



High-resolution impacts of green areas on air quality in Madrid

Roberto San Jose¹ · Juan L. Perez-Camanyo¹

Received: 20 January 2022 / Accepted: 21 September 2022 / Published online: 11 October 2022
© The Author(s) 2022

Abstract

This study numerically investigates the influence of trees on air quality in Madrid urban area (Spain). Simulations are performed using the mesoscale model WRF/Chem (EPA, US) and the microclimate computational fluid dynamics (CFD) model PALM4U (IMUK, DE) configured as LES (Large Eddy Simulation). PALM4U is running over one of the 1 km × 1 km grid cells with 5 m very high spatial resolution using three different scenarios. In the simulation domain, there is a zone (approximately 25% of the domain) of vegetation where the dominant species are broadleaf trees included in the BAU (Business as Usual) scenario. The second scenario is focused on changing the type of the tree from broad leaf at BAU scenario to needle leaf the so-called ND scenario and the third scenario called NOTREE which comprise the replacement of the trees located in the green zone. The base simulations (BAU) are compared with data from the Madrid air quality monitoring network for the evaluation of the simulation results. The effects of the trees are calculated comparing scenarios (BAU-NOTREE and BAU-ND), so a brute force methodology has been used. This paper shows that the effects of the trees and type of trees are not uniform across the urban area because there are variations in the energy fluxes and the aerodynamic effect and there are important interactions of trees with wind flow dynamics. The mitigation potential effect of trees on gaseous air pollutants concentrations is showed and also may enhance substantially air pollution in other areas.

Keywords Urban air pollution · CFD PALM4U · Tree effects · Pollutant dispersion

Introduction

Air quality is currently one of the priority environmental problems in large cities. High concentrations of pollution are often found in urban areas, where there is a high population density and emissions due to road traffic are very high. Exposure to air pollution has been demonstrated to have serious health effects, e.g. it increases the number and severity of respiratory and cardiovascular diseases, which in turn leads to increased mortality (Pope and Dockery 2006). Urban air quality is controlled both by large-scale background characteristics of the atmosphere and by local-scale dynamic and chemical processes, mainly driven by turbulence. In addition, in urban areas the air encounters a large number of obstacles (buildings, trees...) that give complex flow patterns in the streets. All of the above, together with the

heterogeneity of pollutant emissions, which in cities mainly come from road traffic (NO_x), produce strong concentration gradients, there can be large variations in concentrations between one side and the other of the same street. Mesoscale chemical transport models simulate the instantaneous mixing of emission sources within each of the individual grid cells, even if a point emission is homogeneously distributed over the whole grid cell, which does not allow modelling the spatial variability of urban air quality because the grid cells are too coarse (Wang and Shallcross 2000). Mesoscale models (with a spatial resolution of up to 1 km) do not allow us to capture local phenomena and high spatial variability due to too coarse a resolution of the emission model and insufficient representation of the urban surface (including different three-dimensional obstacles, such as buildings and trees), as described in Beevers et al. (2012) and Choudhary and Tarlo (2014). Another limitation of mesoscale models is that they cannot accurately simulate the turbulent transport generated by larger eddies. In order to be able to simulate this phenomenon, high-resolution models (metre-resolution cells) are needed in which at least the larger transport eddies are explicitly resolved. In addition, the layout and effect of

✉ Roberto San Jose
roberto@fi.upm.es

¹ Environmental Software and Modelling Group, Computer Science School, Technical University of Madrid (UPM), Madrid, Spain

buildings, streets and other objects on the urban surface that affect the atmospheric flow and thus the turbulent diffusion of pollutants must be taken into account.

