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# PROGRESS IN URBAN AIR QUALITY ASSESSMENT: CFD MODELLING OF A WHOLE TOWN IN SPAIN

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**Abstract**: The WA CFD-RANS (Weighted Averaged Computational Fluid Dynamic– Reynolds-Averaged Navier–Stokes simulations) methodology applied throughout the entire city of Pamplona to compute the hourly $NO_2$, NO and $NO_x$ maps at pedestrian level for annual and seasonal averaged days during 2016, is presented in this paper. This modelling approach has been evaluated with measurements from 3 air quality monitoring stations in the city and with experimental data from cyclists who carried portable sensor in their bikes through Pamplona. The proposed maps can be very useful for studying the health impact of these pollutants and their associated externalities in the city and for planning healthy routes of cyclist and pedestrian.

***Key words:*** *CFD-RANS, $NO_2$, NO, $NO_x$, microsensors, urban air quality, evaluation.*

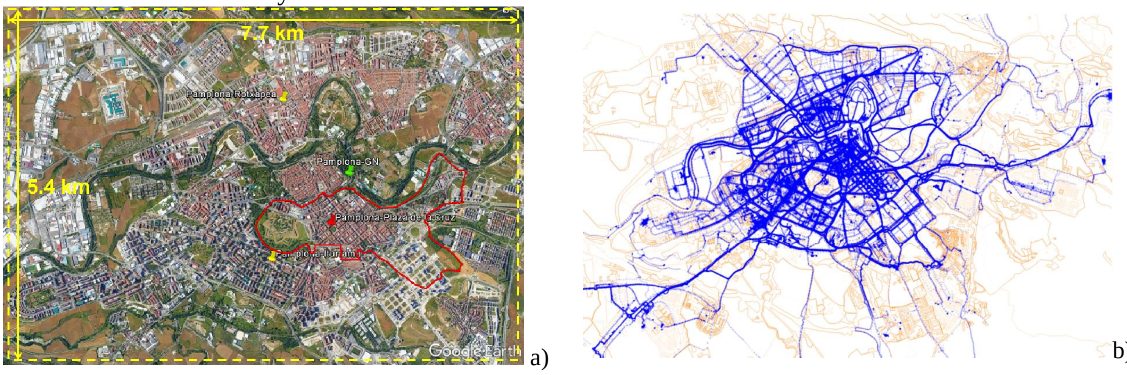
## INTRODUCTION

Limit values for $NO_2$ established by the European Directive 2008/50/EC on ambient air quality and cleaner air for Europe (EC, 2008) are currently being exceeded at many cities throughout Europe (EU, 2016). The impact of air pollution on human health is well documented through long- and short-term epidemiological cohort studies (Brunekreef & Holgate, 2002). In order to consistently address health and regulatory issues related to urban air quality, both the spatial distribution and temporal variability of air pollution must be estimated at high resolution (hourly time step and few-meter horizontal resolution), and the contributions from different emission sectors must be assessed separately (Berchet et al., 2017). The main source of several pollutants (e.g. $NO_x$) in cities is road traffic. These pollutants are emitted close to the ground and are dispersed by atmospheric circulation that is affected by perturbation from buildings. Therefore, the distribution of pollutants in cities gives rise to very complex patterns with high concentration gradients.

One of the main targets of the LIFE+ RESPIRA project is developing a specific tool able to reproduce the pollutant maps in Pamplona´s city (Spain) accurately and with the highest possible resolution to estimate the population exposure. In this framework, the objective of this work is to develop modelling approach to compute detail concentration maps of $NO_x$, $NO_2$ and NO for the whole Pamplona´s city. This information could be used to calculate the health impacts of pollution and to propose low pollution routes for cyclists and pedestrian. For this purpose, a CFD modelling and a methodology based on RANS-CFD simulations have been used to compute the 2016 hourly annual and seasonal mean day concentration maps. This methodology has been evaluated with air quality monitoring stations of the city and experimental data from microsensors carried by cyclists.

