Evaluation of a CFD modeling approach by means of an intensive experimental campaign using passive samplers in an urban area of Madrid

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dated: 8 June 2015

1. Introduction

Computational Fluid Dynamics (CFD) models, based on the resolution of the Reynolds Average Navier Stokes (RANS) Equations are being increasingly used to simulate the dispersion of air pollutants in urban areas. Their ability to reproduce the air flow modifications induced by the buildings at a fraction of the computational time required by Large Eddy Simulations (LES) models, make them an attractive choice for real world applications (air quality assessment or network design, microscale air pollution abatement strategies, etc.). Parra et al. (2010), Santiago et al. (2011) and Santiago et al. (2013) developed a methodology based on a set of steady state simulations for a range of wind directions, that allowed to compute average concentration maps over large periods of time (weeks, months). In this work, this methodology is further validated using measurements of NO_2 from two intensive experimental campaigns lasting several weeks that were carried out deploying a large number of passive samplers distributed in a heavily trafficked district in the city center of Madrid. The CFD-RANS simulations were done assuming that: a) road traffic is the dominant air pollutant source, b) chemical reactions can be neglected, and c) thermal induced circulations can be also neglected. Data of daily mean traffic intensity, used as proxy of the traffic emission, were provided by the Madrid City Council. The methodology to obtain average concentration maps is evaluated by comparing measured values with the time averaged NO_2 predictions in the locations of passive sampler tubes.

2. Numerical methodology

High resolution maps of average concentration over a large period of time are necessary for air quality management and the assessment of abatement measures. Due to computational loads, it is not possible (within a reasonable CPU time) to run an unsteady CFD simulation of several weeks or months. The solution proposed (Parra et al., 2010; Santiago et al., 2011; Santiago et al., 2013) is to run only a set of scenarios (16 inlet wind directions) using steady CFD-RANS simulations (STAR-CCM+ code from CD-Adapco). The pollutant emissions are modelled with a line source inside each street and several tracers (one for each street) are emitted in each simulation. The final map of average concentration is made by means of a combination of the simulated scenarios considering concurrent wind patterns within the period analyzed.

Pollutant concentration is computed assuming: 1) non-reactive pollutants, thermal effects negligible in comparison with dynamical effects, 2) emissions inside each street at a given hour are proportional to the number of cars at that hour and tracer concentration at a certain hour depend only on emissions and background pollution at that hour. It should be noted that the two periods simulated in this study correspond to winter conditions, where the pollutant concentrations are less affected by atmospheric chemistry and thermal effects are not important.

In addition, the dynamic effects of vegetation are included in CFD simulations assuming the trees as a porous medium (Santiago et al., 2013). The background concentration at each hour from an urban background station is added to the results of the simulations as they only represent the local traffic contribution. Finally, some modifications to the methodology of Parra et al. (2010) are introduced to take into account weak winds. For these cases, several assumptions are not fulfilled (e.g. thermal effects have more importance, concentration is not proportional to 1/v, etc). Taking into account all of these assumptions, for wind speed higher than 2 m s^{-1} at 10 m height a concentration proportional to the observed one at time t is computed using CFD results and Eq. 1. Note that we do not obtain the observed concentration because the number of vehicles inside each street is used as proxy of traffic emissions.

$$C_{\text{Observed}}(t) - C_{background} \propto C_{\text{computed}}(Sector(t)) = \sum_i C_i(Sector(t)) \cdot \frac{L_i}{Vsource_i} \cdot N_i(t) \cdot \frac{1}{v_{in}(t)} \quad (1)$$

where $C_{\text{Observed}}(t)$ and $C_{\text{background}}(t)$ are the observed and background concentration at time *t*, $Sector(t)$ is the