Urban air pollution is also driven by the medium- and long-term transport of gaseous and particulate pollutants from surrounding areas. This is also an important factor to be taken into account in modelling the air quality of a city at the local scale, so tools to simulate the transport of pollutants in the areas outside cities will have to be added, as is done in this work. The ideal tool to solve this aspect are mesoscale models that can provide boundary conditions for simulation at the microscale (local scale). The dispersion of urban pollutants in the urban environment, with trees, buildings, etc. is intrinsically a multi-scale problem, and we will have to simulate from the global scale (data from global models) to the local scale (city) through the mesoscale models. We propose to combine the advantages of three-dimensional Eulerian models, which can simulate urban background concentrations of the main air pollutants of interest, and the three-dimensional urban model, which can simulate air pollutant concentrations in complex urban canopy configurations.

One of the most important issues in using CFD technology to research atmospheric environment problems on the street level is to obtain accurate initial and boundary conditions (Ehrhard et al. 2000). To solve this problem, the multi-scale coupling method is revealed as a good solution, which uses information from mesoscale model as the initial and boundary conditions to drive CFD (Nelson et al. 2016) in order to take into account both short range and long-range transport and chemistry effects. Grid nesting is the most common method, being employed in most of the chemical transport models (WRF/Chem, CMAQ, CMAx). The long-range transport of air pollutants is an important fact and it has influence in local air quality (Bae et al. 2020). The regional influences in the local concentrations depends of the meteorological conditions but the pollutants can travel from the regional domains to the local domain, so local pollution can be strongly influenced by regional emissions and transport. The proposed nesting-based architecture has already been used by the authors in other works (San José et al. 2021). In the previous work, it is shown how the nesting of domains with the WRF/Chem model allowed to obtain satisfactory results when comparing the simulated concentrations with the concentrations measured by the network of stations of the Madrid City Council, but in some stations the WRF/Chem model was unable to reproduce high NO₂ peaks and when introducing the CFD driven by the WRF/Chem BCs these peaks were reproduced. The general pattern of NO₂ concentrations over time was determined by the WRF/Chem and it was the CFD that was able to reproduce the large fluctuations at some specific points in the city. Others studies have shown the advantages of the nesting approach

to provide BCs to CFD simulations (Kadaverugu et al. 2019; Kwak et al. 2015; Michioka et al. 2013); the meteorological mesoscale and air quality multiscale models coupled with CFD models are used to develop urban air quality modelling systems which shown better performance than the mesoscale models in simulating NO₂ and O₃ concentrations.

If we apply a pollution dispersion model over an urban area, we must take into account what happens in and on the urban canopy to determine the spatial–temporal variation of the simulated air pollutants. The complexity from a computational point of view is how to solve the equations describing the behaviour of the flows, which in these areas are turbulent and therefore unstable and heterogeneous. In this context, computational fluid dynamics (CFD) models are powerful modelling tools to reproduce the dispersion of pollutants taking into account the realistic characteristics of urban environments. Microscale models, such as CFD models, can be used to solve the turbulent flow equations at a higher spatial resolution (on the order of metres) to reproduce in detail the atmospheric processes in the urban canopy layer. These numerical tools assist urban planners and other decision makers by providing them with detailed knowledge on the possible air pollution mitigation strategies to be implemented in order to be able to assess in advance the different actions within this objective (Caplin et al. 2019).

Computational fluid dynamics (CFD) models are high in computational demand, but thanks to the increased computing power of computers and the availability of high-performance systems to scientific groups, the use of CFDs has become widespread in the scientific community. Such models provide a detailed three-dimensional representation of the energy flows, wind and concentrations of a city at high resolution (metres), and are capable of modelling the effects of obstacles such as trees and buildings. There are mainly two types of turbulence models in CFD models, based on their ability to resolve turbulent flow. The CFD RANS which are based on the Reynolds-averaged Navier–Stokes equations with parameterised turbulence and the LES for the simulation of large eddies. RANS assumes that non-convective transport in a turbulent flow is governed by a stochastic three-dimensional turbulence that has a broadband spectrum with no distinct frequencies and therefore models all eddy length scales without distinction. This method has obvious weaknesses and poses serious uncertainties in flows where large-scale organised structures dominate. In addition, RANS models often assume gradient transport, which may not be the case for pollutant exchange within street canyons. Large eddy simulation (LES), although more computationally expensive, has the advantage over RANS in that it explicitly resolves most energy transporting eddies and internally or externally induced periodicity, and only universally small eddies are modelled. The similarity hypothesis dictates that the statistics of the small eddies are universal and they