## AREA OF STUDY AND EXPERIMENTAL DATA

The area of study is Pamplona, a city in the North of Spain (~200000 inhabitants), representative of about 80 % of cities in Europe. Most buildings in the area have a height between 21 m and 30 m, although the tallest building is 70 m high approximately. Meteorological data of the city were provided by a meteorological station, *Pamplona-GN*, located approximately 200 m outside of the Ensanche´s district (**Fig 1 a)**). Concerning pollution data, the network of air quality monitoring stations in Pamplona consist of one traffic station, *Pamplona-Plaza de la Cruz*, located in the Ensanche´s district of the city (is one of the most crowded district in the city, surrounded by several streets and avenues with intense road traffic, (**Fig. 1 a)**), and two background stations, *Pamplona-Iturrama* and *Pamplona-Rotxapea*, which are located on the south and north peripheries of the city respectively. This network provides hourly mean values of $NO_2$, NO and $NO_x$. In addition, an experimental campaign of volunteer cyclists carrying microsensors took place during LIFE+RESPIRA project. In this study, data from 2016 were used (**Fig 1 b)).** Approximately 10 million data records from microsensors were treated in order to remove outliers, pooled by hour and subsequently spatially-averaged in cells of 50 × 50 $m^2$ (hereafter 50m-averaged cyclists maps). This cell size is related with the sampling period (10 s) and the average speed of the cyclist, 5 m $s^{-1}$. Then, the spatially-averaged hourly maps of $NO_2$ concentrations, for the 2016 mean annual day, have been built from these measurements. Note that maps cover only the roads, streets, and other areas accessible to cyclists.



a) b)

**Figure 1.** a) Aerial view of Pamplona´s City (Source: Google Earth). Modeling domain, ~42 $km^2$ (dotted yellow box), Ensanche´s district (continuous red line) and location of traffic monitoring station (red pushpin), background monitoring stations (yellow pushpins) and meteorological station (green pushpin) within it. b) Roads traveled by cyclists during 2016.

# MODELLING APPROACH

## Numerical Methodology

CFD modelling is applied to obtain high spatial resolution distributions of pollutants. In addition, concentrations representative of long time periods (e.g. annual averages) are required. Due to unsteady simulations during long time periods being very time consuming, a numerical methodology based on weighted averaged of Computational Fluid Dynamic–Reynolds-Averaged Navier–Stokes (WA CFD-RANS) simulations is used (Parra et al. 2010; Santiago et al. 2011; Santiago et al. 2013; Santiago et al. 2017). It consists on running only a set of scenarios (16 inlet wind directions) using steady-state CFD-RANS simulations. In this case, the final averaged concentration maps are made by means of a combination of the simulated scenarios considering wind patterns within the periods analyzed. Pollutant concentration is computed assuming: 1) non-reactive pollutants, 2) thermal effects negligible in comparison with dynamical effects and 3) tracers concentration depend only on emissions and wind speed. To determine the meteorological conditions during the studied periods, data from meteorological station were used. In this way, the average $NO_x$ concentration maps are computed as,

$$C_M(t) = \left[ \sum_{i=1}^{16} f_i(t) \cdot \left(C_{CFD}\right)_i \cdot \frac{v_M}{\left(\overline{v_{ref}(t)}\right)_i} \right] \cdot E(t) \tag{1}$$

where $C_M\,(t)$ is the modeled time average concentration at time $t$ (time resolution used is 1 h), $i$ indicates the wind direction sector at inlet in CFD simulation, $f_i\,(t)$ is the statistical frequency of wind direction sector $i$ at time $t$ during the modeled period, $(C_{CFD})_i$ is the concentration computed by CFD for the wind direction sector $i$ (i.e. results from the corresponding steady state CFD-RANS simulation), $\left(\overline{v_{ref}(t)}\right)_i$ the average wind speed of wind direction sector $i$ measured at meteorological station at time $t$ during the modeled period, $v_M$ inlet wind speed simulated and $E\,(t)$ a emission factor at time $t$ during the modeled period. $E\,(t)$ is an unknown parameter in our simulations; therefore it is fitted assuming that:

$$\overline{C_O(\vec{r}_0, t)} = C_M(\vec{r}_0, t) \tag{2}$$

where $\overline{C_O(\vec{r}_0,t)}$ is the average concentration measured at time *t* at *Pamplona-Plaza de la Cruz* air quality monitoring station and $C_M(\vec{r}_0,t)$ the modeled concentration at time *t*.