wind direction sector at time *t*, *i* indicates the tracer emitted inside each street, $C_i(Sector(t))$ is the concentration computed for $Sector(t)$ for a given emission from street *i* and for a given inlet wind speed, L_i is the length of the street *i*, $Vsource_i$ is the volume of the row of computational cells where emission of the street *i* is located, $N_i(t)$ is the number of cars per unit time in street *i* and $v_{in}(t)$ is the inlet wind speed. In the case of weak winds (lower than 2 m s^{-1}) the methodology was modified. For these cases, thermal effects are not negligible and we assume that the pollutant concentration is independent of wind direction and it is modelled depending on traffic intensity and mixing height along the day. This assumption allows taking into account indirectly the thermal effects.
As for emission sources, only those of road traffic are considered. According to previous source contribution analysis, NO_2 ambient concentration levels in Madrid, particularly in the innermost area of the city where de modelling domain is located, are strongly dominated by road traffic (Borge et al., 2014).

3. Description of modeling domain, experimental campaigns and simulation setup

The methodology presented in the previous section was evaluated by Parra et al. (2010) for an urban area of Pamplona using measurements from experimental campaigns using passive samplers and monitoring data. However in this work the evaluation is done by means of a denser network of passive samplers providing more information about the spatial distribution of the time averaged NO_2 concentrations. Two different experimental campaigns were carried out and simulated in the same urban area in Madrid.

3.1 Location and urban environment

The urban area analyzed is located in Madrid City close to El Retiro park. In this zone there are several streets and avenues with intense road traffic and also there is a large green urban area (El Retiro). Buildings with different heights are located in this area; most of them have a height between 18 m and 24 m, although the tallest building is 90 m high approximately. A traffic air quality monitoring station (EA) is located in a garden very close to the sidewalk in the intersection of the two more important avenues (Figure 1). Meteorological data were provided by AEMET (Spanish Meteorological Agency) from the meteorological station located in El Retiro (the urban park South of EA station), approximately 200 m outside of the numerical domain (Figure1). The urban park produces not negligible dynamical effects on pollutant dispersion.

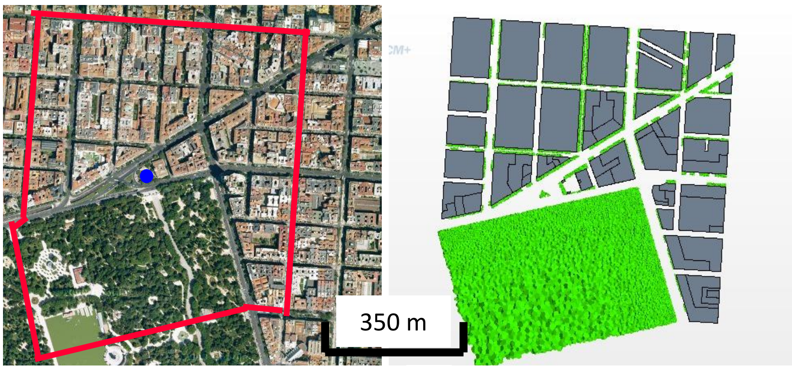

Fig. 1. Escuelas Aguirre district. Left: Aerial picture of the modeling domain (red line) including the location of the air quality monitoring station (blue dot)). Right: Modeled geometry of the domain including street and park vegetation.

3.2 Simulation set-up

The size of the modelling domain is 700 m x 800 m, approximately (Fig. 1). Hourly traffic data inside each street is estimated from the daily average traffic intensity (TI) data provided by the city council of Madrid, considering typical traffic patterns for different types of days (working days and weekend days) and the corresponding diurnal variation (TF). 29 passive tracers were released (one for each street) within the modelling domain. An irregular mesh of $3{\cdot}10^6$ grid points with a resolution of about 1 m^3 close to the buildings is used. The dynamical effects of the vegetation are modelled considering trees as porous medium. More details can be found in Santiago et al. (2013), Santiago et al. (2014) and Krayenhoff et al. (2015). Inside the park, vegetation is represented in the numerical cells located from the ground to 18 meters-height (average height of trees) but for the trees within the street only the canopy level is considered.

