Urban scale air quality modelling using detailed traffic emissions estimates

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Abstract

The atmospheric dispersion of NO_x and PM10 was simulated with a second generation Gaussian model over a medium-size south-European city. Microscopic traffic models calibrated with GPS data were used to derive typical driving cycles for each road link, while instantaneous emissions were estimated applying a combined Vehicle Specific Power/Co-operative Programme for Monitoring and Evaluation of the Long-range Transmission of Air Pollutants in Europe (VSP/EMEP) methodology. Site-specific background concentrations were estimated using time series analysis and a low-pass filter applied to local observations. Air quality modelling results are compared against measurements at two locations for a 1 week period. 78% of the results are within a factor of two of the observations for 1-h average concentrations, increasing to 94% for daily averages. Correlation significantly improves when background is added, with an average of 0.89 for the 24 hours record. The results highlight the potential of detailed traffic and instantaneous exhaust emissions estimates, together with filtered urban background, to provide accurate input data to Gaussian models applied at the urban scale.

Keywords

Urban air quality; Gaussian model; traffic modelling; emissions modelling; monitoring campaign; background concentration

1. Introduction

In the European Union 72% of the population lives in urban areas, a rate that is projected to increase (EEA, 2015a). Despite significant efforts to improve urban air quality, namely by reducing traffic emissions (Tente et al., 2011; Cyrysa et al., 2014), air pollution is still the single largest environmental health risk in Europe (EEA, 2015b). Over the past years, and due to policy pressures requiring more detailed assessment of air pollution at local and urban scales, there has been a growing need to simulate meteorological and air quality fields at higher spatial resolutions than the ones obtained with mesoscale models (Coelho et al., 2014). Regardless the increasing application of high-resolution computational fluid dynamics (CFD) models over cities (Amorim et al., 2013a; Martins et al., 2009), the large demand of input data and the computationally expensive simulations still represent an obstacle when dealing with large areas and/or long-term periods. Hence, Gaussian models constitute a natural choice for the urban scale air pollutant dispersion modelling with regulatory or policy assessment purposes (Zawar-Reza et al., 2005; Gidhagen et al., 2009), especially in the simulation of short-range (up to a few tenths of kilometers from the emission source) dispersion processes from different sources over topographies of varying complexity, inclusively accounting for building-induced effects (Denby, 2011). Also, background concentrations are of particular interest, because they are a critical source of uncertainty in the prediction of ambient levels (Stein et al., 2007; Arunachalam et al., 2014). Reliable estimates of background concentrations are indispensable for accurate air dispersion modelling results. However, there are several techniques that may be used for this purpose and their selection may influence the final results.

Despite the developments on air quality models, road traffic emissions are still a variable of fundamental relevance in the global accuracy of simulations, especially at the urban scale. Whereas instantaneous emission models (such as CMEM and VT-micro) are based on second-by-second vehicle dynamics and clearly include congestion in the modelling process, the emission rates used by average speed models (such as COPERT) are calculated based on standardized driving cycles (Smit et al., 2008). Although Ahn and Rakha (2008) pointed out that the use of instantaneous emission models is the most appropriate method to assess different operational traffic scenarios, the majority of the studies linking road traffic, emission, air quality and human exposure at the urban scale usually use average speed emission models (Mensink and Cosemans, 2008; Amorim et al., 2013b). As exceptions one can mention the studies conducted by Amirjamshidi et al. (2013) and Misra et al. (2013), in which PARAMICS traffic model was linked to CMEM emission model and an air quality model to estimate the levels of carbon monoxide (CO), nitrogen oxides (NO_x) and hydrocarbons (HC).

Given this background, the present paper proposes the simulation of air quality at the urban scale based on a detailed traffic modelling approach that uses microscopic traffic models calibrated with real world GPS data in order to establish typical driving cycles for each link within the road network. The atmospheric dispersion of NO_x and particulate matter (PM), both pollutants posing serious health concerns in urban areas, is calculated with a second generation Gaussian model, accounting for the effect of buildings. Background contribution to urban air pollution levels is estimated with a low-pass filter applied to local observations. Modelling results are compared against field observations in a south-European city.

2. Methodology

The Portuguese city of Aveiro was selected as study area because of the adequate size and relevant road network for the purpose of the work, the prior availability of traffic volume data (both from Aveiro municipality as from previous measurements performed by the authors), as also the facilitated logistics in the set-up of experimental campaigns. This medium-size city, with approximately 198 km^2 and 78 thousand inhabitants (INE, 2013), is located at the Norwest coastline at 70 km south of Porto. The following sections describe the experimental observations (section 2.1) and the numerical modelling approach (sections 2.2 to 2.4).

2.1. Experimental field campaigns

The experimental work consisted in the monitoring of road traffic, meteorological conditions, and air pollutant concentrations for selected periods in different locations within the city, as hereafter described. Emissions were not directly measured during the field campaigns.

To assess the road traffic network several variables were collected. Firstly, ten different routes with heterogeneous traffic conditions across the study domain were covered using GPS data-logger equipped vehicles to collect second-by-second vehicle dynamics (speed, acceleration/deceleration and road grade). GPS data includes road traffic field campaigns performed during peak (7-10h and 17-19h) and non-peak (10-17h) periods on typical weekdays (Tuesdays to Thursdays) and under dry weather conditions in February/March 2011, February/March 2012 and May/June 2013. Approximately 550 km of GPS data over 15 hours were considered during peak hours, allowing the coverage of congested periods. For validation purposes, the authors used 15 data sets of vehicle dynamic data from 10 different routes. Such monitoring routes included urban roads, arterials, and motorways over the study domain (with different traffic flows and speed limits). In addition, aiming to reduce systematic errors, road tests were performed using different drivers and vehicles.