NO and $NO_2$ are reactive and this methodology can only be applied for non-reactive pollutants. To solve this problem, the experimental ratio $NO/NO_x$ and $NO_2/NO_x$ measured at the station during each period is applied to NOx concentration maps:

$$\left(C_M(t)\right)_{NO\ or\ NO_2} = \left(C_M(t)\right)_{NO_x} \cdot \frac{\left(\overline{C_O(\vec{r}_0,t)}\right)_{NO\ or\ NO_2}}{\left(\overline{C_O(\vec{r}_0,t)}\right)_{NO_x}} \quad (3)$$

**CFD model description and simulation setup**

The numerical domain covers the whole city and a 3D full-scale geometrical model has been constructed which considers the actual height of buildings (an average height per block is assumed). The computational grid has a resolution of 5 m in built areas, presenting refinements close to urban surfaces (ground and buildings) and in narrow streets where the resolution is close to 1 m. The total number of cells is approximately 45 million. Numerical simulations are based on steady-state RANS equations and *k*-*ε* turbulence models. The pollutant concentrations are simulated using additional transport equations. 16 different wind directions are simulated. Inlet profiles of wind speed are logarithm, and profiles of turbulent kinetic energy (*k*) and turbulence dissipation rate (*ε*) are computed following the equations of Richards & Hoxey (1993). The pollutant emissions are modeled by means of a source terms in the transport equation. The emission sources are placed inside each street, where the roads are located up to 1 m height. Traffic emissions inside each street are assumed proportional to the daily average traffic intensity (*ATI*) of each street.

**RESULTS**

Hourly concentration maps of $NO_2$, NO and $NO_x$ of a mean day during 2016, and for seasonal mean days (i.e. winter, spring, summer and autumn) are computed as described in previous Section. In **Fig. 2**, time evolution of the average annual high-resolution $NO_x$ map is shown as example.

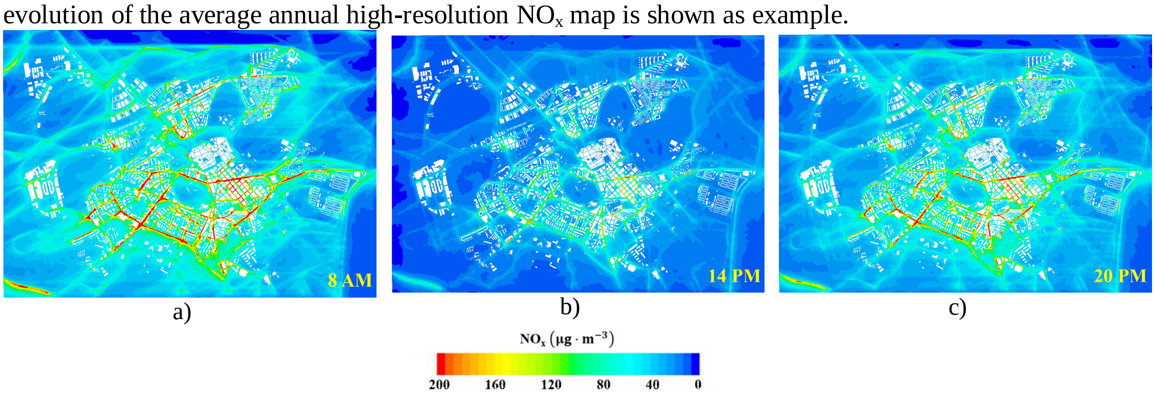



**Figure 2.** High resolution hourly maps of $NO_x$ annual averaged concentration during 2016: a) 8AM, b) 2PM, c) 8PM, all of them local time.

**Model evaluation with air quality monitoring stations**

Modeled hourly $NO_2$, NO and $NO_x$ are compared with measurements from the air quality monitoring stations for annual and seasonal averaged days. In **Fig. 3**, $NO_x$ concentration is shown as example.

The simulated concentrations fit well the observations from both stations, especially during daytime hours (from 8AM to 8PM, local time). The observed average daily concentration evolution is captured by the model despite of the underestimation during night-time hours (from 8PM up to 8AM, local time). The daily concentration peaks (at 8AM and 8PM) are slightly underestimated at *Pamplona-Rotxapea* but fit very well at *Pamplona-Iturrama*. Similar agreement is obtained for NO and $NO_2$ (not shown here).