3.3 Experimental campaigns

Two different campaigns were carried out in this zone. The first campaign was took place from January 26th to February 16th 2011. 26 passive samplers were deployed in the simulation domain (Fig. 2). The second campaign was done from November 6th to December 1st 2014. In this campaign the number of passive samplers deployed within the modelling domain was increased to 95 (Figure 3).

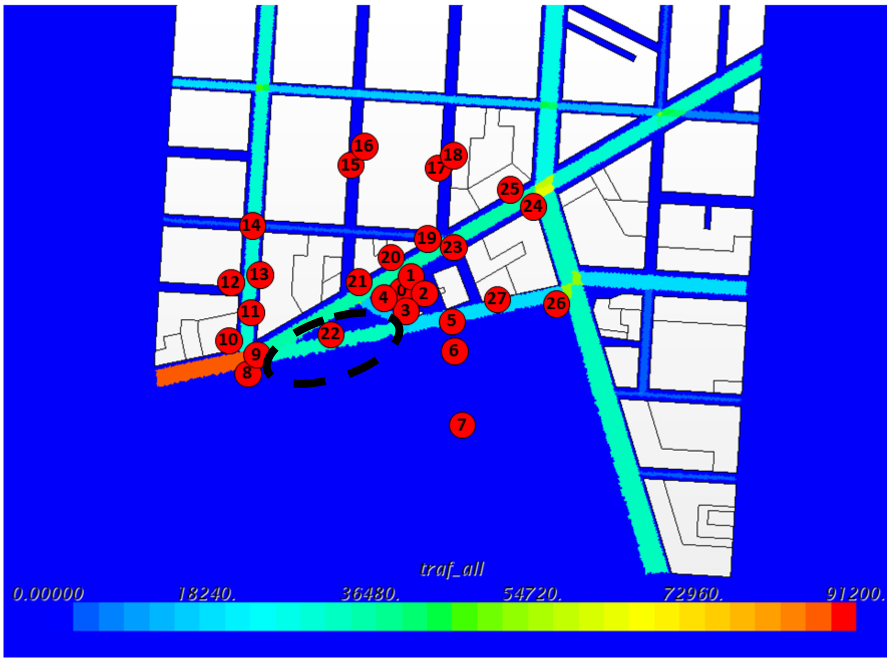

Fig.2. Daily mean traffic intensity for 2011 campaign (vehicles day^{-1}), location of passive samplers, and the zone B (dashed line).

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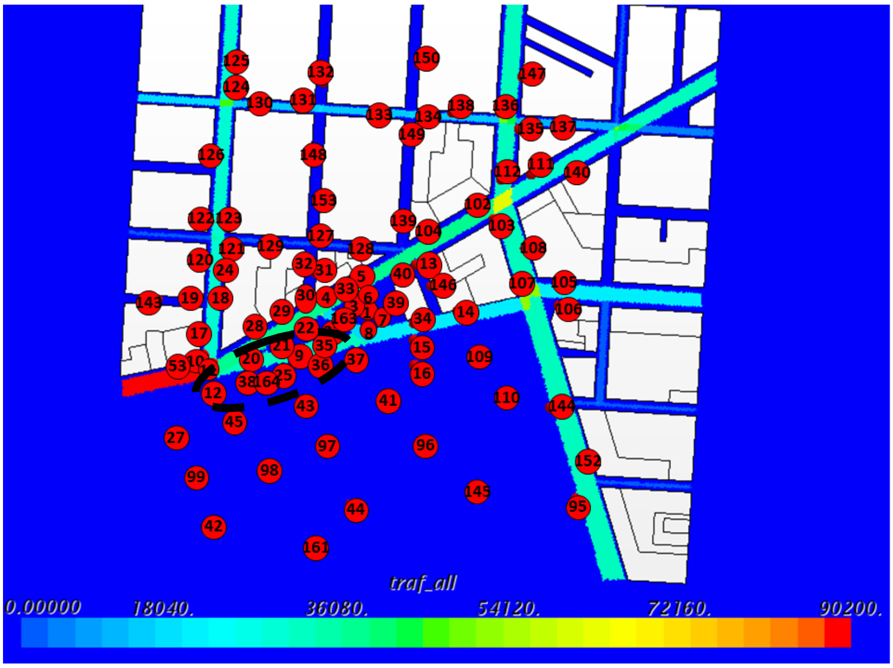