Traffic was monitored in 56 strategic points that allow the connection among the most important roads within the study network, as shown in Figure 1. Based on the above data, time dependent origin-destination (O/D) matrices were defined for each intersection and assigned to the overall study domain. To monitor traffic signals timing, the cycle length and phasing was measured six times in the traffic lights in five points of the domain. A detailed description of the field work for vehicle dynamics assessment and traffic monitoring can be found in Bandeira et al. (in press) and Fontes et al. (2014).

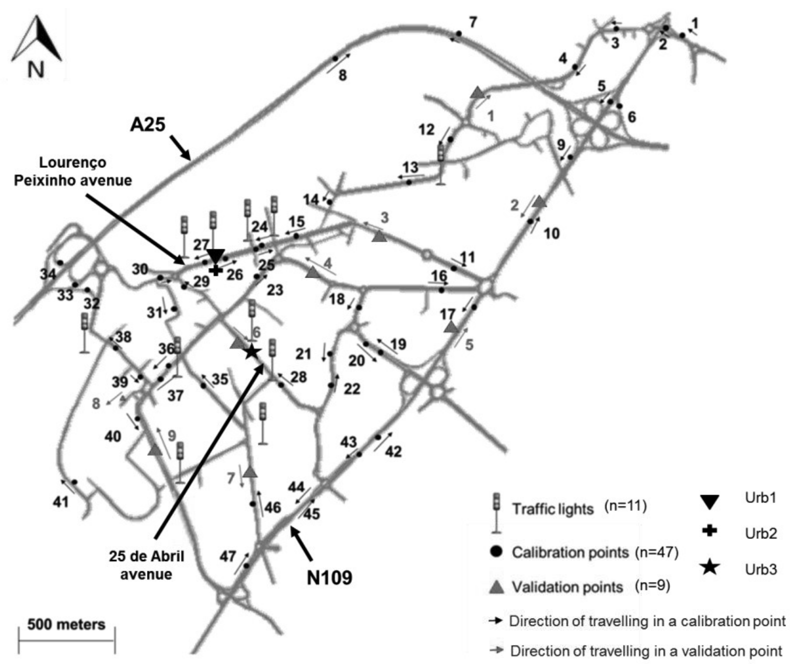


Figure 1. Study domain showing the traffic collection points and the location of the urban air quality stations (the suburban background station is outside the domain). Main roads are indicated: A25 (motorway), 'Lourenço Peixinho' (city avenue), '25 de Abril' (city avenue), and N109 (interurban road).

Aiming to capture the spatial variation of air quality a monitoring network consisting of four stations was designed, as shown in Figure 1 and Table 1. The air pollutants addressed in this paper are NO_x and particles with an aerodynamic diameter smaller than 10 µm (PM10). Air quality monitoring equipment with similar technical specifications was used in the different stations. Two of them were located in major thoroughfares of the city, the 'Lourenço Peixinho' avenue (labelled as Urb1 and shown in Figure 2a) and the '25 de Abril' avenue (Urb3). The Urb2 station (Figure 2b) was positioned in a pedestrian zone with very low traffic density. Although it was located at close distance from the avenue, the buildings geometry protects this location from the direct influence of traffic emissions. Finally, data from a suburban background station (Sub), located at approximately 6.5 km from Urb1, are included in the analysis.

(a) (b)

Figure 2. Mobile air quality monitoring stations (a) Urb1 (b) and Urb2.

Table 1. General description of the air quality stations.

Station ID	Classification	Type	Location
Urb1	Urban (traffic)	Mobile	Central sidewalk of the 'Lourenço Peixinho' Av. 40°38'31'' N; 8°39'03'' W
Urb2 [1]	Urban (traffic)	Mobile	Square in front of the 'Manuel Firmino' market (ca. 100 m from Urb1) 40°38'30'' N; 8°38'58'' W
Urb3 [2]	Urban (traffic)	Fixed	Front yard of the 'José Estêvão' School, in the '25 Abril' Av. (ca. 570 m from Urb1) 40°38'08'' N; 8°38'48'' W
Sub [2]	Suburban (background)	Fixed	'Gabriel de Ançã' School, in Ílhavo town (ca. 6.5 km from Urb1) 40°35'23'' N; 8°40'14'' W

[1] Used to characterize background concentration (cf. sections 2.4 and 3.1)
[2] Station from the national network QUALAR (http://www.qualar.org), managed by the Portuguese environmental agency APA.

In addition, wind velocity, wind direction, temperature, and relative humidity were measured using 10 m high meteorological masts installed in the mobile labs. A 1 week study period was defined between the 1st (9h) and the 8th (14h) of June 2013, in a total of 174 hours. In the case of Urb1 observations of PM10, the time period covered by this analysis is shorter (91 hours) in order to fulfill with the minimum data acquisition efficiency of 75%.

2.2. Road traffic modelling

The simulation of road traffic at the urban scale was carried out applying the VISSIM ('Verkehr In Städten SIMulationsmodell') microscopic traffic model (PTV, 2011) tuned with the traffic data field measurements. This model was selected because of the possibility of defining different road-user behavior parameters and selecting sub-models (car following, lane change and gap acceptance) for distinct vehicle types. Additionally, it allows the definition of vehicles performance outputs, such as desired maximum speed per vehicle and class (PTV, 2011). Several studies have documented the effective use of this tool in assessing management strategies in real world case studies (Mahmod et al., 2010; Fontes et al., 2014; Fernandes et al., 2016).

