Downscaling WRF-Chem: Analyzing urban air quality in Barcelona city

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Abstract. Improving air quality in highly polluted cities is a challenge for today's society. Most of the proposed strategies include green policies that aim to introduce green infrastructures helping to improve air quality. To design new cities with more green infrastructures, the WRF-Chem model is used to analyze the evolution of the most common pollutants and their dispersion due to the meteorology of the moment. Most of the studies, however, are off an urban scale (hundreds of meters of resolution), and those cases that simulate the meteorology at this resolution need to consider the city's morphology. Using the city of Barcelona as a case study, this paper confirms that the modeling methodology used up to now must be reviewed to design green cities. Certain limitations of the WRF-Chem model have been analyzed, including the BEP-BEM as an urban canopy layer, and the reasons for such limitations are discussed.

Keywords: WRF-Chem · BEP-BEM · Air Quality · Urban scale · Green Infrastructures

1 Introduction

Air quality is a major issue in urban areas where the population's exposure to air pollution directly impacts citizens' health [12]. The main reason for this is that big cities and their metropolitan areas are almost the main contributors to injecting the atmosphere with different kinds of pollutants ([4], [2]). Therefore, new governmental policies devoted to creating smart and green cities should be designed to transform our current cities into resilient cities that provide citizens with a good and healthy life. One of the trends in this area is to reconfigure the current morphology of the cities by including green infrastructures that help to reduce pollutant concentrations in the underlying urban area. The urban planners, however, must be aware that specific green designs that include urban trees can sometimes produce the opposite effect than the desired because they can obstruct the wind flow and, consequently, lead to higher pollutant concentrations [27].Therefore, green urban infrastructures should be designed considering those contradictory aspects. Consequently, it is necessary to test different vegetation

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combinations and analyze their implications for the air quality to select alternatives that improve human life quality in the long term. In order to tackle this challenge, one needs to rely on different simulation engines. On the one hand, numerical atmospheric models are required to simulate the atmosphere's behavior in urban areas. Furthermore, the chemical processes associated with pollutant and vegetations interactions must also be considered. Therefore, the models of the atmosphere must be coupled to a chemical model to evaluate the influence of the meteorological variables provided by atmospheric models on these chemical processes involved in the reduction of the air pollution. Moreover, we need to analyze the impact of green infrastructures in urban zones, the city's morphology (also called urban canopy) is the another key factor that will affect the dispersion of the pollutant particles. These three puzzle components (atmosphere, chemistry, and city morphology) should, somehow, be simulated, and their interrelations must also be considered. For that reason, the coupled model WRF-Chem+BEP-BEM has been used in this work. WRF (Weather Research and Forecasting) model is one of the most commonly used atmospheric mesoscale models ([21]) worldwide. The model offers many physical options and can be coupled with the online numerical atmosphere-chemistry model WRF-Chem ([7]) for Air Quality applications. Furthermore, the BEP-BEM urban multilayer scheme is also included in the system to analyze the influence of the urban canopy while extending the green infrastructures in the city. However, the main concern when using this multi-model system for air quality evaluation is to deliver high-resolution results useful at urban scales (around 300m). Reaching such a resolution is not easy because there are performance aspects regarding execution time and downscaling numerical processes that should be carefully analyzed. A first step through analyzing the influence of coupling WRF and BEP-BEM urban canopy model into the air quality and simulation execution time was presented in [26]. Other works on the effects of downscaling WRF-Chem at an urban scale are reported in [28]. Wang et al. (2022) claim in those cases that it is possible to achieve a resolution of 100 meters to determine air quality aspects. For this purpose, they use WRF-Chem, including the Large-Eddy-Simulator (LES) module, since otherwise, it is not possible to reach out such high-resolution simulations. However, in Wang et al. (2022), there is no consideration of the urban canopy layer, and it should be taken into account because it makes the results useful in urban areas.

On the other hand, one can find works that analyzing the influence of including trees as green infrastructures in urban areas [23]. The main conclusion of these works is that any modification of the urban morphology may have both: the positive and the negative influence on the quality of the urban air. Consequently, the authors conclude that a deep study on both effects must be done appropriately to determine how to configure green areas in urban zones to be sure that, as a result, the air quality is improved instead of worsened. This paper shows several reasons why the current state of the art regarding theair quality simulation at urban resolution must be re-oriented to consider the effect of green

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infrastructures properly. For this purpose, we have selected the city of Barcelona (Spain) as the case study.