are not dependent on properties of the fluid while the large-scale structures are directly affected by the geometry and the boundary conditions. The ability of LES to reproduce the unsteady and intermittent fluctuations of the flow fields and thus to capture the transient mixing process is what makes it numerically superior to conventional RANS, in particular for studies dealing with complex geometries and pollutant dispersion problems, such as the one we will address in this paper.

Previous work has already shown the advantages of coupling mesoscale numerical models to microscale models, as substantial improvements in wind field predictability were observed when using the results of a mesoscale meteorological model as CFD initial and boundary conditions (Miao et al. 2013). In subsequent work, turbulence-resolving large eddy simulation models have already been applied to cities to investigate air pollution (Abhijith et al. 2017), for example to simulate the spatial distribution of NO₂ in a city with high (metre) horizontal resolution (Buccolieri et al. 2018). Usually when CFD models are used to understand air quality in cities, several meteorological scenarios are considered, but without coupling a mesoscale model to provide initial and boundary conditions, which allow the CFD simulation with real meteorological data, that aspect is one of the novelties of this work. In other research, urban CFD simulations have been performed considering an idealised two-dimensional street canyon or a simplified urban topology (Baik and Kim 2002); in this work, a real complex urban area is modelled, using real 3D tree, street, and building data. Therefore, this work proposes a novel approach by combining complex mesoscale and microscale air quality models with traffic simulation tools that take into account emission data, regional and urban meteorology, and various chemical and physical mechanisms to simulate air pollution concentrations at different spatial scales; a complete modelling system is applied that tries to simulate the atmospheric dynamics of a city as realistically as possible.

Urban vegetation is an important element influencing the dispersion of pollutants in the cities. In fact, the impacts of vegetation in urban areas and its application as a mitigation measure for urban air pollution are currently under discussion. This work tries to supply new scientist data to the urban air quality community. The motivation is related to the complex processes that make it difficult to extract general conclusions due to the high dependence on local conditions. With several modelling techniques, especially through CFD, models are being applied to study the impact of urban vegetation on pollutant dispersion. The impact of vegetation is produced by the aerodynamic effect, altering fluxes, and by the emission and deposition process, adding and removing pollutants to and from the air through their leaves. Several studies have found that the aerodynamic effect is greater than pollutant emitted or removal by deposition. In some

studies, the inclusion of vegetation has been shown to be beneficial by decreasing pollutant concentrations through deposition on trees, leaves, and other green infrastructure (Pugh et al. 2012). However, vegetation may also increase pollutant concentration in street canyons by obstructing wind circulation. In this study, we analyse and quantify the positive and/or negative impacts of trees and type of trees in a downtown area of the city of Madrid (Spain) in a real scenario. The experiment takes into account the atmospheric conditions of the environment, the micro-meteorology of the area, the solar radiation and flow energy balance, traffic emissions, chemical reactions, deposition of pollutants, and the dispersion of pollutants in a 3D obstacle (buildings and trees) environment.

