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# Modeling air quality at urban scale in the city of Barcelona: A matter of green resolution[☆]

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## ABSTRACT

Improvement of the air quality in highly polluted cities is a challenge for today's society. Many of the strategies that have been proposed for this purpose promote the creation of green infrastructures. The Weather Research and Forecasting model coupled with chemistry (WRF-Chem) is used to analyze the behavior of the most common pollutants and how they are dispersed as a result of different meteorological conditions. To also consider the impact of including green infrastructures on urban morphology, the BEP/BEM (Building Effect Parameterization/Building Energy Model) multi-layer urban scheme is also included in the system. Using the city of Barcelona as a case study, this paper confirms that the modeling methodology used up to now needs to be reviewed for the design of green cities. Certain limitations of the WRF-Chem+BEP/BEM coupled model when applied in urban resolution are discussed, as well as the reasons for such limitations, being the main contribution of this paper to show that an alternative paradigm such as Machine Learning techniques should be considered to address this challenge.

## 1. Introduction

Air quality is a major issue in urban areas where the population's health is directly impacted by exposure to air pollution [1]. Large cities and their metropolitan areas tend to be the main contributors to the release of different kinds of pollutants into the atmosphere [2,3]. New governmental policies should therefore be designed to promote smart green cities that are better prepared to ensure a healthy life for their inhabitants. One of the trends in this area is to reconfigure the morphology of modern-day cities by introducing green infrastructures that will help to reduce concentrations of pollutants. Urban planners must however be aware that trees can sometimes produce the opposite effect to the desired one because they can obstruct the flow of wind, thus leading to even higher concentrations of pollution [4].

These contradictory aspects should therefore be considered in the design of green urban infrastructures. This includes the need to verify different plant combinations and analyze their implications for air quality, so as to be able to choose the best alternatives for improving the long-term quality of human life. Different simulation engines can be used for this purpose. Numerical models are required to simulate the atmospheric behavior, and these must be coupled with the chemical processes associated with interactions between plants and pollutants. Moreover, the impact of green infrastructures on urban morphology (also called urban canopy) is another key factor affecting the dispersion of pollutant particles. The influence of the city's design on air quality must therefore be analyzed.

The three parts of the puzzle (the atmosphere, chemistry, and city morphology) should be considered together, including their interactions. In our research, the WRF-Chem+BEP/BEM coupled model has been applied. The WRF (Weather Research and Forecasting) model is one of the most commonly used atmospheric mesoscale models worldwide [5]. It offers many physical options and can be coupled with the online numerical atmosphere-chemistry model WRF-Chem [6] for air quality applications. Furthermore, the BEP/BEM (Building Effect Parameterization/Building Energy Model) multi-layer urban scheme is also included in the system to analyze the influence of the urban canopy when green infrastructures are introduced to a city. The main concern when using this multi-model system is the delivery of high-resolution results that are useful at urban scales (around 300 m). Such a resolution is not easy to achieve because there are performance concerns in terms of execution time and the downscaling of numerical processes. One of the earliest analyses of the influence of coupling WRF and the BEP/BEM urban canopy model on air quality measurement

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[☆] This document is an extended version of the conference paper titled "Downscaling WRF-Chem: Analyzing Urban Air Quality in Barcelona city", which was originally presented at the International Conference of Computational Science (ICCS2023) from July 3rd to 5th.

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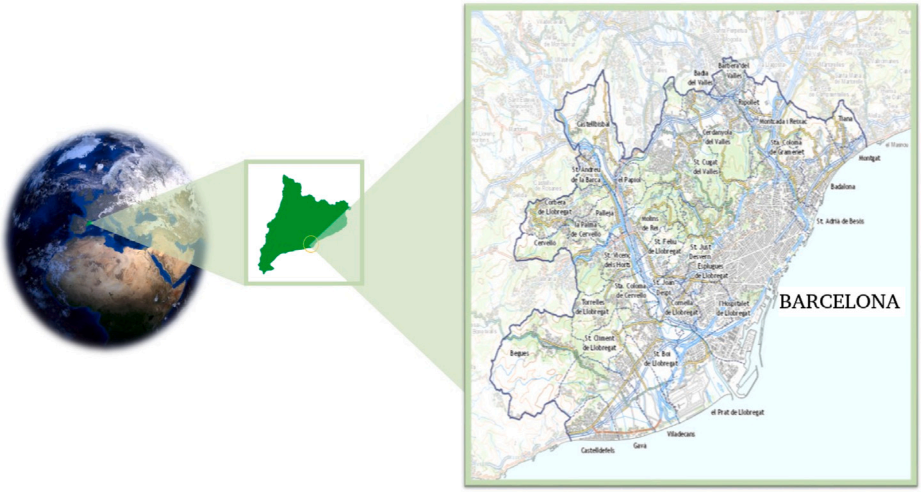


**Fig. 1.** Our case study focuses on the city of Barcelona in Catalonia, in the northeast of Spain.

and simulation execution time was presented in [7]. The effects of downscaling WRF-Chem to urban scale are also reported in [8], where Wang et al. claim that it is possible to achieve a resolution of 100 meters to determine air quality. They use WRF-Chem, including the Large-Eddy-Simulator (LES) module, since it is not otherwise possible to achieve such high-resolution simulations, but include no consideration of the urban canopy layer, which makes the results useless for urban areas.

Other studies have achieved spatiotemporal variability of pollutants on an urban scale by coupling mesoscale air quality forecasting systems with dispersion models [9]. Such systems are, however, primarily designed for describing pollutant dispersion on street maps rather than analyzing the effect of green infrastructures on urban air quality.

Other studies have analyzed the influence of including trees as green infrastructures in urban areas [10]. Their main conclusion is that any modification of the urban morphology may positively or negatively influence the quality of the air. The authors conclude that an appropriate in-depth study of both effects is required to determine how green areas should be configured in urban areas to ensure that the air quality is improved and not worsened.

The present study analyzes the state of the art of air quality simulation at urban resolution and argues why it needs to be reassessed to properly consider the effect of green infrastructures. For this purpose, we have selected the city of Barcelona (Spain) as a case study. With the aim of analyzing in detail the influence of green areas on air quality, this article proposes a hybrid classification of land use maps, in which new categories designed specifically for urban green areas have been included. This map has been obtained at a resolution of 100 m, which allows us to capture changes in the green morphology of the city of Barcelona, however, the results obtained with classic strategies are not capable of capturing these land use improvements.

The main characteristics of the case study and the air quality model setup are described in Section 2. Section 3 presents the experimental results, and the main conclusions are summarized in Section 4.

## 2. Data, materials and methods

### 2.1. Case study

The case study used is the city of Barcelona (Fig. 1), which is located in the Catalonia region in the northeast 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.

In Barcelona, annual reports consistently highlight some of the highest air pollution rates in Europe, primarily driven by elevated levels of $NO_2$, $O_3$, $PM_{10}$, and $PM_{2.5}$ pollutants [11]. Fig. 2 shows how $NO_2$ levels in 2021 exceeded WHO recommendations across the region, with even higher levels observed in previous years. For instance, in 2015, the mean $NO_2$ concentrations surpassed the 2005 WHO guideline of $40\ \mu g/m^3$, ranging between 5.6% and 41.2% depending on the monitoring station [12]. During the same period, the mean $PM_{10}$ concentrations also exceeded the 2005 WHO guideline of $20\ \mu g/m^3$ at all urban stations in the city, ranging between 47.4% and 133.8% [12]. These elevated levels pose significant health risks to the public [11,13]. The WHO Global Air Quality Guidelines (AQG) serve as crucial benchmarks for assessing and addressing such air quality concerns, providing clear standards and targets to guide pollution reduction efforts worldwide.

This study focuses on $NO_2$ pollution from 16 to 20 July 2015, an episode of high temperatures and high pollution levels in the studied area, which would typically entail excess of 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 new air pollution recommendations were introduced. For example, the threshold value for $NO_2$ was reduced from $40\ \mu g/m^3$ to $10\ \mu g/m^3$. In light of the updated threshold values in the 2021 WHO guidelines, it is noteworthy that, based on these new recommendations, the exceedances of $NO_2$ levels in Barcelona during the year 2015 would have ranged between 220% and 464% depending on the air quality monitoring station.