VISSIM was used to simulate individual vehicle movements during peak and non-peak periods aiming to consider the variability in traffic dynamics throughout a typical working day. Traffic model parameters were calibrated by modifying vehicle performance and driver behavior parameters and examining their effect on traffic flows and speeds in 47 points of the study domain, as depicted in Figure 1. The driver behavior parameters included car-following (average standstill distance, additive and multiple part of safety distance), lane-change and gap acceptance (front gap, rear gap, safety factor, anticipate route), and simulation resolution. The methodology presented in Fontes et al. (2014) was followed.

Traffic model validation focused on comparing estimated and observed hourly traffic flows in the points that were not used for calibration, as well as travel time, average speeds and cumulative VSP modes distributions for each monitoring route. This procedure was conducted with a preliminary number of simulation runs (between 10 and 20, as suggested by Hale, 1997). The widely-accepted FHWA (Federal Highway Administration) practice Geoffrey E. Havers (GEH) statistic was used to compare estimated and observed traffic flows. The advantage of using GEH is that it avoids divisions by zero and is independent of the order of the values. Aiming to satisfy the validation criteria, the GEH should be less than 5 for at least 85% of the monitoring points (Dowling et al., 2004).

For travel time and average speed, the root-mean-square percentage error (RMSPE) was used to measure the magnitude of the errors between data samples. This goodness-of-fit measure was selected for two main reasons: it provides comparing forecasting errors of different models for specific variables; and the validation parameters values are significantly higher than zero which avoids extremely skewed distributions (Hyndman and Koehler, 2006).

Lastly, the observed (GPS runs) and estimated (VISSIM output) VSP modes distributions were calculated from travel time data of each monitoring route, and further compared using the two-sample Kolmogorov-Smirnov test (K-S test) for a 95% confidence level. K-S evaluates the consistency between the estimated and observed VSP mode distributions, and it is suggested when a natural ordering of the modes of data samples occurs (Fontes et al., 2014).

2.3. Vehicles emission modelling

As mentioned, vehicular emissions were not measured at the site. Thus, emission estimates were carried out by using two complementary methodologies: VSP (EPA, 2002; Frey et al., 2008; Coelho et al., 2009) was used to estimate the emissions of NO_x and PM for passenger cars and light duty vehicles, while for heavy duty vehicles and motorcycles, the EMEP/EEA methodology (EEA, 2013) was applied since there is a lack of VSP emission factors adapted to the European situation. The VSP methodology allows estimating second-by-second emissions based on vehicle's dynamics (speed, acceleration and road grade) in accordance to the specified level of detail of the road traffic model used previously. Because of its direct physical interpretation and strong statistical correlations with vehicle emissions, VSP has become a widely recognized approach for emission micro simulation from both gasoline (EPA, 2002; Frey et al., 2008) and diesel (Zhai et al., 2011) light passenger vehicles. Total emissions by segment can be derived based on the time spent in each VSP mode multiplied by its respective emission factor (EPA, 2002; Frey et al., 2008). More information on the VSP methodology is described in Frey et al. (2008), EPA (2002), and Coelho et al. (2009). In the EMEP/EEA methodology (EEA, 2013) the emission factors depend on the speed, age and engine size or tonnage of each vehicle category. Although this methodology is based on the average speed, in order to maintain consistency, the emission factors were adapted to consider the spatiotemporal resolution of the other models.

Emissions estimates using VSP/EMEP methodologies were based on vehicle dynamics data (instantaneous speed, acceleration/deceleration) gathered from VISSIM traffic model which had been calibrated with GPS data. A console application in C# programming language was developed to compute second-by-second vehicle dynamics data from VISSIM output. Passenger cars total emissions were based on Portuguese fleet according to the information given by the Portuguese Automotive Association (ACAP): 57.5% passenger gasoline vehicles and 42.5% of passenger diesel vehicles (ACAP, 2010).

2.4. Air quality modelling

Air pollution levels at the urban scale were simulated applying the air quality modelling system URBan AIR (URBAIR) (Borrego et al., 2014; Valente et al., 2014). In its core is an improved version of the second generation Gaussian model POLARIS (Borrego et al., 1997), which is differs from traditional Gaussian dispersion models because its dispersion parameters have a continuous variation with the atmospheric stability and accounts for building-induced dispersion mechanisms. This steady state atmospheric dispersion model is based on boundary layer scaling parameters and is suitable to be used for distances up to about 10 km from the source. A pre-processor calculates the meteorological parameters needed by the dispersion model, such as atmospheric turbulence characteristics, mixing height, friction velocity, Monin-Obukov length and surface heat flux. The inputs consist of meteorological measurements from a local synoptic surface station (located at the University of Aveiro, 1 km from Urb1) and twice-daily upper air soundings (station 08001 over La Coruna, Spain, available at http://weather.uwyo.edu/upperair/sounding.html). NO_x is treated as a non-reactive tracer, allowing that the atmospheric chemistry involved is simplified to a steady state solution. Dry deposition fluxes of particulate and gases are described applying conventional resistance schemes by Wesely et al. (2002).

The simulation domain defined over Aveiro, with dimensions of 3.9 x 4.5 km^2, coincides with the one considered for the estimation of traffic dynamics and related emissions, covering the entire urban zone, as shown in Figure 1. In order to use the emissions as estimated in section 2.3, URBAIR's road traffic emissions module was deactivated. Line sources are discretized into a series of point sources with diameters matching the road dimensions, following Karamchandani et al. (2009). No industrial sources exist within the simulation domain, being the nearest one at approximately 5 km from the city center. The contribution of industrial areas around the city is accounted in the urban background concentration, as also for other point sources inside the domain (e.g., some bakeries using wood burning ovens).