Material and methods

Modelling tools

The CFD simulation presented in this work were ran using the Parallelized Large-Eddy Simulation Model (PALM) adapted to urban areas (PALM4U) for atmospheric flows (Maronga et al. 2015). PALM4U solves the three dimensional fields of wind and scalar variables (e.g. potential temperature and scalar concentrations). The performance of PALM over an urban-like surface has been validated against wind tunnel simulations, previous LES studies and field measurements (Park et al. 2015). Buildings are represented as solid obstacles that react to the flow dynamics via form drag and friction forces. Natural and paved surfaces in urban environments are simulated using a multi-layer soil model. It is well known that vegetation canopy effects on the surface-atmosphere exchange of momentum, energy and mass can be rather complex and can significantly modify the structure of the ABL, particularly in its lower part (Dupont and Brunet 2009). It is thus not possible to describe such processes by means of the roughness length and surface fluxes of sensible and latent heat. To describe the complete 3D structure of individual trees, the plan canopy model uses canopy leave area density (LAD) and basal area density (BAD) as inputs. The plant canopy model is integrated within the detailed radiation model (which includes shadows). The direct, diffuse, and reflected short-wave and long-wave radiations are partially absorbed by individual grid boxes of plan canopy and transformed to sensible heat flux inside the vegetation. This heat flux is consequently transformed to increase of the corresponding air mass. The plant canopy also emits the long-wave radiation according its current local temperature. An important part of the heat balance in the urban canopy represents the latent heat fluxes from the vegetation. A fully “online” coupled chemistry module is integrated into PALM. The chemical species are treated as

Eulerian concentration fields that may react with each other, and possibly generate new compounds; in this experiment, the chemistry mechanism CBM4 Carbon Bond Mechanism (Gery et al. 1989) with 32 compounds and 81 reactions was used. Gases are deposited using the DEPAC module (Van Zanten et al. 2010).

The mesoscale modelling tool is the Weather Research and Forecasting and Chem model (WRF/Chem) (Grell et al. 2005). The model simulates the emission, transport, mixing, and chemical transformation of trace gases and aerosols simultaneously with the meteorology. The main advantage of this model is that chemistry and meteorology are solved simultaneously thanks to their coupling, therefore both processes use the same advection, convection, and diffusion scheme, on a common grid and without the need for interpolations. This model is widely used by the scientific community and has been evaluated in many experiments (Fast et al. 2006). The WRF/Chem model was configured as in phase 2 of the International Air Quality Model Assessment Initiative (AQMEII) (San Jose et al. 2015). The Carbon Bond Mechanism version Z (CMBZ) is the atmospheric chemical mechanism (Zaveri and Peters 1999) used for gas phase chemistry. Aerosol chemistry is represented by the Model for Simulating Interactions and Aerosol Chemistry (MOSAIC) (Zaveri et al. 2008). Dry aerosol deposition is simulated following the approach of Binkowski and Shankar (Binkowski and Shankar 1995) and the wet deposition approach follows Easter (Easter 2004). Photolysis rates are obtained from the photolysis scheme in Fast-J (Williams et al. 2006). We include aerosol-radiant feedback in our simulation. The Rapid Radiative Transfer Model (RRTM) scheme (Mlawer et al. 1997) is used to represent both short-wave and long-wave radiations. The Lin cloud microphysics scheme (Lin et al. 1983) is setup and Grell 3D ensemble cumulus parameterisation scheme (Grell and Dévényi 2002) is used.

The initial and boundary meteorological conditions for the WRF/Chem model have been obtained from the global NCEP-GFS (National Centers for Environmental Prediction Global Forecasting System) model with a resolution of 0.5° (NCEP 2015). These data are available to the scientific community and are often used in regional modelling processes. The chemical conditions of the lateral boundaries for mother domain were taken from prescribed profiles. The profile is based upon northern hemispheric, mid-latitude, clean environment conditions. The idealised profile is obtained from climatology with data based upon results from a NOAA-Aeronomy Laboratory Regional Oxidation Model (NALROM) (Liu et al. 1996).

One of the most important data for pollutant dispersion simulations is emissions. It is necessary to produce very detailed and high-quality emission data in order to know the amount of each pollutant that is injected into the atmosphere. In the case of urban simulations, road traffic emissions are

the most challenging to estimate as we need to have detailed information on traffic flows as vehicles are the main emitting sources in the city. In this work we have performed a traffic microsimulation with SUMO (Krajzewicz et al. 2012) that allows us to know the traffic flow intensities and vehicle speeds. Simulation of urban mobility (SUMO) is an open source software for the simulation of traffic flows continuously in space and discretely in time, with a maximum temporal resolution of 1 s. Each vehicle is explicitly simulated so that we know the vehicle's route through the network, departure time, arrival time, and its position every instant of time, so it is a microscopic traffic flow model. The speed of a vehicle through the network depends on the vehicles in front of it and the maximum speed of the network segment. Once the vehicles passing through each cell are known in detail for the calculation of the amount of emissions injected into that cell, we have coupled an emissions model which is detailed below.