**Model evaluation against experimental data from cyclists with microsensors**

Based on the corresponding high-resolution hourly CFD maps, equivalent spatially-averaged maps in cells of 50 x 50 m$^2$ (hereafter 50m-averaged CFD maps) have been computed. The comparison between cyclist measurements and modelling results presents several difficulties, namely:

1) In 50m-averaged maps, CFD concentration represents the average value over all cell, while the cyclist measurements represent the average value but only over the portion of the cell where the cyclist travel, which consists mainly of roads, sidewalks, and bike paths, where traffic-borne, point-source pollutants may be locally higher. Therefore, it is expected that CFD values underestimate the concentration measured by cyclists.

2) Measurements from cyclists are accompanied by a certain spatial uncertainty due to the microsensors sampling period and the movement of cyclists. These instruments send data every 10 s (time averaged concentration and GPS position) while the cyclist can run several tens of meters, but during this period there are uncertainties about the actual route traveled by cyclists while microsensors were measuring.

3) In addition, the total number of cyclist measurements in some cells should not be enough to obtain a representative average concentration.

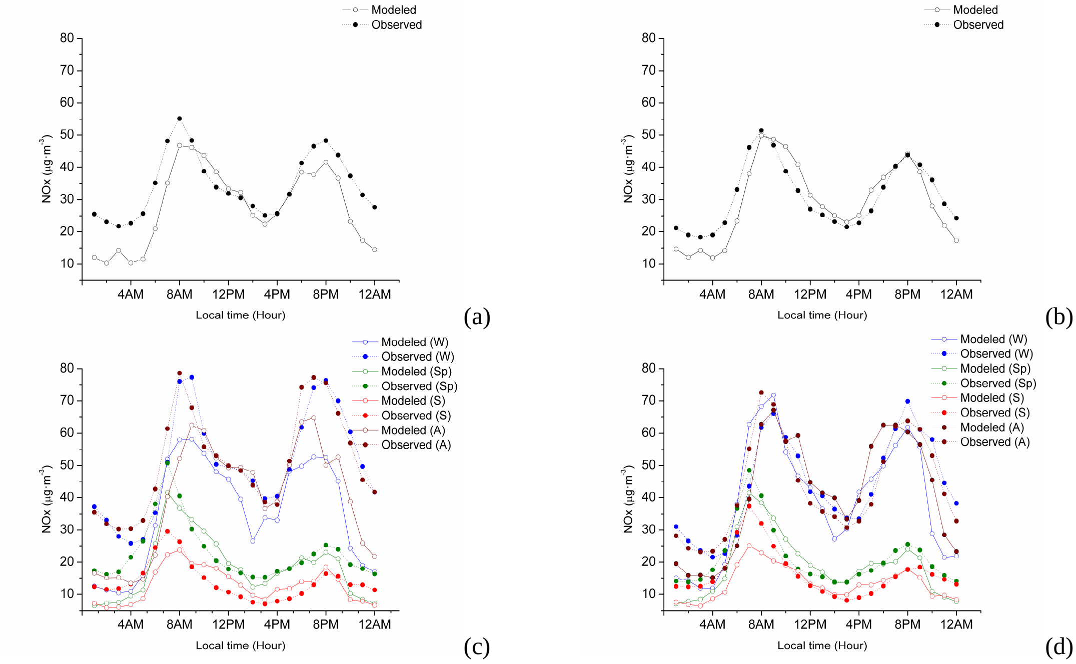



**Figure 3.** Comparison between modeled and observed hourly $NO_x$ concentrations. Average annual day at: a) *Pamplona-Iturrama*, b) *Pamplona-Rotxapea*. Average seasonal day at: c) *Pamplona-Iturrama*, d) *Pamplona-Rotxapea*.