The study case an the air quality model set up is described in Section 2. Section 3 includes the experimental results of this paper and, finally, the main conclusions of this work are summarized in section 4.

2 Data, materials and methods

2.1 Case Study

The case study used is located in the city of Barcelona (Figure 1), inside the Catalonia region, in northeastern part of the Iberian Peninsula (Spain). The Metropolitan Area of Barcelona (MAB) with more than 3 million people, is the most populated urban area on the Mediterranean coast. The city of Barcelona reports annually one of the highest air pollution levels in Europe. The most problematic pollutants are NO_2, O_3 and particulate matter (PM_{10} and $PM_{2.5}$) [17]. In figure 2, one can observe how in 2021, the levels of NO_2 in the city of Barcelona exceed the recommended WHO (World Health Organization) levels in almost all its territory and, if we take previous years into account, the situation was even worse. In particular, in 2015 the NO_2 annual mean exceeded the 2005 WHO guideline (40 $\mu g/m^3$) in the high traffic urban air pollution ground monitoring stations (*Eixample* and *Gràcia-Sant Gervasi*) [16]. The same year, the mean value for $PM_{2.5}$ and PM_{10} was above the 2005 WHO guideline (20 and 10 $\mu g/m^3$, respectively) in all urban stations in the city [16]. Exceeding these air quality reference levels is associated with significant risks to public health [13,17].

Fig. 1. Location of the study case, Barcelona, indicated with a yellow mark in the map

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For that reason, in this work, we will focus in the NO_2 and the time period studied belongs to this year and, in particular, we have selected from 16th to 20th of July 2015 for being a part of an episode of high temperatures and high pollution levels in the studied area what could, typically, lead to exceeding the limits recommended by the WHO in 2005. In 2021 the WHO guidelines were updated in order to reduce air pollution levels in European cities and the new air pollution recommendations have been established. For example, recommended value of the the NO_2 has been reduced from 40 $\mu g/m^3$ to 10 $\mu g/m^3$. To achieve these levels, the governments of cities like Barcelona, must invest in green policies that have a direct positive the urban air quality. One key point to consider is to redesign cities taking advantage of including green infrastructures (trees, green roofs,...). However, to design it in a smart way, reliable simulations at urban resolution must be done. In the next section the models required for this purpose and, then, the models are used in the experimental section to determine whether they are useful in the way they are currently used or not.

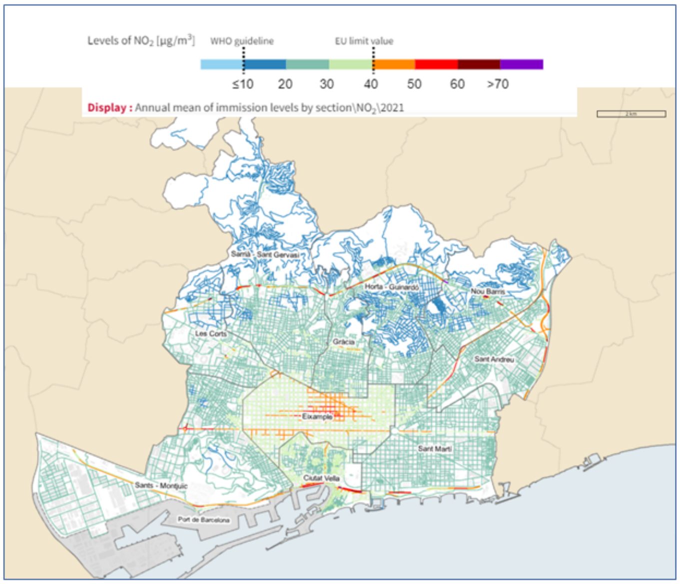

Fig. 2. NO_2 concentration levels in Barcelona in 2021. Data taken from https://ajuntament.barcelona.cat/mapes-dades-ambientals/qualitataire/ca/

2.2 Model description, chemistry and physics schemes

The WRF-Chem model is set up with three nested domains covering the Iberian Peninsula, which is the parent domain(D01) with a 9km x 9km horizontal resolution (WE: 1350 km, NS: 1305 km), followed by the second domain comprehending region of Catalonia at a 3km x 3km horizontal resolution and, finally, followed by the third and finer domain of the Metropolitan Area of Barcelona (MAB) at 1km x 1km horizontal resolution. Vertically, the three domains are described by 45 vertical layers up to 100 hPa (Figure 3).