In order to generate the routes followed by each car, it is necessary to know the destinations demanded by the vehicles and SUMO allows to generate these routes based on the data measured by the traffic detectors. The streets and roads of the simulation domain have been imported from OpenStreetMap (OSM) which, in addition to the location, contains characteristics about the streets (number of lanes, direction, roundabouts...) and traffic lights; all these data are used by SUMO for the simulation of road traffic. Some of the data, such as allowed turns, do not reflect reality, so a process of fine-tuning of the input data is required in order to achieve the most realistic simulation possible. The road and street network of Madrid consists of more than 100,000 streets and road segments. Through an iterative process, we have tried to ensure that no intersection represented an unrealistic bottleneck for traffic flows. This iterative process has been necessary to generate the road network that SUMO needs to provide realistic vehicle flow data for all streets in Madrid. For the simulation, first of all, random traffic is generated that travels through the Madrid network, and then road detectors have been used as calibrators, which are entering or removing cars to best simulate the traffic demand of the domain. In Madrid, there are more than 3000 vehicle detectors located on the streets and roads of Madrid and 2/3 of them have been used to calibrate the traffic simulations; the remaining 1/3 has been used to evaluate the performance of the simulation by comparing the traffic flow estimates from SUMO with that measured by the evaluation detectors. One of the main challenges of the traffic simulation has been to ensure a configuration that does not produce unrealistic traffic blockages and congestion. The calibration process is an iterative process in which the model configuration parameters are modified until the measured traffic flow values do not cause congestion in the traffic network.

In each simulation, by visual observation and counting vehicles in street segments, blockage areas are identified and the parameters of the streets involved are modified, a time-consuming task that we will try to automate in future work.

In such highly detailed simulations, it is necessary to have emission data, especially from traffic, at a high level of detail. Traffic emissions are calculated following the detailed methodology (Tier 3) described in the EMEP/EEA Air Pollution Emission Inventory Guidebook (EMEP/EEA 2016). In this methodology, specific emission factors are detailed for each vehicle category and are dependent on the ambient temperature, which can be derived from the mesoscale simulation. The following vehicle categories are considered: passenger cars, light commercial trucks, heavy duty vehicles including buses and motorbikes. These categories are further subdivided into new subcategories according to fuel type, vehicle weight, vehicle cubic capacity, and vehicle technology (associated with age). In the simulation, the percentage of each type of vehicle was

known based on the vehicle registration data for Madrid for December 2016, published by the Madrid City Council.

Experiment

The study urban area for this work is located in Madrid (Spain). The simulations are performed for the period June 12, to June 18, 2017, when high levels of ozone were observed. Figure 1 shows the 1 km×1 km area of interest for the CFD simulations. Roads, buildings and trees data were integrated to build a 3D CFD grid. In the area, there are two main roads with very high traffic flows and many street canyons. The area also experiences high pollution NO_x episodes during the winter time periods. One air quality monitoring station is located in the domain (red star of the Fig. 1). This station, called E. Aguirre is classified as traffic station. Part of one big park (Retiro Park) with a lot of trees is present in the south-west of the domain. The total area covered by trees represents 9.9% of the modelled area and the total area covered by buildings represents 43.9% of the modelled area, also the 1.4% of the area are water surface. The horizontal