To achieve recommended levels, the governments of cities like Barcelona need to invest in green policies that directly impact their urban air quality. One key issue here is the redesign of cities to include more green infrastructures (trees, green roofs, gardens between blocks of buildings, etc.). For this reason, we need a land-use classification system.

### 2.2. Land use

Our study uses the hybrid land-use classification system that was previously used in [14]. This is based on the Local Climate Zones (LCZ) classification, a micro-level land use classification that is widely applied to classify urban landscapes. The hybrid scheme we used is based on the United States Geological Survey (USGS), which is known to perform better for non-urban areas than the European Corine Land Cover (CLC) project [15]. We expanded the USGS to include the ten urban categories described in the LCZ at a spatial resolution of 100 m. We also introduced two new classifications for urban categories: land cover type E from LCZ, corresponding to paved areas, and a new type of classification defined as green urban areas, including parks and other similar features. Fig. 3 presents this hybrid classification system, which also includes the conversion into the applied numeric classes.

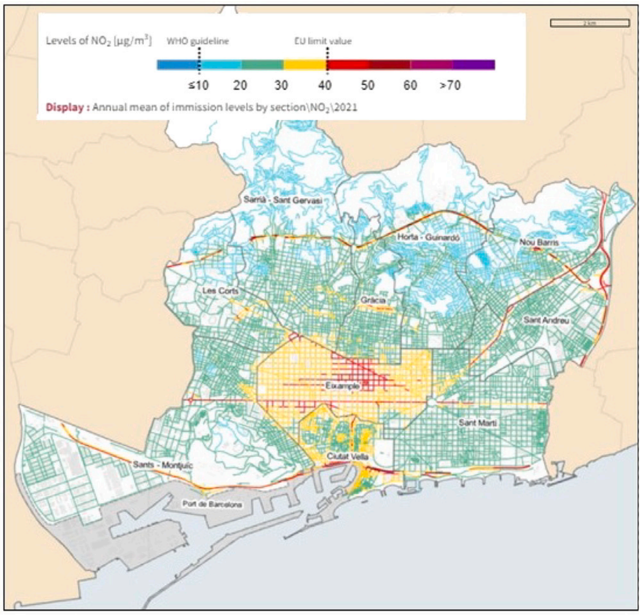


**Fig. 2.** Nitrogen dioxide ($NO_2$) concentration levels of Barcelona in 2021. The information obtained from https://ajuntament.barcelona.cat/mapes-dades-ambientals/qualitataire/ca/.

To ensure smart design, reliable simulations at urban resolution need to be performed. The following section describes the models required to do so, which are then used in the experimental section to determine whether they are useful in their current form.

### 2.3. Model description and configurations

As mentioned earlier, the interaction between the atmosphere, chemical reactions, and green city morphology is a critical matter that must be addressed smartly in order to design healthy, resilient cities. But making a city "greener" does not necessarily imply improvements to its air quality. Accurate analysis of the effect of including green infrastructures is therefore required in order to determine which urban canopy modifications are useful and which are not. As noted earlier, the WRF-Chem model considers all these aspects, including the BEP/BEM urban multi-layer scheme.

The Weather Research and Forecasting (WRFV4) model is an atmospheric modeling system designed for numerical weather prediction [5]. The Advanced Research WRF (ARW) Dynamics Solver integrates the compressible, non-hydro-static Euler equations with several physics schemes and dynamic options designed for atmospheric phenomena on a regional scale [5]. The WRF model, which is intended for advanced high-performance computing systems, was developed through a collaborative partnership between various organizations, including the National Center of Atmospheric Research (NCAR), the National Centers for Environmental Prediction (NCEP), the NOAA Earth System Research Laboratory (ESRL), the U.S. Air Force, the Naval Research Laboratory, the University of Oklahoma, and the Federal Aviation Administration. As of 2021, WRF has an extensive global community of over 57,800 registered users across more than 160 countries, and NCAR regularly hosts workshops and tutorials to support its users [16].

WRF-Chem is WRFV4 coupled with a complete online atmospheric chemistry model offering a wide range of options and certain interactions with physics aerosols affecting radiation and microphysics. This coupled system typically requires the emission source maps as additional inputs [5,6], as introduced later in this paper.

The WRF-Chem model was set up with two nested domains. The parent domain ($D01$) covers the Iberian Peninsula at a horizontal resolution of 9 km × 9 km (WE: 1350 km, NS: 1305 km), the second domain ($D02$) covers Catalonia at a horizontal resolution of 3 km × 3 km (WE: 348 km, NS: 348 km) and, finally, the third and most detailed domain ($D03$) covers the Metropolitan Area of Barcelona (MAB) at a horizontal resolution of 1 km × 1 km (WE: 119 km, NS: 119 km). The atmosphere is divided into 45 vertical layers from the surface up to the top of the atmosphere, at 12–15 km in altitude, where the pressure level is 100 hectopascals (100 hPa). You can see the three domains in Fig. 4.

#### 2.3.1. Physical and chemical schemes

We represented the urban areas using a multi-layer urban canopy scheme, i.e. Building Effect Parameterization (BEP) coupled with the Building Energy Model (BEP/BEM, [17]). This canopy layer considers the energy consumption of buildings and anthropogenic heat, which has previously been validated for the area under study [18,19]. We use the Local Climate Zones (LCZ) classification [20] to associate a specific value to the thermal, radiative, and geometric parameters of the buildings and land in the Metropolitan Area of Barcelona (MAB). The BEP/BEM urban canopy scheme uses 11 urban classes to compute heat and momentum fluxes (for further details on the use of LCZ and urban morphology, see [19]). The configuration of the WRF model is shown in Table 1, where the parameterizations used in the configuration file (namelist.input) are listed. Also you can see the execution process scheme in Fig. 5.

For the gas-phase chemical scheme, we used the Regional Acid Deposition Model (RADM2, [21]) that accounts for 63 chemical species, 21 photolysis reactions and 136 gas-phase reactions. In WRF-Chem, RADM2 is coupled with the MADE/SORGAM aerosol module [22,23]. RADM2 has been widely used in the air quality studies across Europe [24,25]. The configuration file (namelist.input) contains the chemical scheme and all its associated parameters.

#### 2.3.2. Model inputs

The initial and lateral meteorological boundary conditions (IC/BCs) were obtained using the ERA5 global model from the European Centre for Medium-Range Weather Forecast (ECMWF), see Fig. 5. ERA5 benefits from a decade of advances in model physics, core dynamics, and data assimilation. It also has a significantly enhanced horizontal resolution of 31 km (0.28125 degrees) in its HRES version, 137 levels from the surface up to approximately 80 km in altitude (0.01 hectoPascals -hPa- in pressure), and also provides hourly output throughout [26].

We utilized the Community Atmosphere Model with the Chemistry (CAM-Chem) model to establish the initial and lateral chemical boundary conditions (see Fig. 5). The CAM-chem model, part of the NCAR Community Earth System Model (CESM), is equipped with the MOZART chemical mechanism and provides various options for tropospheric and stratospheric chemistry complexities. This model is extensively employed for conducting global simulations of atmospheric composition in the troposphere and stratosphere. Its resolution is 1.9 $x$ 2.5 deg with 56 vertical levels [27].

In order to determine the anthropogenic and biogenic emissions (see Fig. 5), we utilized two powerful tools: the High-Elective Resolution Modelling Emission System version 3 (HERMESv3;[28];[29]) and the Model of Emissions of Gases and Aerosols from Nature v2 (MEGAN; [30]). HERMESv3 is an open-source preprocessing tool that is specifically designed to compute gaseous and aerosol emissions for atmospheric chemistry models. It is a multi-scale framework that can work in parallel and series. Biogenic emissions, on the other hand, were computed online using MEGAN, a modeling system used for estimating the emission of gases and aerosols from terrestrial ecosystems into the atmosphere. Both emission inputs have a resolution of 1 km.