The meteorological and chemical initial and lateral boundary conditions (IC/BCs) were determined using the ERA5 global model [10] and the CAMS-Chem model [5], respectively. The HERMESv3 preprocessor tool [9] was used to create the anthropogenic emissions files from the CAMS-REG-APv3.1 database [6]. Biogenic emissions have been computed online from the Model of Emissions of Gases and Aerosols from Nature v2 (MEGAN; [8]). For the gas-phase chemical scheme, we used the Regional Acid Deposition Model (RADM2, [24]) that accounts for 63 chemical species, 21 photolysis reactions and 136 gas-phase reactions. In WRF-Chem, RADM2 is coupled with MADE/SORGAM aerosol module [3,19]. RADM2 has been broadly used in the air quality studies across Europe [11,25].

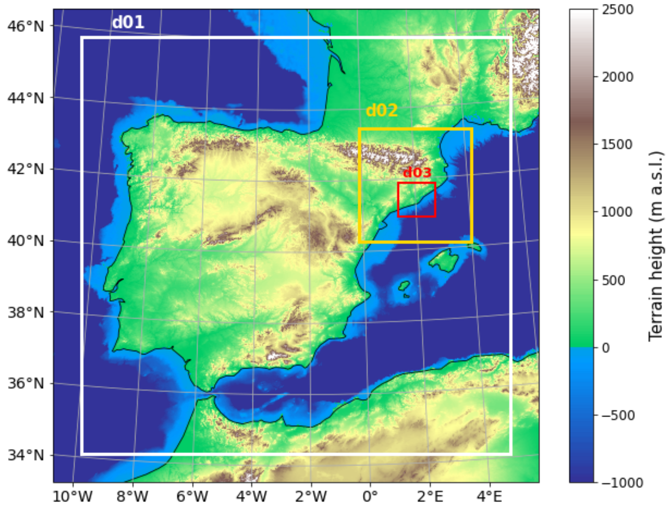

Fig. 3. WRF domains used in our simulations over the Iberian peninsula. Three two-ways nested domains D01: Iberian peninsula (IP), D02: Catalonia region (CAT) and D03: Metropolitan Area of Barcelona (MAB) with 9km x 9km , 3km x 3km and 1km x 1km horizontal resolution, respectively.

In order to represent the urban areas, we used a multi-layer urban canopy scheme, the Building Effect Parameterization (BEP) coupled with the Building

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Energy Model (BEP-BEM, [18]). This canopy layer takes into account the energy consumption of buildings and anthropogenic heat, which has previously been validated for the area under study [14,20]. We use the Local Climate Zones (LCZ) classification [22] to associate a specific value of the buildings and ground's thermal, radiative, and geometric parameters in the region of the Metropolitan Area de Barcelona (MAB). The BEP-BEM urban canopy scheme uses 11 urban classes to compute the heat and momentum fluxes in the urban areas (for more details on the use of LCZ and urban morphology refer to [20]). The principal configuration of the model is presented in Table 1.

Table 1. Parameterizations used (same as in [15]

WRF schemes	
Urban scheme	BEP-BEM
Land Surface Model	Noah LSM
PBL scheme	Bougeault-Lacarrère PBL (BouLac), designed to use with urban schemes
Microphysics	WRF Single Moment 6-class scheme
Long- and short-wave radiation	Rapid Radiative Transfer Model for General circulation models (RRTMG) scheme

3 Experimental results

As it has been mentioned in the previous sections, the experimental study reported in this paper, has been oriented to if the urban air quality simulations must be redefined or not, to be able to play with all the elements that affect the pollutants dispersion in the cities with a high level of the air pollution. The pieces to consider must include the impact of the green urban infrastructures on the chemical processes and also the influence on the meteorological factors. Therefore, the results shown in this section contemplate both: the meteorological and air quality aspects. The results analyzed correspond to the simulation results obtained from $D02$ and $D03$ domains, that is, the results have a resolution of 3km and 1km respectively. In order to capture the imprint of two Barcelona's zones that have opposite green morphologies, we have selected *Eixample* and *Ciutadella* areas for the experiments and analysis. The former, is the representative zone of the dense traffic, especially at rush hours and, the second one corresponds to a large green park close to the seaside. Although the meteorological stations and the air quality measurement stations chosen for this work are in different places, the distance between them is irrelevant because we are interested in the station type and its surroundings. However, it is worth noting that the experimentation described below for the selected locations has been carried out for all meteorological and air quality stations in the city of Barcelona. Finally, due to space issues, it was decided to choose two representative areas, one

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with a no-green and the other with a green urban canopy, since they facilitated the explanation of the objective of this work.