Fig.3. Daily mean traffic intensity for 2014 campaign (vehicles day^{-1}), location of passive samplers and and the zone B (dashed line).

4. Results

The two different campaigns are modelled following the methodology described in section 2. Firstly, modelled hourly data for NO_2 were compared with observed data in the air quality monitoring station (Figs. 4 and 5) for both periods. The results were quite good showing that the simulated data fit well the observations.

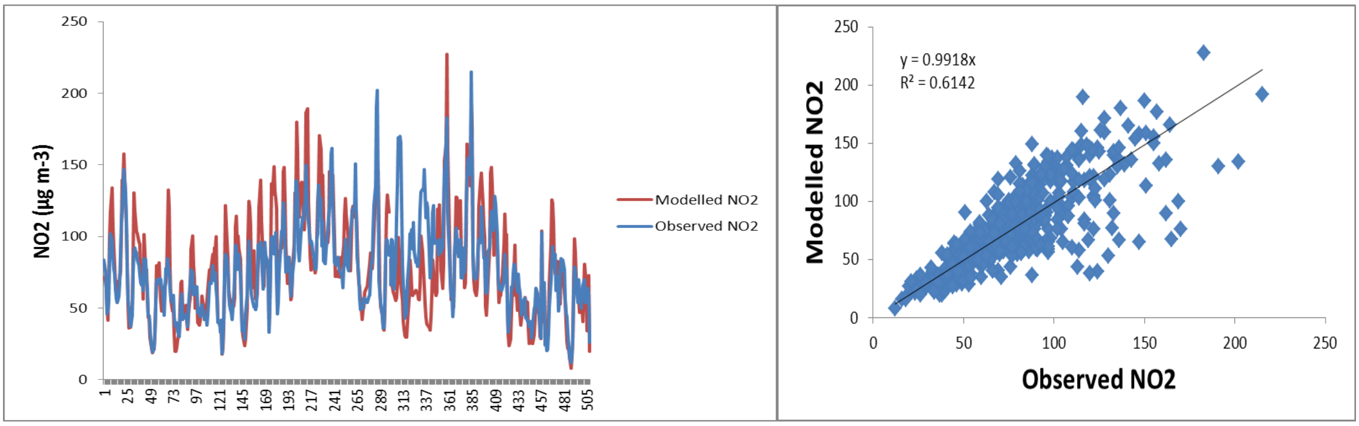

Fig. 4. Comparison between modeled and measured hourly NO_2 concentrations recorded at EA air quality monitoring station for the 2011 campaign. Left: Time series. Right: Scatter-plot.