Input data describing the spatial variation of terrain surface elevation, buildings 3D coordinates and roads 2D coordinates are required. Local Geographic Information System (GIS) shapefiles complemented with aerial imagery were used for this purpose. For simplicity, buildings were assembled based on proximity and geometry criteria. Direction-specific downwash parameters, in the form of projected building height and width dimensions, are estimated using an approach similar to the one implemented in EPA's Building Profile Input Program for the Plume Rise Model Enhancements (BPIP-PRIME) model (Schulman et al., 2000; EPA, 2004).

With the purpose of estimating representative background concentrations, several approaches have been tested. In the scope of this work, the background concentration is defined as the concentration that would be measured in the absence of local emission sources that are explicitly considered by the dispersion model. Therefore, the background air quality should include a contribution of all other sources, natural and anthropogenic, except local traffic emissions considered in the model inputs. As a first attempt, measurements from the nearest suburban background station (Sub) carried out in June 2013 were analyzed, but this station poorly explains the fluctuations of the pollution levels within the study area for the period of interest (cf. section 3.1). Therefore, an alternative approach previously developed and validated by Tchepel and Borrego (2010) and Tchepel et al. (2010) was applied to define the background pollution levels. The main idea of the data filtering is based on the assumption that the fluctuations presented in the time series could be analyzed as a linear combination of periodic functions. The contribution of local sources is attributed to high frequencies (short-term fluctuations). Therefore, the filter is designed to remove the high frequencies and to pass the low frequencies presented in the data. It should be noted that due to the filter algorithm, the length of the processed time series is shorter than the original one but the data are still with hourly resolution.

The modelling results were evaluated against the measurements carried out in Urb1 and Urb3 stations applying the model acceptance criteria proposed by Chang and Hanna (2004) for air quality models assessment, which establishes performance measures for the normalized mean square error (NMSE<1.5), fraction of predictions within a factor of two of observations (FAC2>0.5), and fractional bias (|FB|<0.3). Also the correlation coefficient (r) was considered in the analysis. The performance measures were calculated applying the BOOT Statistical Model Evaluation Software Package (Chang and Hanna, 2004).

3. Results and discussion

In the following sections both monitored and modelled results are presented and analyzed.

3.1. Local measurements

Meteorological data on wind direction and velocity collected in Urb1 station from June 1 to 8 reveal a dominant wind from North (24% of the time) and North-northwest (44%) with an average speed of 2 m.s^{-1}. South winds (18%) were registered mainly during the morning hours. The temperature ranged between 12 and 28 °C and the relative humidity from 32 to 90%.

The observed pollutant concentration time series shown in Figure 3 reveals both daily and weekly cycles, with a direct relation with the vehicle traffic and resulting emissions.

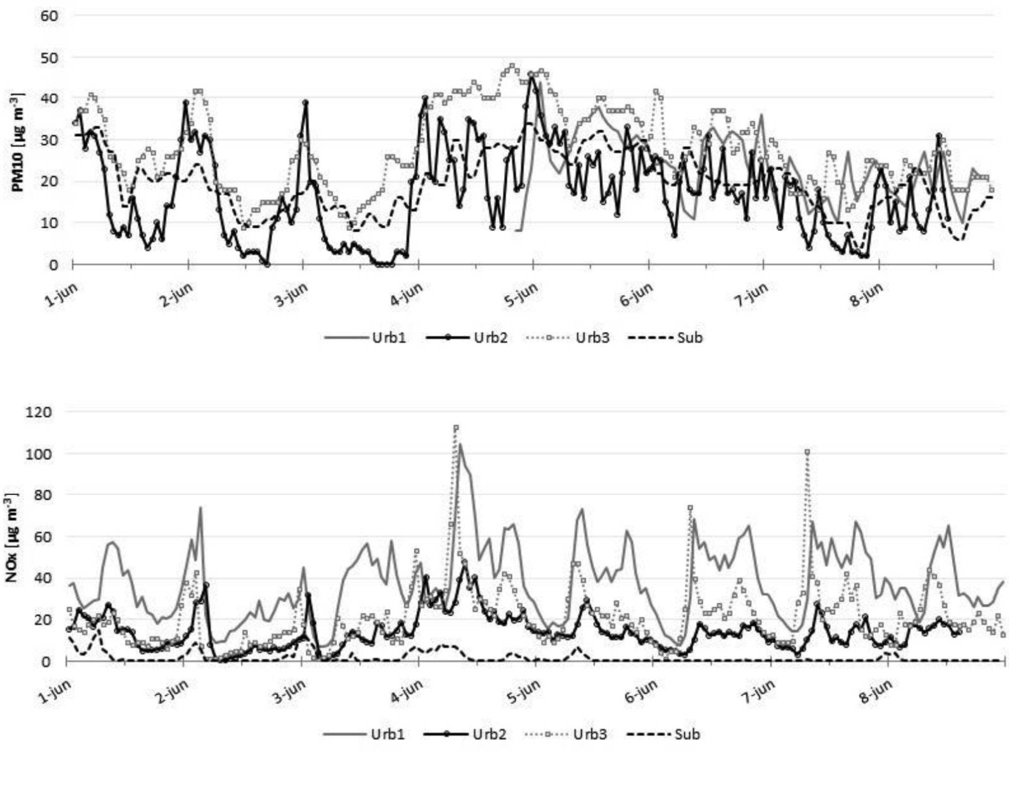


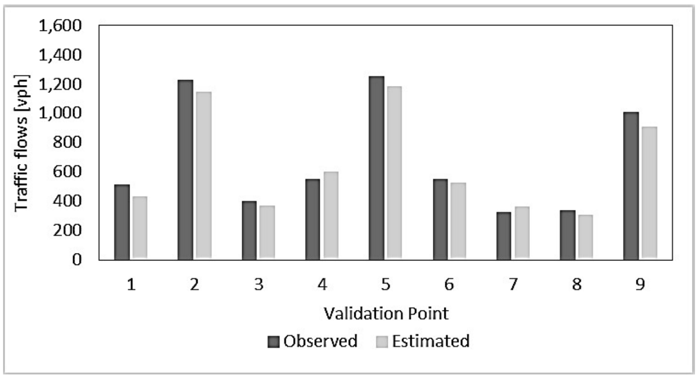
Figure 3. Hourly averaged concentration of PM10 and NO_x measured in the four air quality stations from 1-8 June, 2013.