Table 2. Meteorological Stations from the Network of Automatic Weather Stations of Catalonia (XEMA, catalan acronym)

XEMA Station	Measurements	Lat.(^{o})	Lon.(^{o})	Alt.msl(m)	Alt.agl(m)
Zoo (Ciutadella)	T, RH	41.38943	2.18847	7	2
Raval (Eixample)	T, RH, WS, WD	41.3839	2.16775	33	40

3.1 Meteorology results

The observational data used to evaluate the weather variables from the WRF outputs was provided by the Meteorological Service of Catalonia (SMC) [1] through its Network of Automatic Weather Stations (XEMA, catalan acronym). As we have just mentioned, we have collected the data from two meteorologic stations whose location is shown in Table 2. Figure 4 and figures 5 show, respectively, the relative humidity and the temperature for the *Eixample* (*Raval*) and *Ciutadella* (**Zoo**) locations respectively. As we may observe, for all cases the results obtained for $D03$ are closer to the real observations than the results provided by $D02$ domain. So, as it is was expected, the higher resolutions the better results. However, there is still an improvement gap between the forecasted 1km resolution data and the real observations.

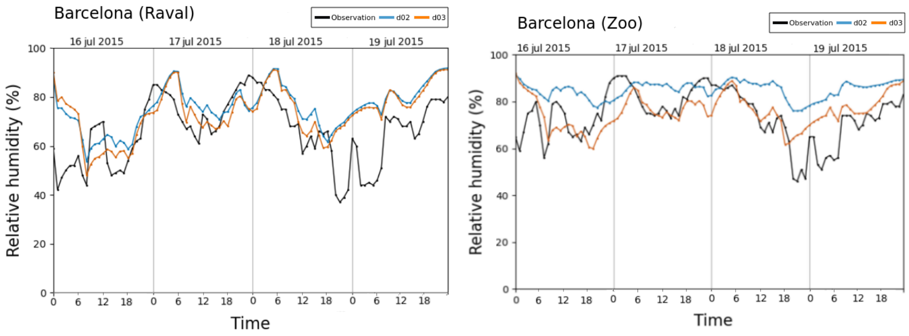

Fig. 4. Evolution of the humidity in the Eixample(Raval) and Ciutadella(Zoo) areas

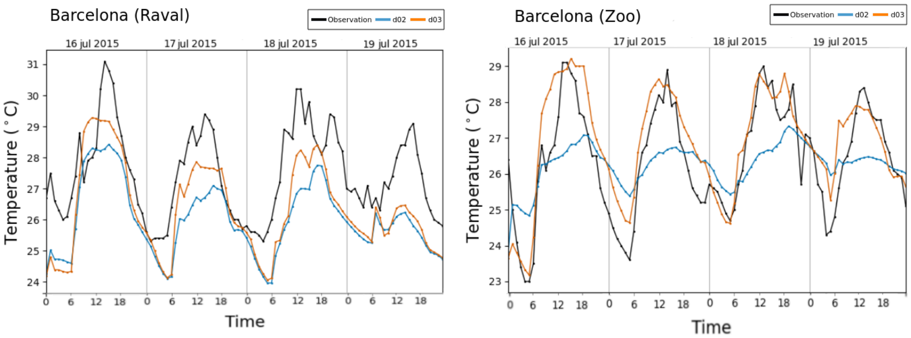

Fig. 5. Evolution of the temperature in the Eixample(Raval) and Ciutadella(Zoo) areas

Table 3. Air Quality Stations from the Atmospheric Pollution Monitoring and Forecasting Network (XVPCA, catalan acronym)

XEMA Station	Measurements	Lat.(º)	Lon.(º)	Alt.msl(m)	Alt.agl(m)
Ciutadella	NO2, O3	41.38640	2.1873	7	2
Eixample	NO2, O3	41.38531	2.15379	26	2