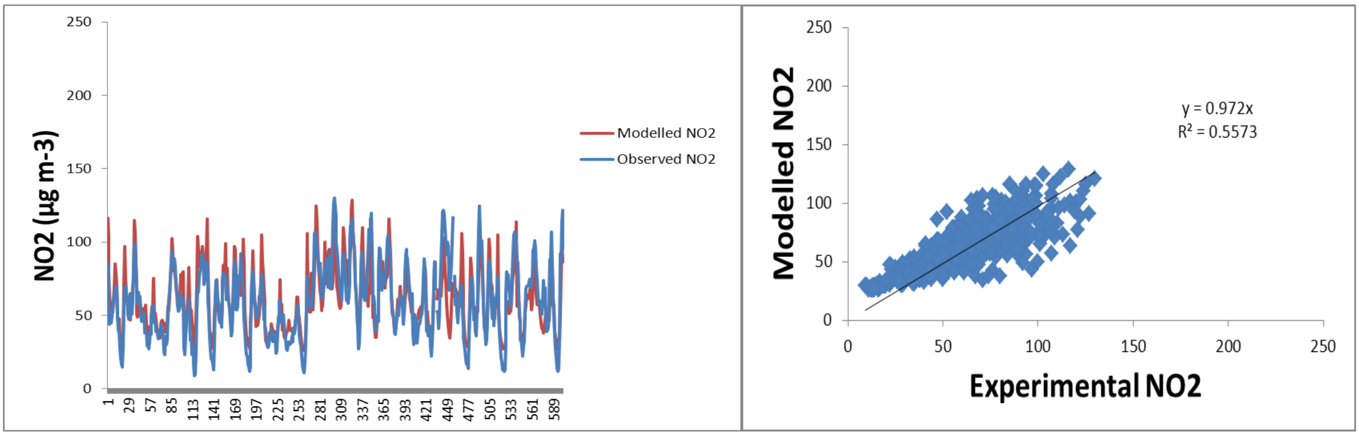

Fig. 5. Comparison between modeled and measured hourly NO_2 concentrations recorded at EA air quality monitoring station for the 2014 campaign. Left: Time series. Right: Scatter-plot.

Following the methodology described in the previous sections, maps of the time averaged NO_2 concentrations were produced for the two experimental campaigns (Fig. 6 and 7). Higher concentrations in 2011 campaign were observed are essentially due to a higher background concentration.

Comparing modelled concentrations with passive sampler measurements, a good correlation agreement is found. However, model performance varies spatially. It was found that the correlation improves if measurements in the locations within the zone marked with a dash line (hereinafter, zone B) in Figs. 2 and 3 are not considered. Figs 8 and 9 show the scatter plots of NO_2 modelled concentration against NO_2 experimental concentration with and without measurements in zone B for the two campaigns. The problem found in the comparison with the zone B could be due to unrealistic emission representation in this particular area. In Fig. 10, it can be observed that the real distribution of the street in this zone which is more complex than the distribution of the emissions (a triangle) used in the simulations (Fig 3 and 4). In addition, the number of the vehicles in the street close to the park is not very high but usually there are traffic jams in this street. This fact may imply that the emissions are not proportional to the number of vehicles that is one of the assumptions made and then, our emissions estimates would not be correct for this zone. For this reasons, passive sampler number 22 is not considered in 2011 campaign and numbers 9, 12, 25, 35, 36, 38 y 164 in 2014 campaigns.Taking into account the correlation obtained in the comparison, we can conclude that the methodology using CFD simulations provides realistic NO_2 averaged concentration maps.

