBE parameter, with
533 both models promoting an underestimation (negative values) of modelled concentration data,
534 more pronounced when TREM was used. In general, a good correlation (higher than 0.8) between
535 modelled and measured data was obtained, independently of the emission model used. The
536 conjoint analysis of all the statistical parameters showed that VSP is the model that allows a better
537 performance of the air quality model, and so a better estimation of traffic-related NO_x emission,

538 related to the ability of the model to realistic reproduce the different driving modes (e.g.,
 539 acceleration/deceleration). The results also highlight the potential of detailed traffic and
 540 instantaneous exhaust emissions estimates to provide accurate input data to CFD models applied
 541 at local scale. These findings are in accordance with the outcomes of studies conducted at urban
 542 scale (Borrego et al., 2016; Amirjamshidi et al., 2013; Misra et al., 2013). A slight improvement of
 543 the statistical parameters was obtained when the background contribution was added; however
 544 an overestimation (positive MBE), more pronounced with VSP model, was obtained. These
 545 results reinforced the road traffic as the main emission source at urban areas. A very different
 546 behaviour was obtained for PM10. In general, and for all emission models, the model acceptance
 547 criteria were not fulfilled. In fact, a negative correlation was obtained meaning an inverse
 548 relationship between the modelled and measured data. A clear underestimation of PM10
 549 concentrations was obtained (negative MBE), with high values of both MBE (with values of -20.7
 550 [TREM] and -19.6 [VSP], according to the emission model used) and NMSE. To these results two
 551 main issues may have contributed: i) a underestimation of PM10 emissions, mainly related to the
 552 fact that non-exhaust PM10 emissions has not been estimated; this is particularly important since
 553 during the experimental campaign the roads were dry (no precipitation have occurred during this
 554 period) and so, PM10 resuspension can be an important emission source (the relative importance
 555 of non-exhaust emissions has been increasing as a result of the introduction of vehicle particulate
 556 abatement technologies [EEA, 2017]); ii) influence of other emission sources.

557 A consistent improvement of model accuracy results from adding the background contribution
 558 with a substantial increases of the average r, with values of 0.62 [VSP] (-0.39 without the
 559 background) and 0.76 [TREM] (-0.38 without the background). The model acceptance criteria for
 560 the NMSE and FAC2 were fulfilled, despite some underestimation (by both models), revealed by
 561 the negative MBE. The FAC2 parameter, a robust performance measure in the evaluation of CFD
 562 models, shows that, in average, 100% of the hourly predictions (0% with no background) are
 563 within a factor of two of the observations.

564

565 Table 2. Statistics of VADIS performance of PM10 and NOx evaluated against observations, without and
 566 with (in brackets) the contribution of background concentrations, for the analysed period. In the analysis, 24
 567 data points (hourly averages) were considered for both pollutants. A positive MBE indicates here an over
 568 prediction.

		MEAN ($\mu\text{g}\cdot\text{m}^{-3}$)	SIGMA	MBE ($\mu\text{g}\cdot\text{m}^{-3}$)	NMSE	R	FAC2
	AQS	15.43	6.20	-	-	-	-
NOx	TREM	8.43 (17.89)	8.51 (12.30)	-7.00 (+2.46)	0.49 (0.20)	0.91 (0.91)	0.38 (1.00)
	VSP	14.31 (23.77)	14.87 (18.44)	-1.12 (+8.34)	0.45 (0.66)	0.88 (0.90)	0.63 (0.88)
	AQS	21.10	5.78	-	-	-	-
PM10	TREM	0.43 (20.02)	0.43 (3.45)	-20.66 (-1.08)	50.42 (0.04)	-0.38 (0.76)	0.00 (1.00)
	VSP	1.49 (21.00)	1.49 (3.59)	-19.61 (-0.09)	13.60 (0.05)	-0.39 (0.62)	0.00 (1.00)