No exceedances to the limit values established by Directive 2008/50/CE (200 $\mu g.m^{-3}$ hourly concentration of nitrogen dioxide (NO_2) and 50 $\mu g.m^{-3}$ daily concentration of PM10) were observed during the reporting period. In comparison with the observations carried out in Urb1 station, lower hourly mean concentrations and a smoother variation over time is found at Urb2 location as a consequence of the longer distance to the main road. The statistical comparison between 1 month (June) time-series acquired in Sub and Urb3 shows a low correlation (r=0.21) for daily average NO_x values. Although for PM10 a better agreement (r=0.65) was obtained, the magnitude presented in the suburban measurements is higher than that from the urban station. This indicates that Sub is not representative of Aveiro´s background in the period under analysis, which can potentially be associated with emission sources in the vicinity of Sub, such as from the nearby city of Ílhavo or/and from agricultural practices (given the predominantly rural characteristics of the site).

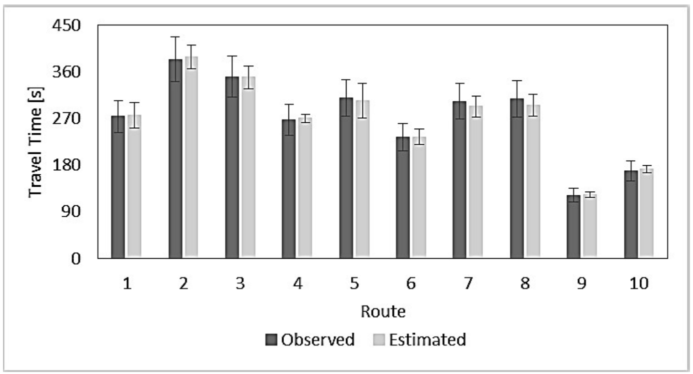
3.2. Road traffic

Figure 4 exhibits the validation results for the modeling platform of traffic and emissions and corresponding statistic test with 10 different runs (stochastic traffic flow), as suggested by Hale (1997). Figure 4a confirms that all traffic points recorded GEH values below 4, meeting the validation criteria (Dowling et al., 2004). These findings are particularly significant since this study domain has a considerable size with different traffic flows along main arterials (300 - 1,250 vph). The comparison between observed and estimated travel time (Figure 4b) and speed (Figure 4c) resulted in a RMSPE below 10% and within confidence level intervals. In such cases, the highest differences were found in routes 7 and 8, which contained several uninterrupted traffic facilities (traffic lights, single or two-lane roundabouts) throughout their length. Concurrently, each monitoring route showed a similar trend for a 97.5% confidence level (p-value > 0.025) concerning the comparison between observed and estimated cumulative VSP modes distributions. Based on these validation results, 10 simulation runs were considered to be appropriate to reproduce site traffic operations in VISSIM model, in agreement with Dowling et al. (2004) and Hale (1997).

(a)



(b)



(c)

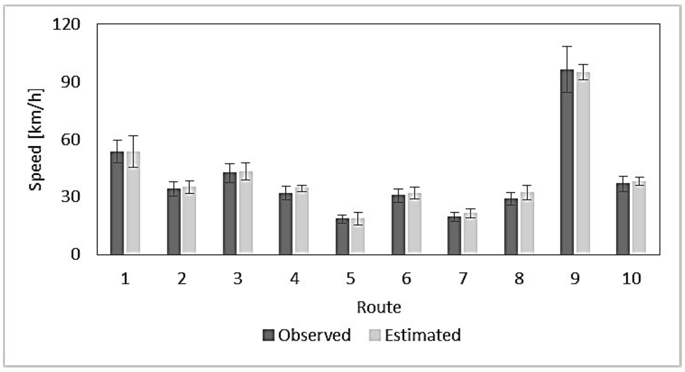


Figure 4. Validation results of traffic model: (a) traffic flow, (b) travel time, and (c) speed. Validation points were randomly selected in order to maintain consistency of the traffic flows and the remaining roads of the study domain.

3.3. Vehicles emission

Figure 5 shows the daily emissions of NO_x and PM10 ($g.km^{-1}$) recorded for the urban area of Aveiro. High emission hot-spots are achieved in the city center, where the daily average speed is low (<50 $km.h^{-1}$), as well as in the interurban road N109 and the motorway A25.