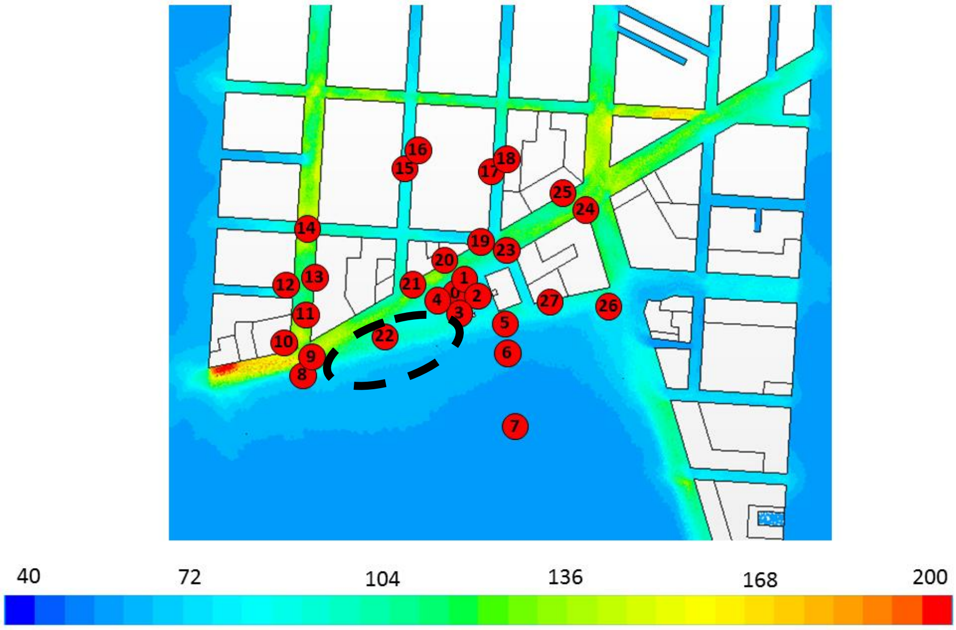

Fig. 6. Map of the time averaged NO_2 concentration in µg m^{-3} (508 hours) and location of passive samplers for 2011 campaign

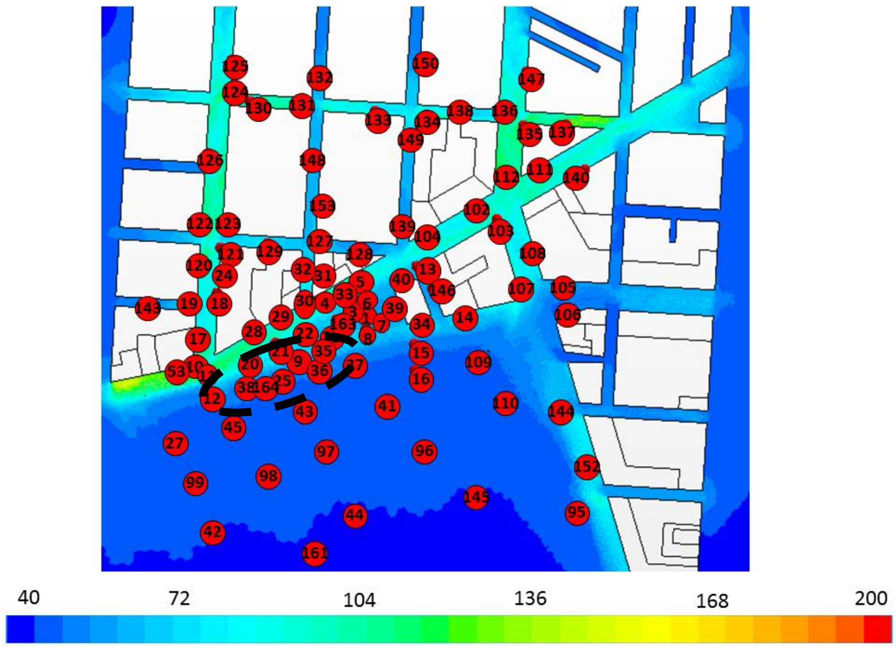

Fig. 7. Map of the time averaged NO_2 concentration in µg m^{-3} (602 hours) and location of passive samplers for 2014 campaign