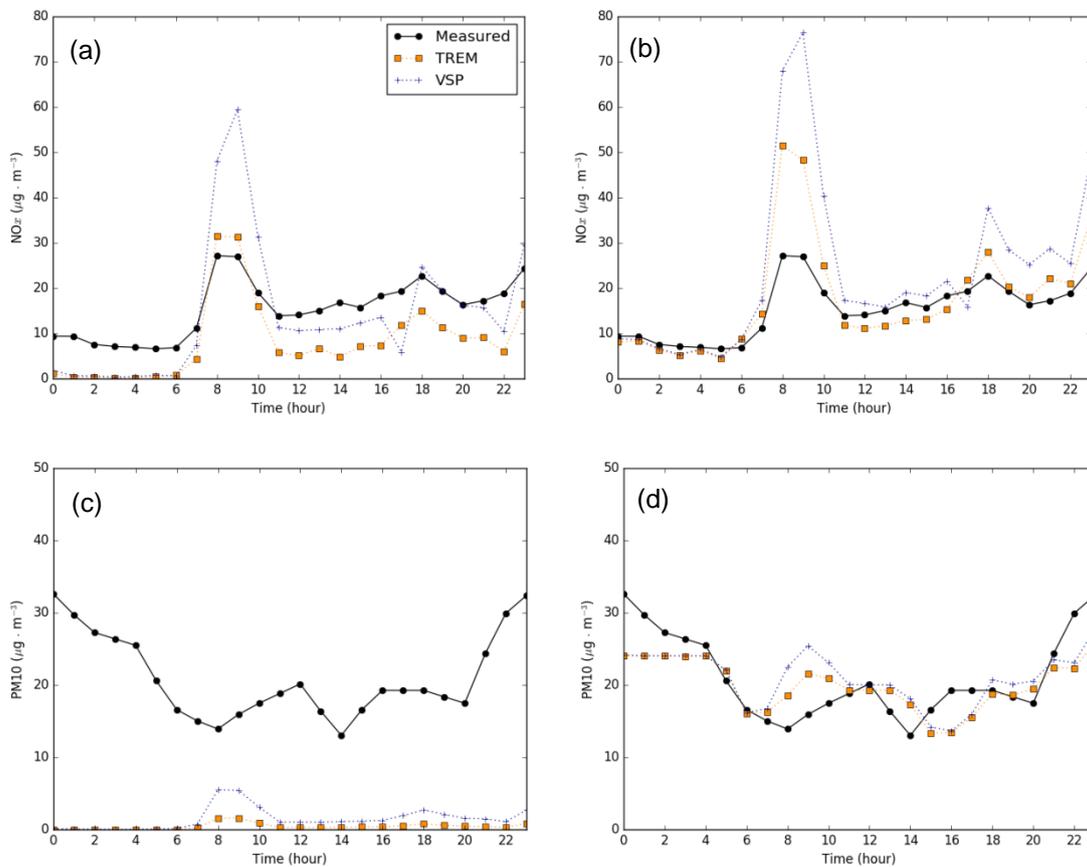
569

570 Aiming to further investigate the dependency of model performance on the time of the day,
 571 measured *versus* modelled daily mean profiles of hourly surface pollutant concentration were
 572 calculated. This analysis is also provided considering the influence of background concentrations.
 573 The measured data was provided by the urban air quality monitoring station. Fig. 9 depicts the
 574 ability of the modelling approach to track the evolution of NOx levels, including the morning traffic
 575 peak at 8-9 a.m. (Fig. 9a). These data shows that in the study area, the NOx concentrations are
 576 mainly caused by traffic-related NOx emission, accounting (in a daily average) for 72.9% [TREM]
 577 and 89.5% [VSP] of the total NOx concentrations measured in the air quality station. Fig. 9 also

578 shows that background concentrations have an influence during off-peak periods (shown by the
579 fit between measured and modelled NO_x concentrations at these periods when the background
580 concentrations are added to the modelled results). The daily profile reveals an overestimation of
581 NO_x concentrations at sunrise (8-9 a.m.), more pronounced when the VSP model is used and
582 when the background concentrations are added to the modelled values. This overestimation
583 reinforces the linkages between road traffic emissions and NO_x concentrations, since considering
584 the influence of other emission sources increases the bias between measured and modelled data.
585 For this pollutant, the background conditions should only be consider when a low road traffic
586 volume is recorded. The origin of this large overestimation is probably due to the conjoint influence
587 of an overestimation of traffic emissions and of unfavourable conditions to air pollutants
588 dispersion. At this period a very low wind velocity (0.9 m·s⁻¹) was modelled. Despite the VADIS
589 model have been validated through time, as discussed by Rafael et al. (2018), a model is merely
590 a model of reality, and so, its use induces a certain level of uncertainty.