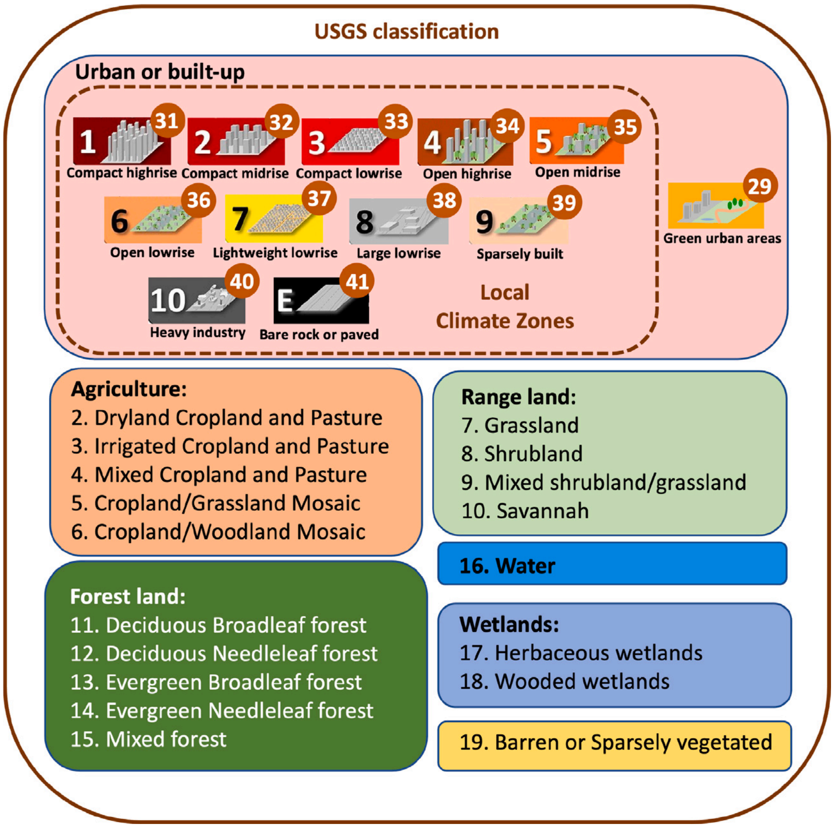


**Fig. 3.** Hybrid land-use classification.

**Table 1**
Model parameterizations.

| 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 |
| Radiation | Rapid Radiative Transfer Model for General circulation models (RRTMG) scheme |
| Chemistry | Regional Acid Deposition Model (RADM2) |

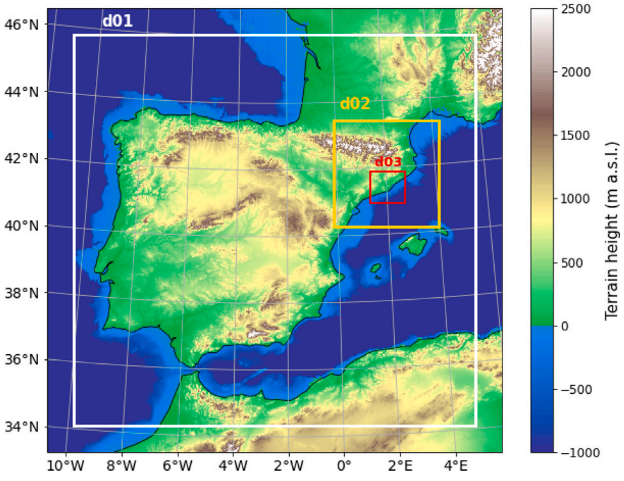


**Fig. 4.** WRF domains used across the Iberian Peninsula. *D*01: Iberian Peninsula (IP), *D*02: Catalonia (CAT), and *D*03: Metropolitan Area of Barcelona (MAB) with horizontal resolutions of 9 km × 9 km, 3 km × 3 km and 1 km × 1 km, respectively.

### *2.4. Model simulations*

All simulations in this study were run in a node with Intel® Xeon® CPU E5-2630 processors totaling 64 cores. The WRF-Chem model was compiled with GNU compilers, including MPI libraries. The experimental study reported herein is divided into two parts. The first is a scalability study to analyze the time performance implications associated with increasing the complexity of the simulation system each time a new model/scheme is coupled/activated. The second is a model evaluation to determine the ability of the simulation system used to evaluate the effects of green infrastructures on the air quality in Barcelona. Although the time period simulated is the same for both experimental parts, the simulated time varies due to time constraints. We call these two methods *Complete Simulation* and *Performance Simulation*. The particular setup of each of these simulations is described below.

#### *2.4.1. Complete simulation*

By *Complete Simulation*, we mean the execution of the complete multi-model configuration including **WRF-Chem+BEP/BEM** Scheme. As mentioned earlier, this method considers atmospheric modeling, chemical processes, and building energy interactions, since all of which are of major relevance when studying the air quality in the city of Barcelona. The simulation covered 20 days from July 1st to July 20th

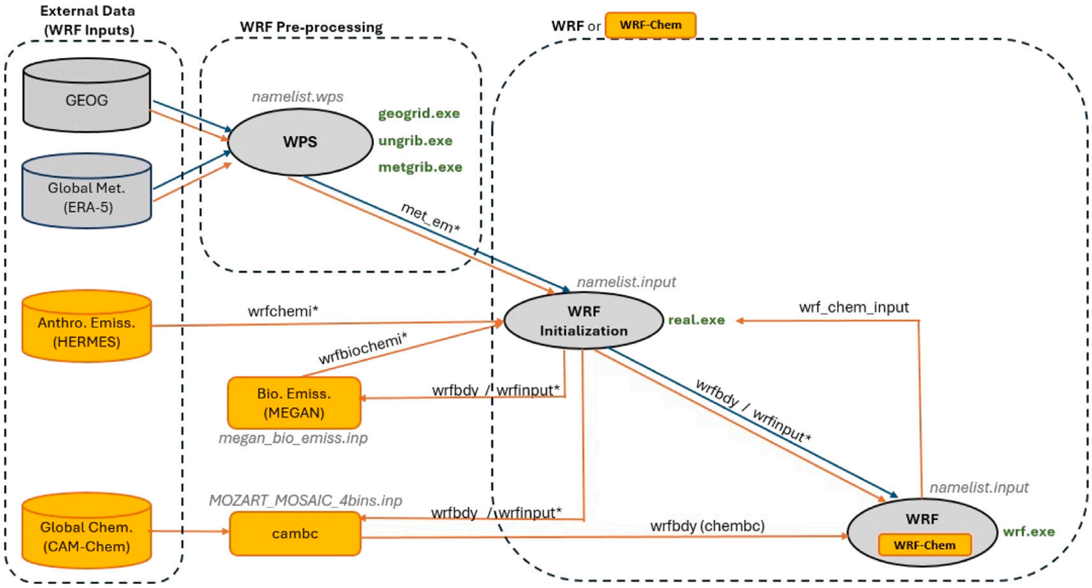


**Fig. 5.** Execution scheme: WRF (+BEP/BEM) depicted by blue arrows, and WRF-Chem (+BEP/BEM) represented by orange arrows.

of 2015. However, the first fortnight was discarded as a precautionary measure due to the lack of consensus regarding the appropriate spin-up duration. Our study therefore considers only the five days from July 16th to July 20th. This complete simulation was used to evaluate the multi-model system's capacity for capturing air quality behavior at the urban scale considering the current green urban canopy.

### 2.4.2. Performance simulation

In order to run the required simulations for performance metrics, they each began immediately after the spin-up period, that is, on July 16th at 00:00. The WRF model can be set with the restart feature, which starts a new simulation from a previously stored state, in this case, the spin-up period. This capacity to reuse the spin-up processing time implies a significant time reduction in the simulations involved in the performance process. It should be noted, however, that this procedure does not affect the obtained results. Considering this restart characteristic, the simulations run in the performance study cover a time of 30 min.

We measured the time executions of the three "partial" simulations (Base WRF, Base WRF+BEP/BEM Scheme and WRF-Chem) for comparison with the time execution and the resources required in each case.

1. **Base WRF:** This configuration is the simplest approach among our simulations; we use the minimum parameters needed to obtain a weather analysis/prediction in our specific case study. This configuration of the WRF model is shown in Table 1, where the parameterizations used are listed.
2. **Base WRF+BEP/BEM Scheme on:** In this configuration, we integrated Building Environment Parameterization (BEP) with the Building Energy Model (BEM) scheme in the WRF model.
3. **WRF-Chem:** In this configuration, we use WRF with the Chemistry (Chem) module, thus enabling atmospheric chemical processes simulation.
4. **WRF-Chem+BEP/BEM Scheme on:** The final configuration used in this study combines all the different pieces of the "puzzle".