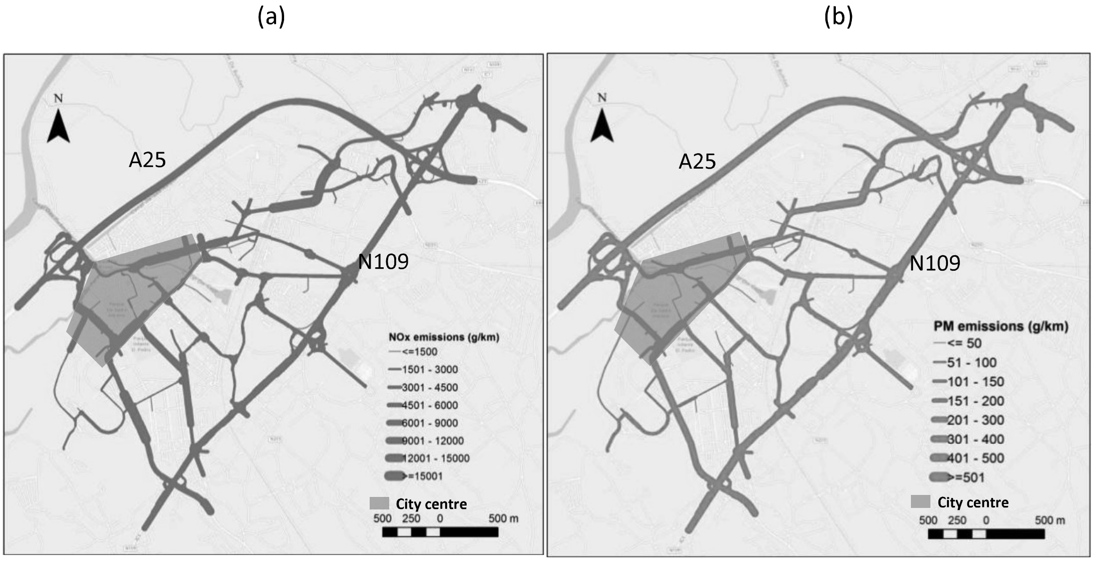


Figure 5. Daily emissions of (a) NO_x and (b) PM10 estimated for the city of Aveiro over a working day.

Figure 6 presents the average emissions by link for PM10 and NO_x ($g.km^{-1}$) as a function of traffic flow (vph) and speed ($km.h^{-1}$). The results show that more than 70% of total PM10 and NO_x emissions are generated in high-traffic demand areas (>800 vph), as depicted in Figure 6a and 6b. In these areas, speed is usually higher than 50 $km.h^{-1}$ (Figure 6c). Two main reasons contribute for these results: firstly, roads with high traffic demand (e.g. N109 and A25) are characterized by high demand of heavy duty vehicles (especially when compared with city center roads); and secondly, traffic flow on the N109 and A25 roads can be severely impacted during peak hours affecting speed and travel time (see the high standard deviation of these links in Figure 6c), and as result increasing vehicular emissions occur. On the other hand, in the city center several intersections with traffic lights and roundabouts are presented (see Figure 1 for those details) which increases stop-and-go situations. Consequently, these speed changes contribute to increased total emission levels per vehicle.

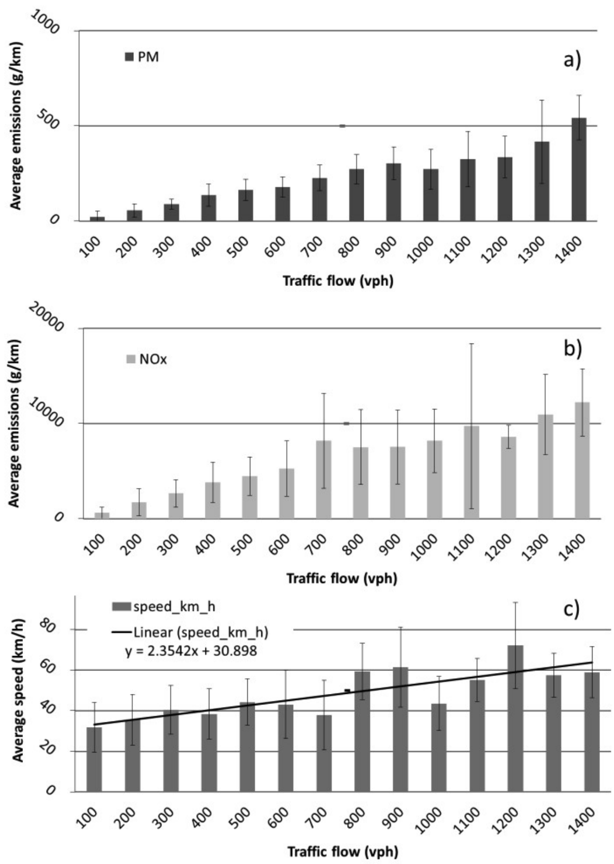


Figure 6. Estimates by link for the city of Aveiro: (a) average PM10 emissions; (b) average NOx emissions; and (c) average speed (c) as a function of average traffic flow.

3.4. Air quality

Figure 7 illustrates the response of URBAIR to peak vs off-peak conditions. The dynamics of traffic (and related emissions, as already discussed in Figure 5) and atmospheric conditions become evident in the magnitude and location of the NO_x hot-spots.