591 An agreement between measured and modelled concentrations was not observed for PM₁₀ (Fig.
592 9c). It is clearly visible that the modelled and measured PM₁₀ concentrations shows a distinct
593 daily profile, which are in line with the statistical analysis (negative correlation factor). The high
594 MBE values obtained in the statistical analysis are also clear along the time series, as well as the
595 response of the CFD VADIS to the different emissions provided (traduced by differences in the
596 magnitude of PM₁₀ concentrations). However, it is evident that these differences were not enough
597 to imply noteworthy differences in terms of the daily profile of the modelled results, being the
598 traffic-related PM₁₀ emissions responsible (in a daily average) for 1.3% [TREM] and 8.4% [VSP]
599 of the total PM₁₀ concentrations measured in the air quality station. These values are in
600 accordance with the air pollution statistical fact sheet (2017) for Portugal (URL1), which shows
601 that road transport contributes 6.7% for the total of PM₁₀ emissions. Maximum linkage were
602 obtained at the morning peak period (8 a.m. – 9 a.m.) with values of 9% [TREM] and 37% [VSP].
603 These results can denote one of two issues: i) the VADIS model is not able to accurately simulate
604 PM₁₀ concentrations; ii) the traffic-related PM₁₀ emission is only one source contributing to PM₁₀
605 concentrations in the study area. When the background concentrations were added to the
606 modelled results (Fig. 9d), it was observed an improvement in the fitting between the measured
607 and modelled daily profile; modelled results obtained by using emissions estimated by TREM
608 model shows a better link with the measured data, which is in line with the statistical parameters.
609 This means that other emission sources, beyond road traffic sector, have an important
610 contribution to PM₁₀ concentrations. The study of Alves et al. (2014) focused in the same study
611 area, have identified a set of PM₁₀ emission sources related to combustion processes coming
612 from nearby restaurants and bakeries with charcoal and firewood use. Additionally, and taking
613 into account that the experimental campaign took place during winter, the contribution from
614 domestic woodstoves and fireplaces should be substantial. In fact, several studies pointed out
615 residential combustion (in particular wood burning) as a major source contributing to PM₁₀
616 concentration levels during winter time in many regions across Europe (Borrego et al. 2010;
617 Bernardoni et al. 2011; Karvosenoj et al. 2011; Fuzzi et al. 2015; Viana et al. 2013; Waked et
618 al. 2014). Borrego et al. (2010) have determined the PM₁₀ diurnal average pattern by season
619 over Portugal, based on the monitoring stations network. In the winter and autumn seasons, two
620 peaks in average concentration were obtained: one in the morning between 7 and 11 a.m., and
621 the other in the evening between 7 and 10 p.m. The existence of these peaks, distinguished from
622 those obtained at spring and summer daily profile, is explained by home heating during the early
623 morning and evening hours. This daily behavior is in accordance with the profile obtained in the
624 urban traffic station, which is well reproduced when the background conditions are added to the
625 modelled results. This issue was recently reinforced by the study of Gama et al. (2018), which
626 provides a long-term characterization of temporal patterns and trends of particulate matter over
627 Portugal. The results showed that the late evening peak is stronger during the winter as result of
628 both the daily evolution of the atmospheric boundary layer, which gets thinner during the night,

629 and the evening contribution of residential combustion; the PM10 late evening peak concentration
 630 can be $20 \mu\text{g}\cdot\text{m}^{-3}$ higher than during summer.



631 Fig. 9. Daily profile of NO_x and PM10 concentrations, for both measured and modelled data, for the
 632 experimental period (a, c). Comparison between the daily profile of modelled data considering the addition
 633 of NO_x and PM10 background concentration and the measured data is also showed (b, d). Modelled results
 634 obtained considering different emission modes are presented.