3.2 Air quality results

The observational data used to evaluate the WRF-Chem outputs was provided by the *Generalitat de Catalunya* from the *Xarxa de Vigilancia i Previsió de Contaminació Atmosfèrica* (XVPCA). As it has been previously mentioned, for comparison, we have chosen the air quality stations located in *Eixample* and *Ciutadella* (see Table 3). In figures 6 and 7, the evolution of the NO_2 pollutant for the *Ciutadella* and *Eixample* measurements stations, are presented respectively. As we may observe, despite the results provided by WRF-Chem at $1km$ and $3km$ are quite similar, there exists a relevant difference for the observations exists. One of the main reasons for such a difference is the model resolution. Figure 8 shows the annual mean value of emissions (NO_2) in two plots of Barcelona, which correspond to the location of *Eixample* and *Ciutadella* air quality measurements stations. The framed area is a square cell with a side of 1km around each selected measurement station. The different colors represent the different levels of NO_2 concentration within these areas. Independently of the particular values of each color, it is easy to directly check that within the purple square there appear more than one color, in fact, for the particular case of *Ciutadella* station, the color distribution goes from 20 to 70 $\mu g/m^3$. Although the model set up incorporates the BEP-BEM urban canopy layer with the objective of taking into account the influence of the buildings morphology in the pollutants dispersion, due to the

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low resolution used, the coupled WRF-Chem model is not able to capture the differences between the parts of the map that are included in the same grid cell. Another aspect to highlight are the differences between the diurnal and night cycles of NO_2 concentration compared to the observations. If one considers as diurnal cycle the time interval that goes from 6:00 to 18:00, we can observe that in the *Ciutadella* station the estimated NO_2 concentration is closer to the observations independently of the day of the week. However, diurnal cycles in the *Eixample* location, are clearly underestimated during business days (2015-07-16 corresponded to a Thursday).

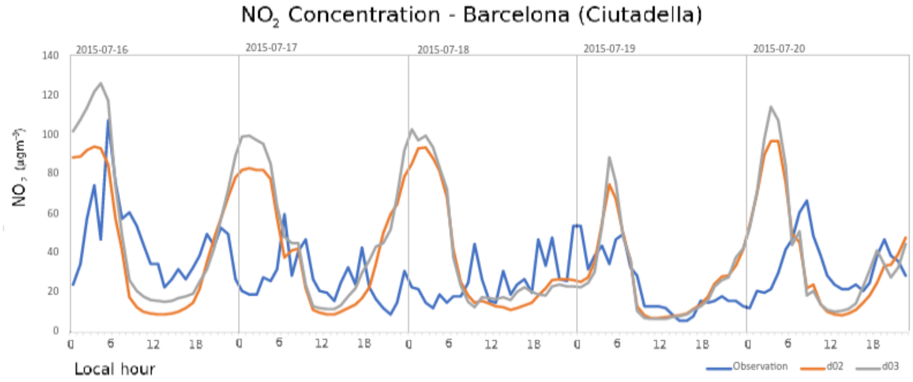

Fig. 6. NO_2 concentration changes in the period of Thursday 2015-07-16 to Monday 2015-07-20 at *Ciutadella* air quality station compared to the results obtained by the WRF-Chem model at $D02$ and $D03$

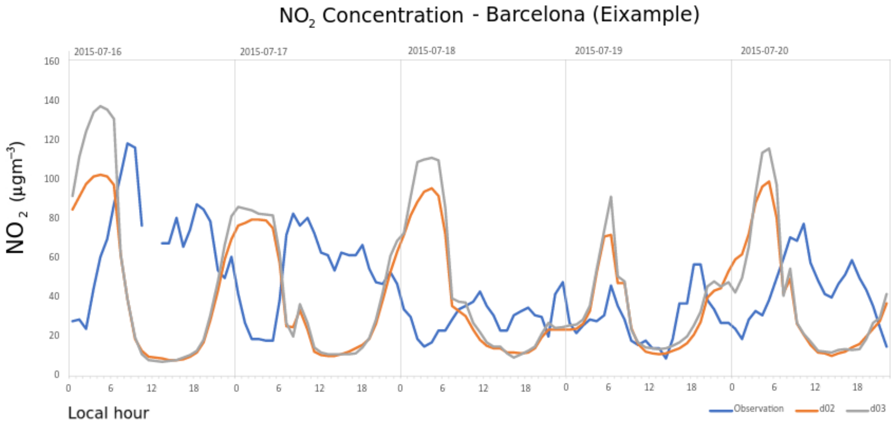

Fig. 7. NO_2 concentration changes in the period of Thursday 2015-07-16 to Monday 2015-07-20 at *Eixample* air quality station compared to the results obtained by the WRF-Chem model at $D02$ and $D03$