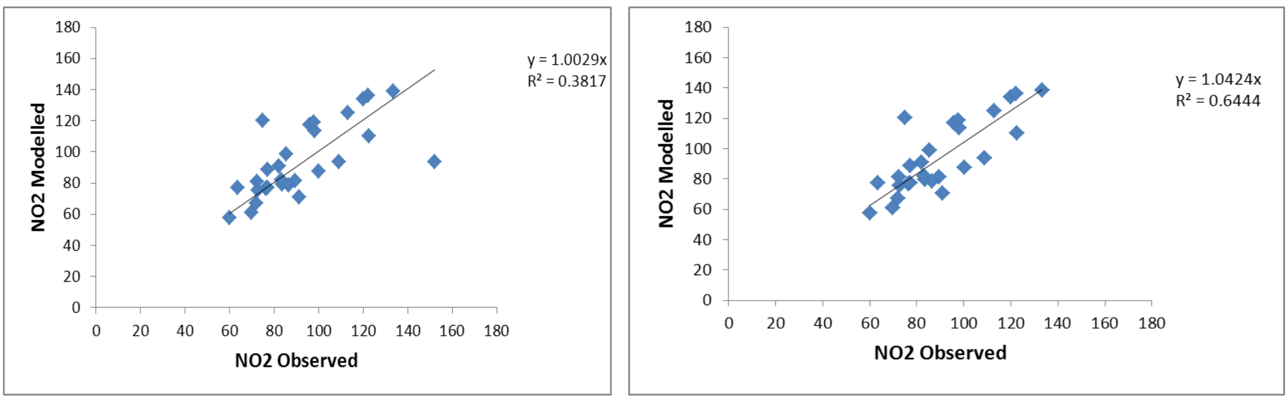

Fig. 8.Left: Scatter plot with all measurements. Rigth: Scatter plot without passive sampler number 22.

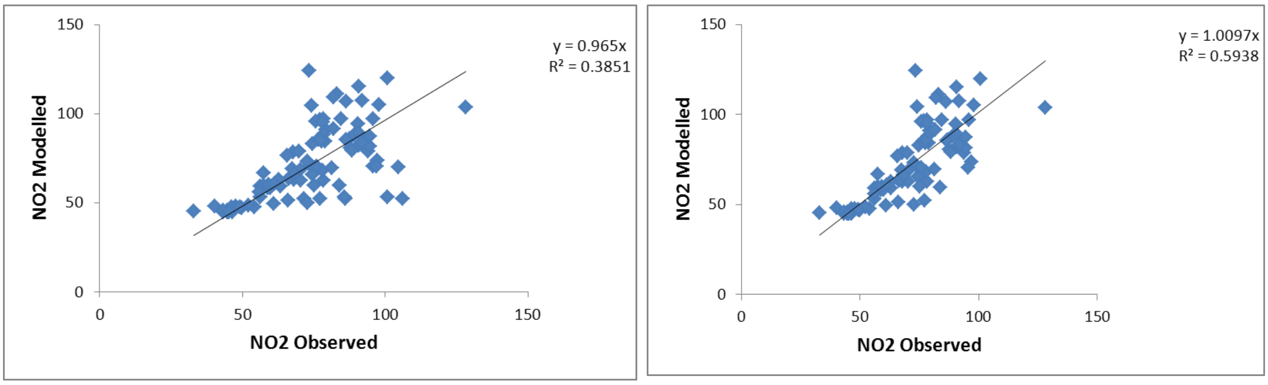

Fig. 9. Left: Scatter plot with all measurements within domain. Rigth: Scatter plot without passive samplers in zone with tunnels and street forks not modeled by emissions (without 9, 12, 25, 35, 36, 38 y 164).

Fig. 10. Image from google maps of the zone B.

5. Conclusions

In the comparison with experimental data from two different campaigns, a good correlation between model estimates and measurements was obtained showing that this methodology, based on the CFD-RANS modelling is able to reproduce the main aspects of several-week averaged pollutant distribution, with resolution of the order of meters. It was observed that in a zone where the traffic distribution was not well estimated due to the complexity (tunnels, street forks,..), the model provided worse results in comparison with passive measurements. We can conclude that the methodology proposed is able to reproduce satisfactorily week-averaged pollutant concentration distribution in an urban area with heavy traffic and shows promising potential to support the analysis of street-scale measures to improve air quality. However, additional research efforts should be done to improve the representation of traffic emissions and the contributions from other sources though dynamic boundary conditions.

Acknowledgment

This study has been supported by the project TECNAIRE (S2013/MAE-2972) funded by The Regional Government of Madrid.

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