### 2.5. Description of observational data

In order to evaluate the air quality forecasting capacity of the WRF-Chem model (including the BEP/BEM scheme) in relation to green city areas, two observational datasets were used: meteorological data and air quality data.

### 2.5.1. Meteorological data

The observational data used to evaluate the weather variables from the WRF outputs was provided by the Meteorological Service of Catalonia (SMC) [31] through its Network of Automatic Weather Stations (XEMA, Catalan acronym). Table 2 lists the four XEMA stations used in this study, including the Land-Use (LU) classification at the location of each specific station, the type of measurements gathered by each one, and their locations. The stations were chosen for their location within the city of Barcelona, as shown in Fig. 6.

### 2.5.2. Air quality data

The observational data used to evaluate the WRF-Chem outputs were provided by the Government of Catalonia from its *Xarxa de Vigilancia i Previsió de Contaminació Atmosfèrica* (XVPCA, Catalan acronym). Table 3 lists the seven XVPCA stations used in this work. As for the XEMA stations, these were chosen because they are within the area of the city of Barcelona. Fig. 7 shows the locations of these stations.

## 3. Experimental results

As mentioned in previous sections, the experimental study reported in this paper was designed to determine whether or not the current methods for conducting urban air quality simulations need to be reviewed in order to account the full range of factors affecting the pollutant dispersion in cities, and to consider air pollution at high-level resolution. These factors include the impact of green urban infrastructures on chemical processes and the influence of meteorological factors. The execution time required to obtain relevant results is, however, not negligible, not only due to the complexity of the simulation system but also to the resolution requirements. The results in this section are therefore organized into two parts, namely a scalability study and the results of the model evaluation. The scalability study is performed to determine the main limitations that make downscaling of this coupled system to the urban scale unfeasible. The results obtained for the three executed domains ($D01$, $D02$, and $D03$) are shown to highlight the impact of downscaling the system. Meanwhile, the results evaluation section contemplates both meteorological and air quality factors. These correspond to the simulation results obtained from the $D02$ and $D03$ domains, at resolutions of 3 km and 1 km, respectively. The $D01$ domain still had to be run as well, although it is not included in this section because its results are not relevant to the present study since we are focusing on high resolution results.

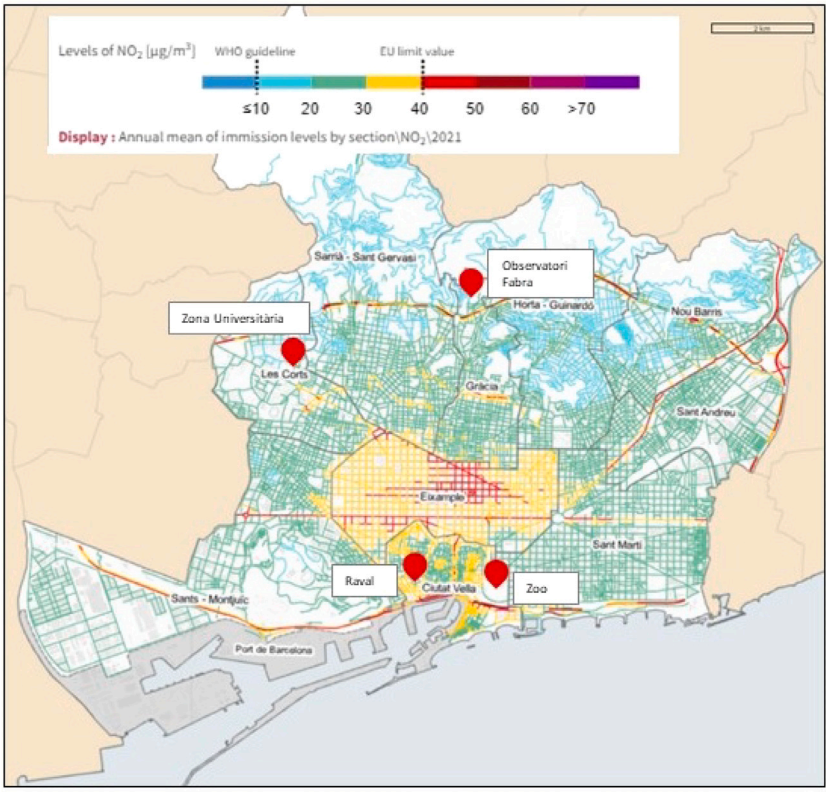


**Fig. 6.** XEMA stations (red dots) in Barcelona measuring temperature, relative humidity, wind speed, and wind direction. The underlying map of Barcelona was obtained from https://ajuntament.barcelona.cat/mapes-dades-ambientals/qualitataire/ca/.

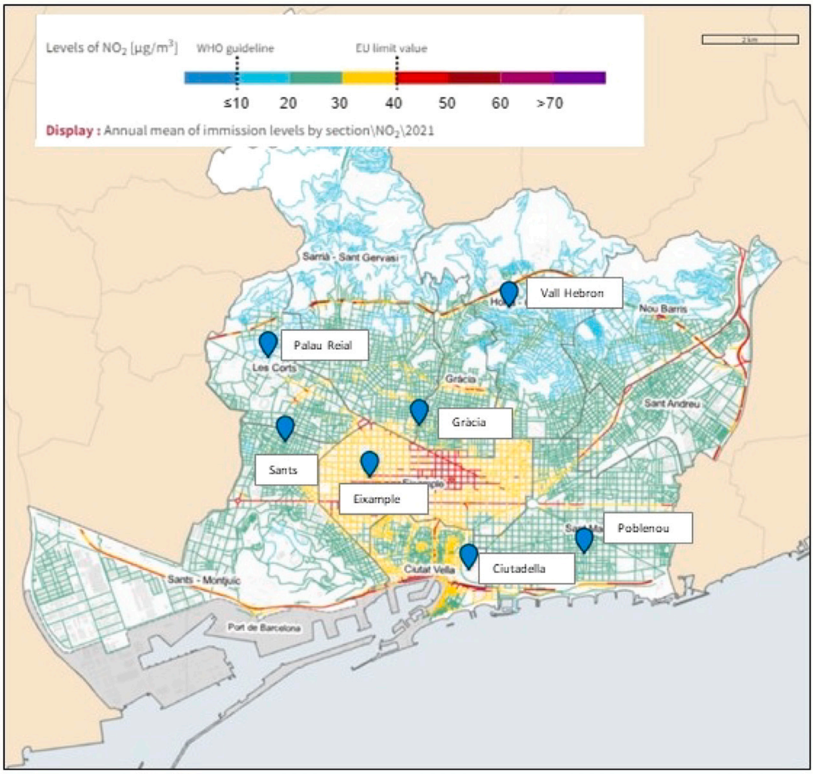


**Fig. 7.** XVPCA stations (blue dots) in the city of Barcelona that measure NO2 and O3 concentrations. The information obtained from https://ajuntament.barcelona.cat/mapes-dades-ambientals/qualitataire/ca/.

**Table 2**
Meteorological Stations in the Metropolitan Area of Barcelona (MAB) belonging to the Network of Automatic Weather Stations of Catalonia (XEMA, Catalan acronym).

| XEMA station | LU | Measurements | Lat.(°) | Lon.(°) | Alt. msl(m) |
|---|---|---|---|---|---|
| BCN(Raval) | 32 | T, RH, WS, WD | 41.3839 | 2.16775 | 33 |
| BCN(Zona Univ.) | 36 | T, RH, WS, WD | 41.37919 | 2.1054 | 79 |
| BCN(Zoo) | 32 | T, RH | 41.38943 | 2.18847 | 7 |
| BCN(Obs. Fabra) | 14 | T, RH, WS, WD | 41.41843 | 2.12388 | 411.2 |

**Table 3**
Air Quality Stations in the Metropolitan Area of Barcelona (MAB) from the Atmospheric Pollution Monitoring and Forecasting Network (XVPCA, Catalan acronym).

| XVPCA Station | LU | Measurt. | Lat.(°) | Long.(°) | Alt. msl(m) |
|---|---|---|---|---|---|
| BCN(Ciutadella) | 32 | NO2, O3 | 41.386406 | 2.187398 | 7 |
| BCN(Eixample) | 32 | NO2, O3 | 41.385315 | 2.153799 | 26 |
| BCN(Gràcia-StGervasi) | 32 | NO2, O3 | 41.398724 | 2.153398 | 57 |
| BCN(Palau Reial) | 38 | NO2, O3 | 41.38749 | 2.115199 | 81 |
| BCN(Parc Vall Hebron) | 32 | NO2, O3 | 41.42611 | 2.148001 | 136 |
| BCN(Poblenou) | 32 | NO2 | 41.40388 | 2.204501 | 3 |
| BCN(Sants) | 32 | NO2 | 41.37878 | 2.133099 | 35 |

### *3.1. Performance study*

As noted in 2.3, we worked with four different configurations: Base WRF, WRF with BEP/BEM, WRF-Chem, and finally WRF-Chem with BEP/BEM, which completes our required configuration. To understand the scalability of our four configurations, including variations with the BEP/BEM scheme and WRF-Chem, and how they are combined using the minimum time execution, we conduct the performance simulations in which we vary the number of CPU cores and measure the corresponding execution times for representative simulations. Analysis of these results offers insights into how efficiently each configuration uses the computational resources when choosing a configuration for a particular case study.