635

636 4. Conclusions

637 In this work the air quality of a main avenue of a medium-size European city was simulated, with
 638 street level resolution, for a weekday period (typical winter day in terms of both emissions and
 639 meteorological conditions). A modelling approach was applied consisting of (1) detailed traffic
 640 flows obtained by an experimental campaign conducted for the study period; (2) exhaust road
 641 traffic emissions estimated by two different approaches, VSP and TREM; and (3) air pollutants
 642 dispersion, focused on NO_x and PM10, simulated by the CFD model VADIS.

643 Both emission models show for NO_x emissions similar patterns in the emissions daily profile with
 644 a good correlation between the traffic dynamics and the emissions daily profile; however, notable
 645 differences in terms of the magnitude of the obtained values were observed. Regarding PM10,
 646 the differences in the complexity level of the emission models were evident in magnitude of the
 647 estimated emissions and at the PM10 concentrations obtained with VADIS. The analysis of model
 648 performance metrics showed that, for NO_x, the data quality objective were fulfilled, with a better
 649 performance (even slight) when the VSP model is used; these findings implies that the NO_x
 650 concentrations are mainly caused by traffic-related NO_x emission, accounting for 72.9% [TREM]

651 and 89.5% [VSP] of the total NO_x concentrations measured in the air quality station. However,
652 an overestimation of the NO_x concentrations (more noteworthy when the background
653 concentrations are added) was observed at the morning peak, independently of the emission
654 model used (but more pronounced when VSP was applied), which can point to an overestimation
655 of traffic emissions. Contrariwise, a negative correlation between measured and modelled values,
656 independently of the emission model used, were obtained for PM₁₀ concentrations. Correlation
657 (0.7 [TREM] and 0.6 [VSP]), as well as all the statistics metrics analysed, were shown to
658 considerably improve when urban background concentration is added. This means that other
659 emission sources, beyond road traffic sector (this only accounts for 1.3% [TREM] and 8.4% [VSP])
660 have an important contribution to PM₁₀ concentrations; taking into account that the experimental
661 campaign took place during winter, the contribution of the residential sector (combustion of fired
662 used in domestic woodstoves and fireplaces) should be substantial.

663 This study showed that despite the developments on air quality models, road traffic emissions are
664 still a variable of fundamental relevance in the global accuracy of simulations, especially at local
665 scale. In general, the results highlight the potential of detailed traffic and instantaneous exhaust
666 emissions estimates, together with urban background, to provide accurate input data to CFD
667 models applied at the local scale. Additionally, since mobility improvement while at the same time
668 reducing air pollution, are common challenges to all major cities in Europe, this type of studies
669 allow an assessment of the different origins of air pollution, and so, the definition of sectoral
670 measures to improve air quality taking into account specific characteristics of each city.

671

672 **Acknowledgments**

673 The authors acknowledge the support of @CRUiSE project (PTDC/EMS-TRA/0383/2014, funded
674 within the Project 9471 – Reforçar a Investigação, o Desenvolvimento Tecnológico e a Inovação
675 (Project 9471 – RIDTI) and supported by the European Community Fund FEDER). CESAM co-
676 authors acknowledge the financial support of the FCT/MEC through national funds, and the
677 cofunding by the FEDER, within the PT2020 Partnership Agreement and Compete 2020, for the
678 research project CESAM (UID/AMB/50017–POCI-01-0145-FEDER-007638). TEMA co-authors
679 also acknowledge: Project CISMOB (PGI01611 funded by Interreg Europe Programme), Strategic
680 Project UID-EMS-00481-2013 (FCT – Portuguese Science and Technology Foundation),
681 CENTRO-01-0145-FEDER-022083, and MobiWise project (P2020 SAICTPAC/0011/2015) (co-
682 funded by COMPETE2020, Portugal2020 - Operational Program for Competitiveness and
683 Internationalization (POCI), European Union's ERDF (European Regional Development Fund),
684 and FCT), FCT Scholarship SFRH/BPD/100703/2014 and Caetano Auto S.A. Portugal
685 (representatives of Toyota).

686

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