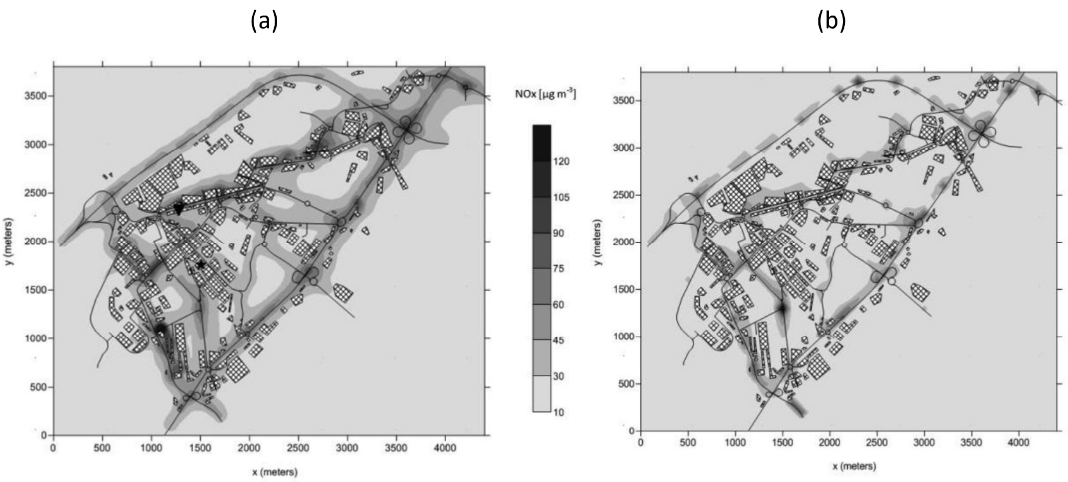


Figure 7. Contours of NO_x concentration fields simulated by URBAIR (with background levels added) over the city of Aveiro for (a) peak (8-9h) and (b) off-peak (13-14h) traffic conditions on the 6th of June 2013 (Thursday). Buildings

shown in crossed pattern. Symbols have the same meaning as in Figure 1. At Urb1 location, observ./model pairs are the following: 68,1/69,4 μg.m^{-3} (peak) and 44,0/39,3 μg.m^{-3} (off-peak).

Aiming to further investigate the dependency of model performance on the time of the day, observed vs computed daily mean profiles of hourly surface pollutant concentration were calculated. Figure 8 depicts the ability of the modelling approach to track the evolution of NO_x levels, including the morning traffic peak at 8-9h. Similar agreement was observed for PM10 (not shown). However, an evident overestimation is reported at the end of the day. This behavior originates from excessively low predicted mixed layer (ML) height (below 200m) at sunset time in three of the days (notice the significant standard deviation of modelled data). This sudden collapse of the ML induces the trapping of pollutants that explains the steep build-up of concentrations at 20h, gradually dispersing within two hours following the decrease in emissions.

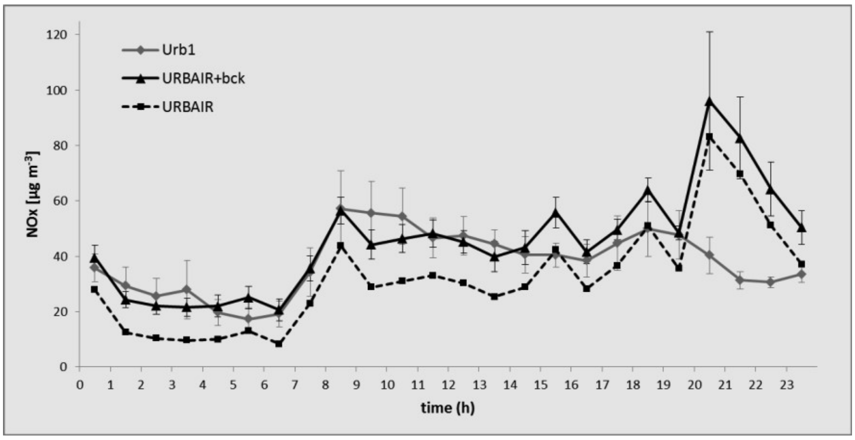


Figure 8. Daily average profile of measured (Urb1) and simulated NO_x concentration for the 1 week study period. Vertical bars indicate standard deviation.

Table 3 compiles the statistics for the comparison between model outputs and air quality measurements of PM10 and NO_x levels considering both hourly and daily averages. Aiming to distinguish the effect of the filtering technique on performance both the direct URBAIR output and with background are shown. As can be seen, model acceptance criteria (cf. section 2.4) are, in general, fulfilled, with a consistent improvement of model accuracy resulting from adding the background contribution, despite some overestimation revealed by the FB, indicating that in some cases the mean bias is not within the threshold of +30% of the mean. In the 24 hours computed record the average r increases significantly from 0.23 to 0.89 by adding the background. Despite the improvement, a poor correlation between observations and predictions is found for the 1h dataset, with an average r of 0.39 (0.08 without the background). This behavior was identified in other studies reporting the application of Gaussian models to line sources emission dispersion (Luhar and Hurley, 2003; Zou et al., 2010; Gibson et al., 2013). The FAC2 parameter, a robust performance measure in the evaluation of Gaussian models, shows that, in average, 78% of the hourly predictions (60% with no background) are within a factor of two of the observations, increasing to 94% (82% without background) for daily averages.

Table 3. Statistics of URBAIR performance for daily and hourly average concentrations of PM10 and NO_x evaluated against observations, without and with (in brackets) the contribution of (filtered) background, for the period between the 1st and the 8th of June. The underlined values indicate that the model acceptance criterion is unfulfilled, while for r (in italic) no criterion is available. In the analysis, 174 data points (hourly averages) were considered, except for PM10 in Urb1 where the sample was of 91 data points. A positive FB indicates here an over prediction.