Fig. 8 shows the execution time of the four different configurations for the three domains executed. In order to facilitate comparison of the performance and scalability between configurations, all graphs use the same time scale. Fig. 8(a) shows the scalability of the basic WRF model, which is typically well-optimized for parallel execution, making it suitable for parallelization on multi-core systems [32]. As the number of CPU cores increases, the execution time decreases. As expected, the third domain is the most costly in terms of execution time. Furthermore, we can observe that above 32 cores, the execution time does not decrease in the same proportion that the number of resources increases. From 32 cores to 64 cores, we only obtain a reduction of 0.426% in the execution time in the first domain. In the second and third domains, the execution time consumed with 64 cores is higher than when we use 32 cores. This poor improvement in performance is due to factors such as communication overhead and memory limitations.

Fig. 8(b) shows the scalability of the BEP/BEM scheme. This configuration introduces additional computational complexity, particularly in simulating the building energy interactions in urban regions. We can see how the execution time decreases as we increase the number of cores. As in the basic WRF model, above 32 cores, communications and memory limitations are the main bottlenecks. An increase in resources does not therefore imply any improvement in performance. For this reason, the execution with 64 cores takes more execution time than the simulation with 32 cores.

Fig. 8(c) presents the time employed by the WRF-Chem model. The simulation of the chemical reactions and interactions in the atmosphere introduces major complexity, which is reflected in the time execution consumption. It is easy to observe that modelization of the atmospheric chemistry implies a sixfold greater increase in execution time than the previous configurations that do not couple the atmospheric and the chemistry model. We improve the performance by adding more cores, but this improvement decreases notably above 32 cores. The improvement is however greater in this configuration than in the previous ones. In the third domain, the improvement in performance is around 20% of the execution time, while in the preceding schemes, the execution time increases.

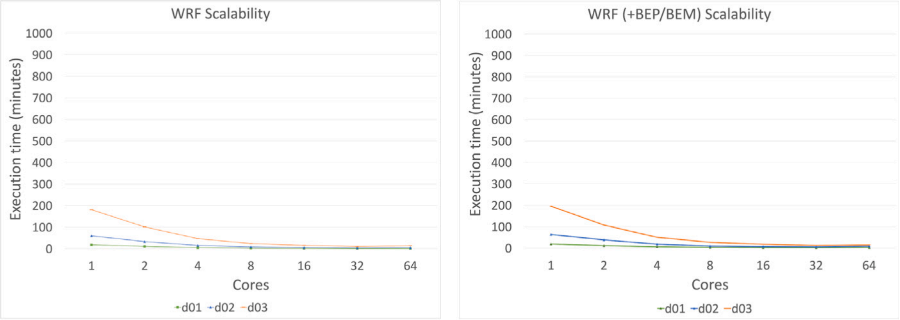
Fig. 8(d) shows the execution time of the WRF-Chem+BEP/BEM model. As in the previous configuration, the modelization of the atmospheric chemistry implies a critical increment in execution time. When the number of cores is lower than 32, the scalability is high. Above this number, the reduction in execution time is around 17% in the third domain, but, as in the WRF-Chem model, there is still a tiny reduction in the execution time.

As shown, the configurations that implement the modelization of the atmospheric chemistry WRF-Chem model and WRF-Chem+BEP/BEM model consume over six times more execution time than the configurations that do not couple the atmospheric and chemistry models. Unlike the basic WRF model, the WRF-Chem model is not well optimized. This is mainly due to the dependencies between the atmospheric chemistry reactions, which are extremely hard to parallelize.

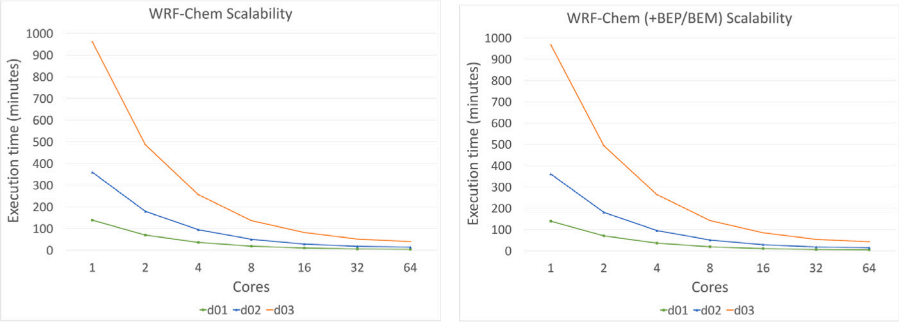
Fig. 9 presents the computed speed-up of the four different configurations for the three domains. As shown, in the configurations that do not simulate the chemical reactions, the basic WRF and BEP/BEM schemes (Figs. 9(a) and 9(b) respectively), speed-up increases until there are more than 32 cores, when the maximum speed-up is reached in the third domain, 17.31 for the basic WRF and 15.93 for the BEP/BEM.

At this point, the speed-up decreases. This behavior indicates that above this number of cores, we enter the memory-bound zone, where simulations are bottlenecked by communication and memory access issues. An increase in resources does not therefore imply any increase in performance. In contrast, in configurations that implement atmospheric chemistry, the WRF-Chem model and WRF-Chem+BEP/BEM model schemes (Figs. 9(c) and 9(d) respectively), speed up continues to increase above 32 cores. In those cases, the maximum speed-up is reached in the first domain, i.e. 32.10 for the WRF-Chem model and 29.41 for the WRF-Chem+BEP/BEM model. In those schemes, when the number of cores is equal to 64, we are in the CPU-bound zone, which means that any increase in computational resources implies a substantial improvement in performance. This is because the modelization of atmospheric chemistry is extremely demanding in terms of computational cost. Hence, the scalability of the WRF-Chem model and WRF-Chem+BEP/BEM model schemes are better than the basic WRF and BEP/BEM schemes for 64 cores.

In order to better understand the scalability of the different configurations used in this study, the efficiency was computed for each. Fig. 10 shows the efficiency of the four different configurations in the third domain. We focus on the third domain because it is the most demanding in terms of execution time. We note that schemes

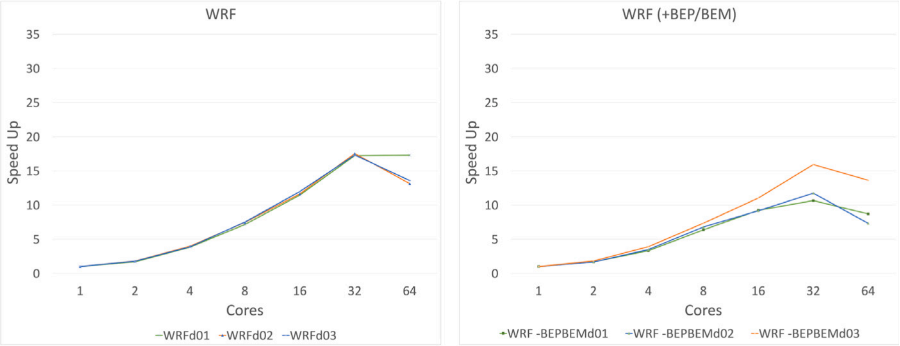


(a) WRF (b) WRFBB

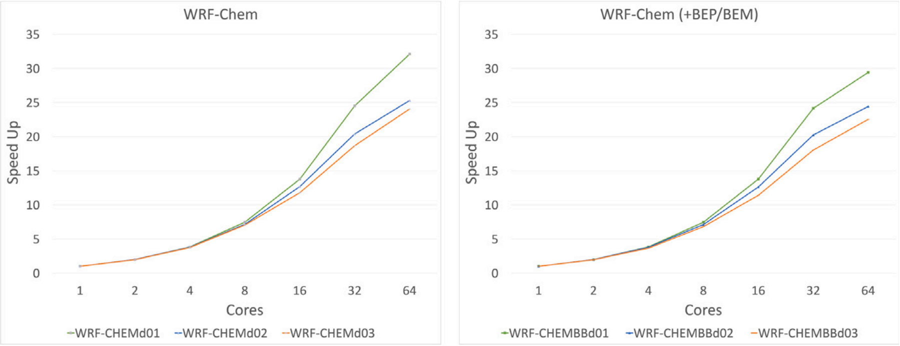


(c) WRFChem (d) WRFBBChem

**Fig. 8.** Execution time depending on configuration. The green line shows the parent domain (d01), the blue line shows the Catalonia region domain (d02), and the orange line shows the MAB region domain (d03).