Therefore, a direct comparison (point-by-point) seems not be suitable. Accordingly, the spatial statistical method "optimized hot spot analysis" (ESRI 2016) is proposed here as evaluating tool of the 50m-averaged hourly maps of $NO_2$ concentrations for the 2016 average annual day. This tool identifies spatial clusters of high values of pollutant concentrations (hot spots) and low values (cold spots) and creates a map of statistically significant spots using the Getis-Ord Gi* statistic (ESRI 2016). It works by looking at each pollutant concentration within the context of neighboring features (calculations based on Euclidean distance). A pollutant concentration with a high value is interesting but may not be a statistically significant hot spot. To be a statistically significant hot spot, a pollutant concentration will have a high value and be surrounded by other pollutant concentrations with high values as well. The local sum for a pollutant concentration and its neighbors is compared proportionally to the sum of all pollutant concentrations; when the local sum is very different from the expected local sum, and when that difference is too large to be the result of random chance, statistically significant z-score results. A preliminary analysis for $NO_2$ concentrations at 8PM (daily concentration peak) has been carried out at district scale in the Ensanche´s district (**Fig. 4**). It shows the Gi_Bin field of 50m-averaged CFD map identifies correctly the statistically significant hot and cold spots, practically the entire district, regarding to the corresponding Gi_Bin field of 50m-averaged cyclist map. Small discrepancies have been found on some streets (**Fig. 4** d), dotted black line), possibly due to traffic emission underestimation. They have been assumed proportional to the daily average traffic intensity (*ATI*), and in this street the *ATI* considered is low but the cyclist measurements indicates that traffic is more intense in this road.

## CONCLUSIONS

The WA CFD-RANS methodology has been modified and applied to the entire city of Pamplona to compute high resolution $NO_x$, $NO_2$ and NO concentration maps at pedestrian level. This modelling approach is able to reproduce the data from air quality monitoring stations located within the domain, especially during daytime hours (from 8 A.M. up to 8 P.M.). However, data from portable sensors carried by cyclists could not be directly compared (point by point), thus a preliminary comparison by using a spatial statistical method that identifies spatial clusters of high and low values of pollutant concentrations is applied in a district. This analysis indicates that similar locations of maxima and minima of concentrations are obtained by both, experimental and numerical results. Therefore, this methodology seems to be adequate to compute high resolution concentration maps for an entire city.

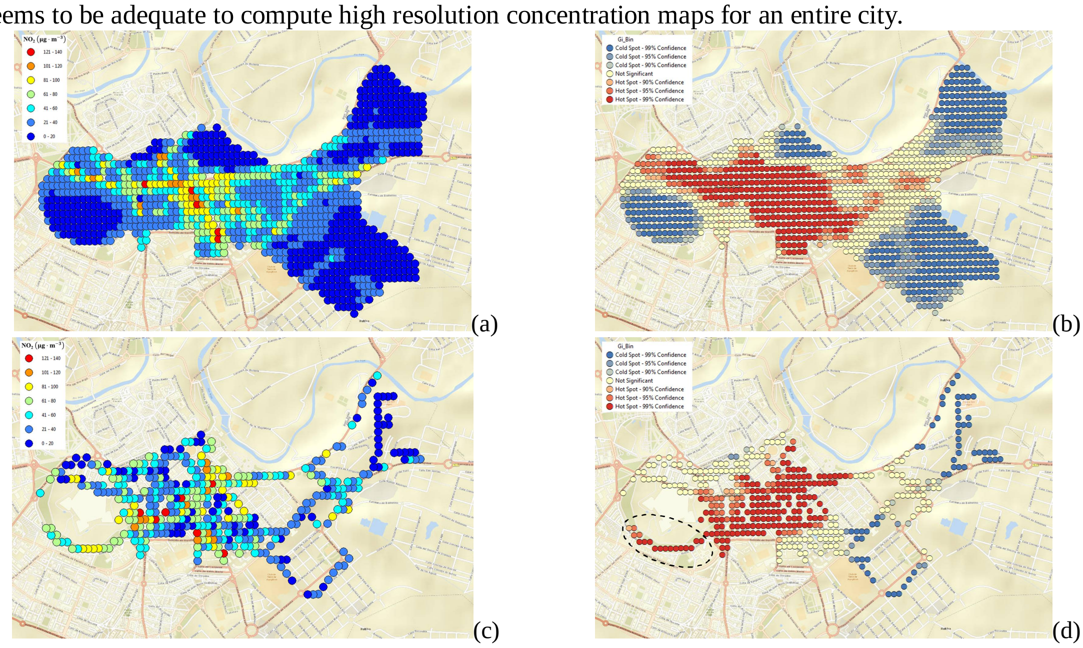


**Figure 4.** (a) 50m-averaged CFD map of $NO_2$ concentration at 8PM on Ensanche´s district, (b) Gi_Bin field of (a), (c) 50m-averaged cyclists map of $NO_2$ concentration at 8PM on Ensanche´s district, (d) Gi_Bin field of (c).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