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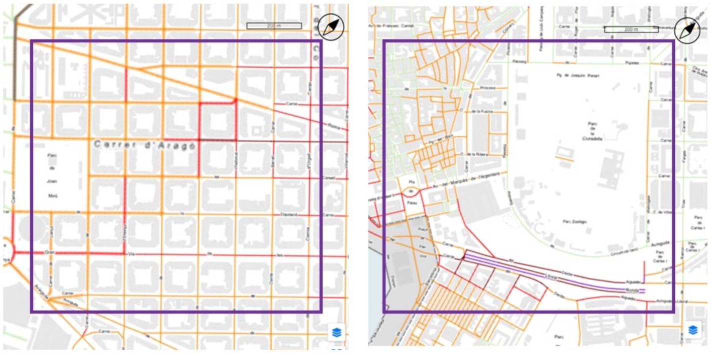

Fig. 8. Annual mean of the $NO2$ concentration in 2018 at the *Eixample* and *Ciutadella* areas of Barcelona (Spain)

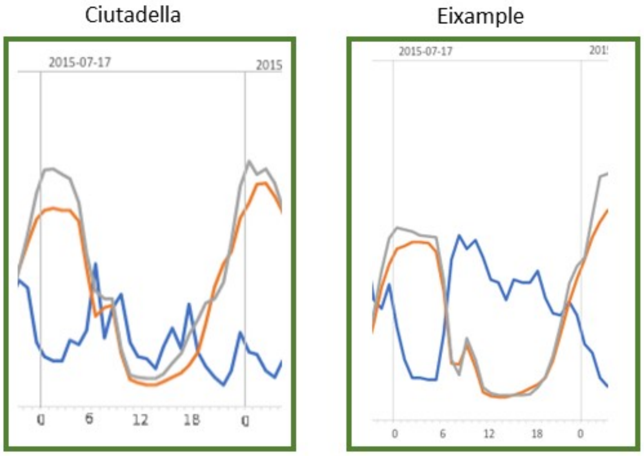

Fig. 9. NO_2 concentration levels for the day 2015-07-17 in the Ciutadella area an in the Eixample

Another issue to analyze is the influence of green areas on air quality. For that purpose, we have cut figures 6 and 7 for Friday 2015-07-17, see Figure 9, but it could be done on any other business day. In the cut corresponding to *Ciutadella*, the behavior of NO_2 during the day and at night is quite regular as far as the observations are concerned, while the models at $3km$ and $1km$, despite coinciding with the results, cannot capture this behavior as it already has been discussed previously.

In addition, it is very remarkable to keep in mind that this plot corresponds to a green zone with practically no traffic in the entire cell except in certain borders. However, the effect of the park on the air quality of the area is altered if we only look at the models. The main reason for this effect is, not having the coupled models at high resolution, taking into account the green layer existing in *Ciutadella*. From the observed data we can deduce that green infrastructure dampens the harmful effects of pollutants, but this effect cannot be reproduced if it is not worked at high resolution. It is true that in *Ciutadella* area, the emissions produced by traffic are lower, but the model does contemplate this lower injection of pollution into the environment. On the contrary, if we analyze the *Eixample* plot, one may observe that the model cannot capture the behavior of NO_2 concentration in its day or night cycle, as has already been commented on. However, the notable effect is also that the improvement that green spaces' inclusion could produce, nor would it be reproducible if the resolution of all the models involved were not increased. Thus, the main conclusion of this study is that although green areas help to reduce environmental pollution, if complete high-resolution models are not used, it will be difficult to obtain effective green designs.

4 Conclusions

Designing green cities to improve their air quality is one of the planned resilience strategies for many highly polluted cities. To achieve an effective design, it is necessary to test the effect that including certain green areas to the urban morphology would have on the city's air quality. For this, it is necessary to reconsider how to run the proper simulations, since according to the authors' knowledge, there are no proposals that allow to model this influence at a resolution of around 100 meters. In this work, the case of the city of Barcelona has been analyzed, emphasizing two areas with opposite characteristics. *Eixample* area has been selected as the area of the high traffic density and many emissions due to the road traffic, and the other area is the *Ciutadella*: Ciutadella: the one that corresponds to a large green park near the sea. The study carried out considering both the meteorological parameters and certain pollutants, has revealed the need of having the complete coupled models (meteorology, chemistry and urban morphology) at urban scale. The main conclusion of this work is that "green resolution matters", that is, downscaling WRF-Chem model without taking green infrastructures into account, may generate designs with the worse air quality for cities than it was before the green modifications.

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