(a) WRF (b) WRFBB



(c) WRFChem (d) WRFBBChem

**Fig. 9.** Speed Up depending on the configuration. Green line shows the parent domain (d01), blue line shows the Catalonia region domain (d02), and the orange line shows the MAB region domain (d03)

that simulate the chemical reactions (WRF-Chem model and WRF-Chem+BEP/BEM model) are more efficient for 2 cores than the other schemes (basic WRF and BEP/BEM). For 4 and 8 cores, the basic WRF and BEP/BEM configurations are more efficient. However, above 8, the

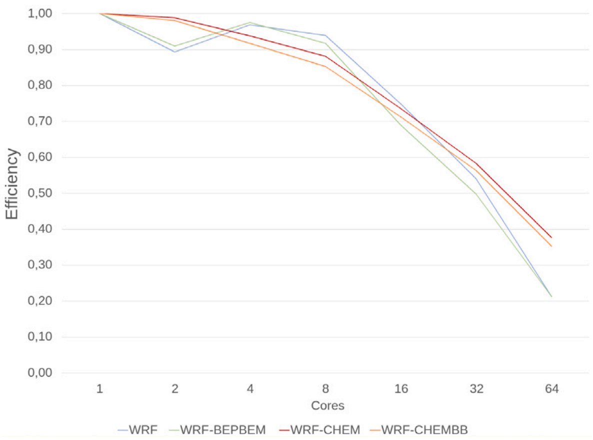


**Fig. 10.** Efficiency depending on the configuration in the third domain. The blue line shows the WRF, the green line shows the WRFBB, the red line shows the WRFChem, and the orange line shows WRFBBChem.

efficiency of the WRF-Chem model and WRF-Chem+BEP/BEM models decreases more slowly than it does for the other schemes. This behavior indicates that the resources are better used in the schemes that simulate atmospheric chemistry. As noted earlier, modelization of chemical reactions is highly complex and demanding in terms of computational cost. Hence, the WRF-Chem model and WRF-Chem+BEP/BEM models use resources more efficiently when the number of cores is incremented.

### 3.2. Model evaluation results

This section evaluates the meteorologic and air quality results. Although the meteorological and air quality measurement stations used in this study are not located in the exact same place in Barcelona, the distance between them is irrelevant because we are interested in the station type and its surroundings. Although the results for all XEMA and XVPCA stations are included in this experimental study, note that in order to capture the imprint of areas that have very different green morphologies, the discussion of the air quality results is sometimes more focused on stations located in dense traffic areas and green urban zones.

#### 3.2.1. Meteorological results

Figs. 11 and 12 show, respectively, the temperature (T) and the relative humidity (RH) for the four XEMA stations in the city of Barcelona. Regarding temperature, note that for all cases, the results obtained for $D03$ (orange line) are closer to the real observations (black line) than the results provided by the $D02$ domain (blue line). So, as expected, higher resolutions produce better results, although there is still a gap in the improvement between the forecast 1 km resolution data and the real observations. However, the mismatch between the observations and forecast values increases when analyzing the relative humidity results. By studying the general behavior of all XEMA stations, the model can capture overall trends in relative humidity but, in all cases, is not so effective at reflecting temperature. In fact, in the transition from October 18 to 19, the observed RH is clearly overestimated.

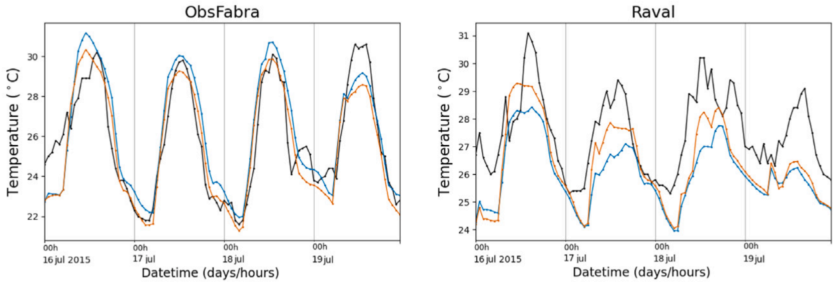
Tables 4 and 5 show the statistical values for $T$ and RH, respectively. In these tables, the Root Mean Square Error (RMSE), Mean Bias (MB), and Correlation (R) for the two analyzed domains ($D02$ and $D03$) are summarized for all four XEMA stations. The correlation column reveals that the poorest correlation for both measures corresponds to the *Raval* and *Zoo* stations. The same behavioral pattern is observed in the other statistical metrics. These two stations are located close to the sea. The *Zoo* station is in *Ciutadella* park, which covers approximately 18 hectares and includes the city zoo. The grid resolution of the inner domain ($D03$) is equal to 1 km and, despite the resolution of the land-use map being 100 m, the land-use class associated with the location of these two XEMA stations is 32, which implies that these areas are classified as compact midrise urban areas. These incorrect classifications, especially that of the *Zoo* station, have a direct impact on the meteorological variables because the model does not properly take into account the influence of the sea on the *Raval* station or the green canopy cover on the *Zoo* station. A high-resolution model that could predict these variables at an urban resolution would allow us to take advantage of the higher resolution of the land-use map to obtain a better description of urban canopy cover. Furthermore, this bias between the observations and the model outputs will directly impact the air quality because the meteorological variables somehow guide the chemical processes performed in the WRF-Chem coupled model.

#### 3.2.2. Air quality results

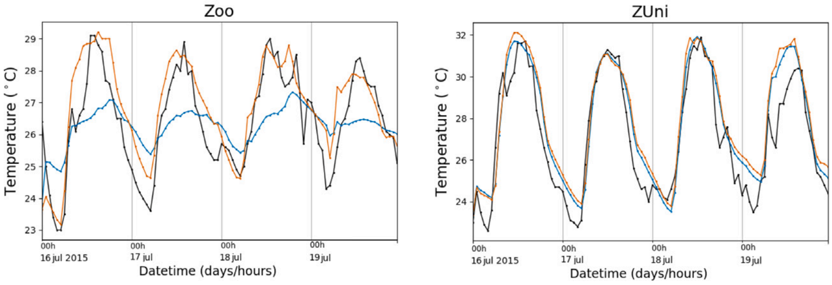
This section is focused on analyzing the evolution of nitrogen dioxide ($NO_2$) during the five days studied. In particular, Fig. 13 shows changes in $NO_2$ concentration from Thursday 2015-07-16 to Monday 2015-07-20 at the seven air quality stations in the city of Barcelona compared to the results obtained by the WRF-Chem model at $D02$ and $D03$. As shown, although the results provided by WRF-Chem at 1 km (red line) and 3 km (blue line) are fairly similar, there is a significant difference from the observations (black line). The station with the lowest mean observation values for the whole period is *Ciutadella*, and this mean value is fairly stable. Although *VallHebron* also has low $NO_2$ concentrations on most days, it presents more significant peaks than *Ciutadella*. *VallHebron* station is located on the outskirts of the city close to a mountain park (*Collserola*) but also next to the city's ring-road, which clearly affects the air quality in that zone. The other five XVPCA stations are located in dense traffic areas, especially *Eixample* and *Gracia*. Since *Eixample* is located in the most polluted area, we have subsequently selected the *Eixample* and *Ciutadella* stations for comparison purposes. The former is representative of a dense traffic zone, especially during rush hours, and the latter is a large green park close to the sea, next to the XEMA *Zoo* station.