	Urb1		Urb3	
	24h	1h	24h	1h
PM10				
NMSE	0.16 (0.15)	0.70 (0.52)	0.91 (0.01)	1.13 (0.08)
FB	-0.33 (0.36)	-0.24 (0.43)	-0.79 (0.03)	-0.78 (0.03)
FAC2	1.00 (1.00)	0.60 (0.79)	0.38 (1.00)	0.42 (0.98)
r	*0.51 (0.95)*	*-0.06 (0.13)*	*0.11 (0.93)*	*-0.05 (0.67)*
NO_x				
NMSE	0.09 (0.04)	0.55 (0.33)	0.19 (0.17)	0.88 (0.50)
FB	-0.19 (0.17)	-0.18 (0.18)	-0.21 (0.38)	-0.21 (0.37)
FAC2	1.00 (1.00)	0.72 (0.78)	0.88 (0.75)	0.66 (0.55)
r	*0.18 (0.79)*	*0.26 (0.40)*	*0.11 (0.90)*	*0.04 (0.37)*

The scatter plot in Figure 9 shows the 1 hour average observed/modelled pairs for different instants in time at each sampling location, the central line indicating a perfect agreement. Figure 9a reinforces the under prediction tendency identified in Table 3 for PM10, while for NO_x a significant dispersion around the 1-to-1 correspondence line is identifiable in Figure 9b, especially at Urb3 spot. The plots (c) and (d) confirm the better agreement between predictions and observations when background is added, despite the overestimation of the lower range of NO_x concentrations at Urb3.

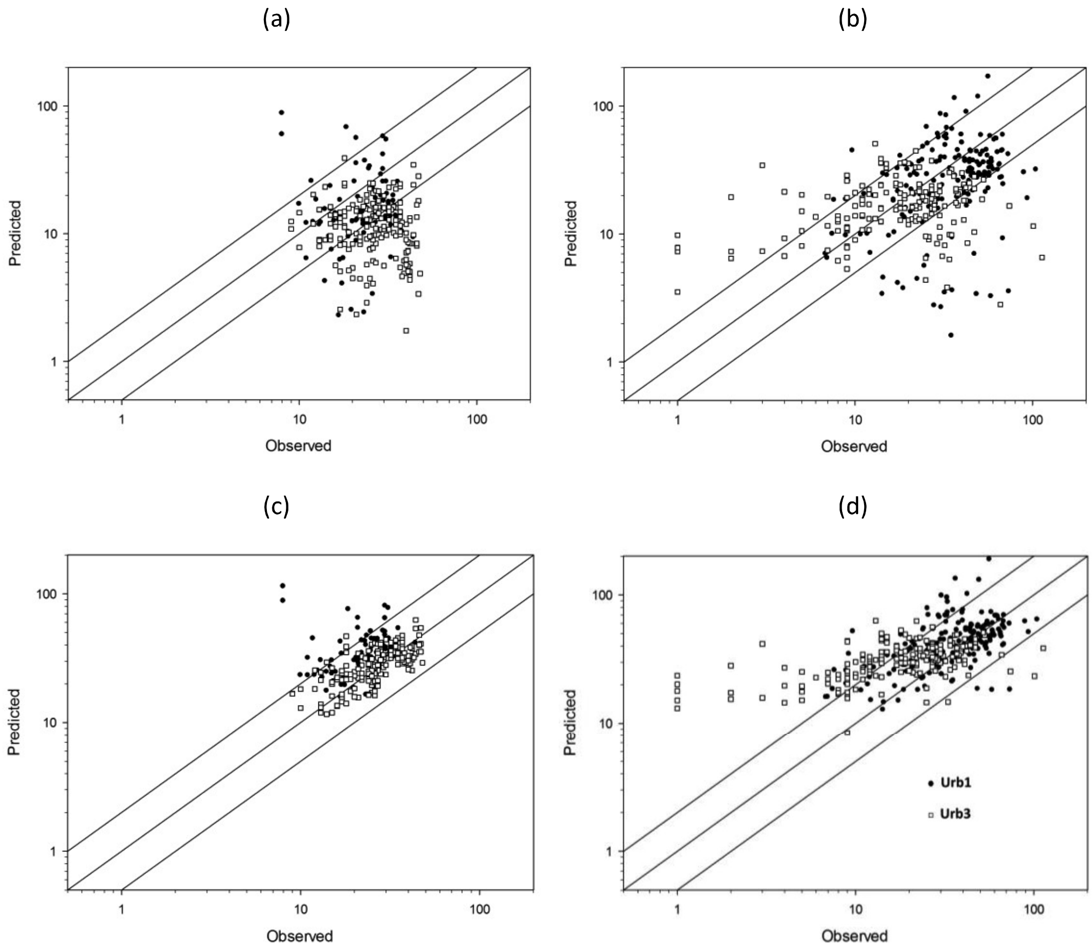


Figure 9. Scatter plot of observed vs predicted hourly average concentrations (in $\mu g.m^{-3}$) of PM10 (a), NO_x (b), PM10 with background (c), and NO_x with background (d). Central line indicates a 1-to-1 correspondence, while the upper and bottom lines indicate respectively a factor-of-2 over- and underestimates.

4. Conclusions

In this work the air quality of a medium-size European city was simulated, at the urban scale, for a 1 week period during which air pollutant concentration measurements were carried out at three distinct spots within the urban area. A modelling approach was applied consisting of (1) detailed traffic flows derived from microscopic traffic models calibrated with GPS data; (2) exhaust road traffic emissions estimated by a combined VSP/EMEP methodology; (3) urban background levels calculated applying a low-pass filter to local air quality observations; and (4) air pollutants dispersion simulated by a second generation Gaussian model accounting for the effects of buildings. The analysis of model performance metrics showed that 78% of the results are within a factor of two of the observations for hourly average concentrations, increasing to 94% when daily averages are considered. The good performance of the model is sustained also by the analysis of the NMSE, which in the great majority of the cases fulfilled the data quality objectives. Despite the low correlation between predicted and observed values for the hourly data series, correlation is shown to significantly improve when urban background concentration is added, with an average of 0.89 for the 24 hours record.

In conclusion, the general good agreement obtained between modelling results and local measurements highlights the potential of detailed traffic and instantaneous exhaust emissions data, together with urban background levels extracted from filtered observations, to provide accurate input data to intrinsically simple Gaussian models applied at the urban scale.

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