Table 6 shows the statistical values for $NO_2$. The Root Mean Square Error (RMSE), Mean Bias (MB), and Correlation (R) for the two analyzed domains ($D02$ and $D03$) are summarized for the four XVPCA stations used in this study. The correlation column reveals that the worst correlation for both measures corresponds to the *Gracia* and *Eixample* stations, which are both close to heavy traffic. In general, the model overestimates the $NO_2$ daily peaks, especially on day 18, Saturday, and the observations show that there was no morning peak. We also can see that the model at a resolution of 1 km overestimates the $NO_2$ peaks more than at 3 km. In general, the model does not capture the behavior of $NO_2$.

Fig. 14 shows the annual mean value of emissions ($NO_2$) in two plots of Barcelona corresponding to the *Eixample* and *Ciutadella* air quality measurement stations. The framed area is a 1 km square cell around each selected measurement station. The different colors represent the different levels of $NO_2$ concentration in these areas. Regardless of the particular values of each color, it is easy to directly verify that more than one color appears in the purple square. In fact, for the particular case of *Ciutadella* station, the color distribution ranges from 20 to 70 $\mu g/m^3$. Although the model setup incorporates the BEP-BEM urban canopy layer in order to take into account the influence of the building morphology on pollutant dispersion, due to the low resolution used the coupled WRF-Chem model is unable to capture the differences between the parts of the map that are included in the same grid cell. Another aspect to highlight is the differences between the diurnal and nocturnal cycles of $NO_2$ concentration compared to the observations. Regarding the diurnal cycle from 6:00 to 18:00 in the *Ciutadella* station, the estimated $NO_2$ concentration is closer to the observations regardless of the day of the week. However, diurnal cycles in the *Eixample* station are clearly underestimated on business days (2015-07-16 was a Thursday).

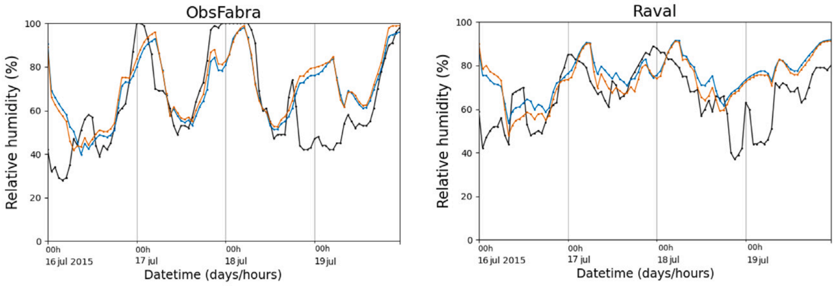


(a) Observatori Fabra (b) Barcelona(Raval)

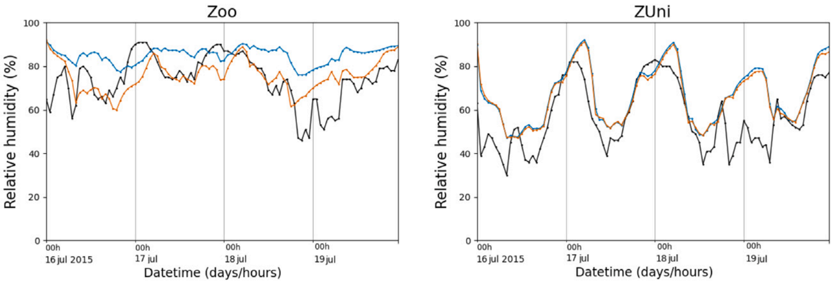


(c) Barcelona (Zoo) (d) Barcelona(Zona Univ.)

**Fig. 11.** Temperature at the XEMA stations in the city of Barcelona (black line) compared to the $D02$ (blue line) and $D03$ (orange line) results of WRF in the same location.



(a) Observatori Fabra (b) Barcelona(Raval)



(c) Barcelona (Zoo) (d) Barcelona(Zona Universitaria)

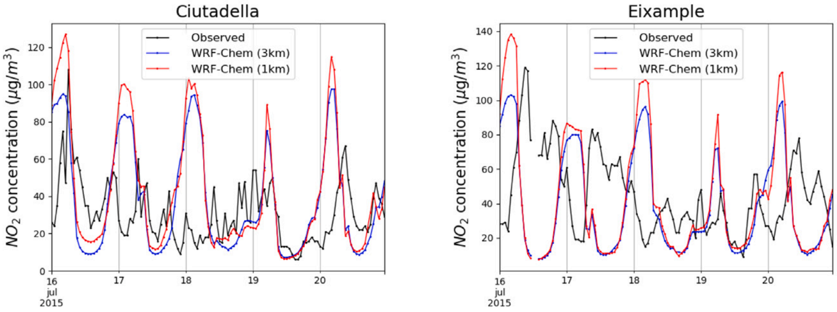
**Fig. 12.** Relative Humidity at the XEMA stations in the city of Barcelona (black line) compared to the $D02$ (blue line) and $D03$ (orange line) results for WRF in the same location.

**Table 4**
Statistics of hourly 2 m temperature for the period from July 16th to 20th of 2015.

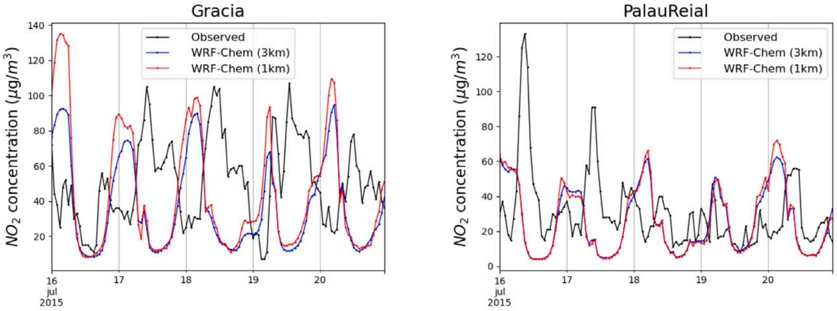
| XEMA station | RMSE D02 | RMSE D03 | MB D02 | MB D03 | R D02 | R D03 |
|---|---|---|---|---|---|---|
| Barcelona(Raval) | 1.6 | 1.6 | −0.2 | 0.1 | 0.42 | 0.47 |
| Barcelona(Zona Univ.) | 1.5 | 1.8 | −0.2 | 0.1 | 0.87 | 0.86 |
| Barcelona(Zoo) | 2.0 | 2.7 | −0.1 | 2.1 | −0.14 | 0.60 |
| Barcelona(Obs. Fabra) | 1.6 | 1.4 | 0.7 | −0.2 | 0.89 | 0.89 |

**Table 5**
Statistics of hourly relative humidity for the period from July 16th to 20th of 2015.

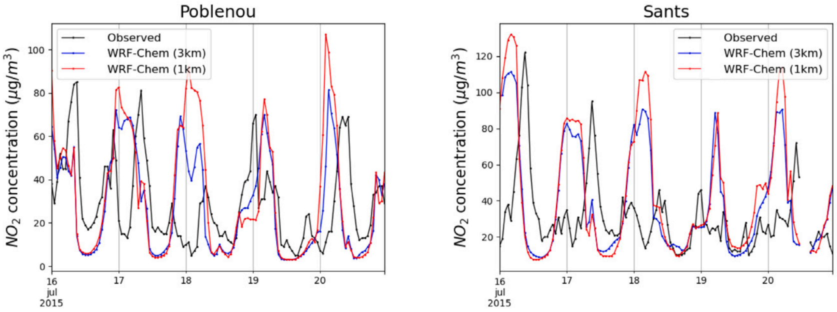
| XEMA Station | RMSE D02 | RMSE D03 | MB D02 | MB D03 | R D02 | R D03 |
|---|---|---|---|---|---|---|
| Barcelona(Raval) | 18.2 | 19.0 | −14.3 | −15.6 | 0.59 | 0.59 |
| Barcelona(Zona Univ.) | 11.7 | 12.3 | −8.1 | −8.9 | 0.76 | 0.75 |
| Barcelona(Zoo) | 12.3 | 29.0 | −2.9 | −25.5 | 0.30 | 0.38 |
| Barcelona(Obs. Fabra) | 13.0 | 11.2 | −7.5 | −4.6 | 0.68 | 0.71 |



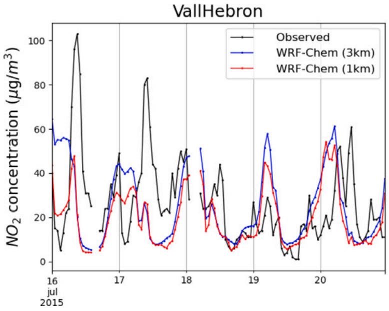
(a) Barcelona(Ciutadella)　(b) Barcelona(Eixample)



(c) Barcelona(Gràcia)　(d) Barcelona(Palau Reial)



(e) Barcelona(Poblenou)　(f) Barcelona(Sants)



(g) Barcelona(VallHebron)

**Fig. 13.** Changes in $NO_2$ concentration in the period from Thursday 2015-07-16 to Monday 2015-07-20 at air quality stations in Barcelona compared to the results obtained by the WRF-Chem model at *D*02 and *D*03.

**Table 6**
Statistics of hourly nitrogen dioxide ($NO_2$) for the period from July 16th to 20th of 2015.

| XVPCA Station | RMSE D02 | RMSE D03 | MB D02 | MB D03 | R D02 | R D03 |
|---|---|---|---|---|---|---|
| Barcelona(Ciutadella) | 31.84 | 35.98 | 0.17 | 0.22 | −7.27 | −11.74 |
| Barcelona(Palau Reial) | 29.77 | 30.57 | −0.05 | −0.05 | 5.57 | 4.85 |
| Barcelona(Eixample) | 42.13 | 46.84 | −0.24 | −0.22 | 4.82 | 0.48 |
| Barcelona(Gracia) | 43.74 | 49.22 | −0.37 | −0.37 | 13.31 | 5.91 |
| Barcelona(Poblenou) | 26.03 | 33.03 | 0.25 | 0.09 | 0.87 | −3.26 |
| Barcelona(VallHebron) | 23.77 | 21.29 | 0.17 | 0.30 | 1.30 | 6.44 |
| Barcelona(Sants) | 36.28 | 41.73 | 0.08 | 0.05 | −9.32 | −12.75 |

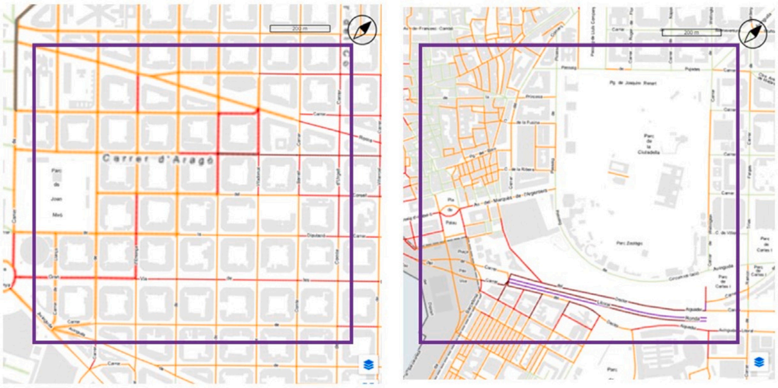
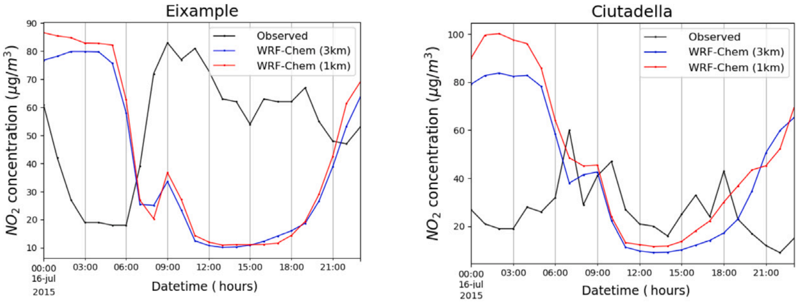


**Fig. 14.** Annual mean of the $NO_2$ concentration in 2021 at the *Eixample* (left) and *Ciutadella* (right) areas of Barcelona.



(a) (b)

**Fig. 15.** $NO_2$ concentration levels for the day 2015-07-17 in the *Eixample* and *Ciutadella* air quality stations.

Another issue to analyze is the influence of green areas on the air quality. For that purpose, Fig. 15 focuses on the *Eixample* and *Ciutadella* stations on Friday 2015-07-17, although we could have used any other business day. In the part corresponding to *Ciutadella*, the $NO_2$ behavior during the day and at night is fairly regular as far as the observations are concerned, while the models at 3 km and 1 km, despite matching the results, cannot capture this behavior as already discussed earlier.

It is also remarkable to note that this plot corresponds to a green zone with practically no traffic anywhere in the cell except in certain border areas. The effect of the park on the air quality in the area is however altered when only modeling at high resolution, considering the green layer in *Ciutadella*. The observed data suggests that the green infrastructure mitigates the harmful effects of pollutants, but this effect cannot be reproduced unless working at high resolution. In the *Ciutadella* area, the emissions produced by traffic are lower, but the model does not reflect this lower release of pollution into the environment. In contrast, the *Eixample* plot shows how the model cannot capture the behavior of $NO_2$ concentration in its day or night cycle, as commented earlier. Another notable effect is that the improvement caused by the introduction of green spaces would not be reproducible without increasing the resolution of all the models involved. Hence, the main conclusion of this study is that although green areas do help to reduce environmental pollution, unless complete high-resolution models are used, it is very difficult to obtain effective green designs.

## 4. Conclusions

The design of green cities is a common strategy to address the issue of poor air quality in highly polluted urban morphologies. To make sure that these designs are effective, their effects need to be thoroughly tested. This requires use of suitable simulation methods but, to the best of the authors' knowledge, until now none have been proposed that are able to model these effects at a resolution of around 100 m. It is only at this kind of resolution that a model can comprehensively account for the full variety of buildings and green areas in highly populated cities, and hence all of the different processes and factors associated to such matters as meteorology, chemical reactions and the urban canopy layer. For that reason, this study has used the WRF-Chem+BEP-BEM model. Furthermore, hybrid land-use classifications were applied in order to consider different urban and green elements. As a case study, we used the city of Barcelona, Catalonia in northeast Spain in the period from 1 to 20 July 2015, although due to model spin-up requirements, a more in-depth study focused on the last five days of this period. Since these coupled models tend to be extremely costly in computational terms, we have done a scalability study to assess the performance of the system. Implementation of city design policies based on these models would require a huge number of simulations with different configurations of the urban canopy layer before being able to determine which would be the best option. Although this study assessed the air quality in the whole of Barcelona, a more in-depth analysis was performed on two areas with very different urban characteristics. The first, Eixample, is an area of very dense traffic, while the second, Ciutadella, is a large green park near the sea. The study considered both the meteorological parameters and certain pollutants, and justified the need for complete coupled models (meteorology, chemistry, and urban morphology) at the urban scale. Although the meteorological model is able to reproduce the observational data at a resolution of 1 km reasonably well, when it is coupled to the chemical system, including the urban morphology, the air quality results fail to reproduce the observations. This behavior is of particular importance in green areas where the observations suggest that the air quality is better, but the model is unable to reproduce this, not even when using a high resolution land-use map that shows these green areas. The main conclusion of this study is that “green resolution matters”. In other words, a downscaled WRF-Chem model that fails to consider green infrastructures might generate green city designs that cause poorer air quality than there were before the green modifications were introduced, therefore, current approaches to this issue need to be revised. Consequently, new strategies need to be designed that are able to address, in a smart manner, the gap between 1 km and 100 m resolution air quality simulations. AI models, such as ML strategies, arise as a promising field to address this problem.

## CRediT authorship contribution statement

**Veronica Vidal:** Writing – review & editing, Writing – original draft, Methodology, Investigation. **Ana Cortés:** Writing – review & editing, Writing – original draft, Supervision. **Alba Badia:** Supervision. **Gara Villalba:** Supervision.

## Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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