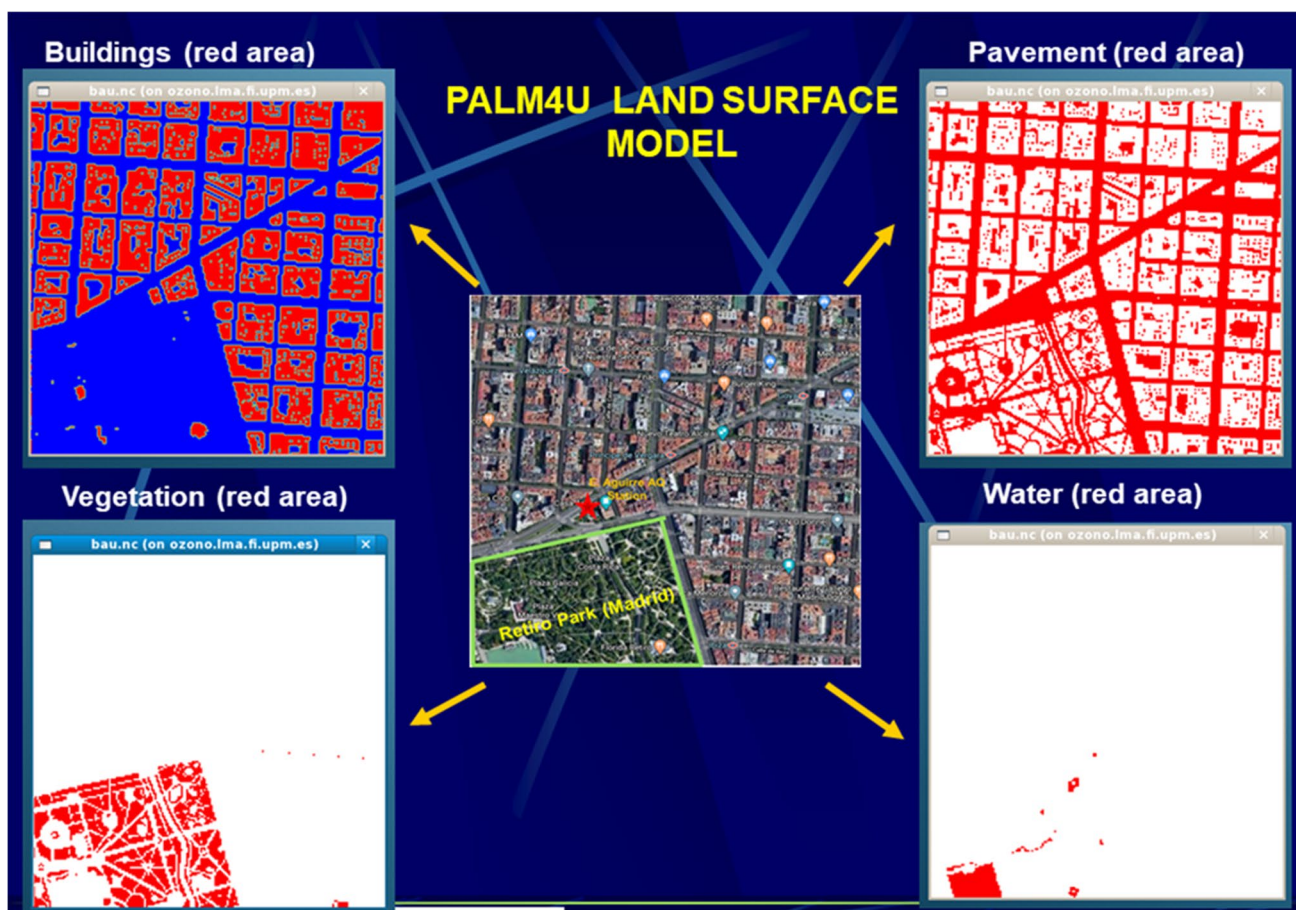


Fig. 1 Simulation area (1 km×1 km) around the E. Aguirre monitoring station (red start) in Madrid (Spain) with the four land surfaces: buildings, pavement, vegetation which includes a green area of the Retiro park and water

and vertical resolution of the 3D CFD grid is 5 m equally spaced. In height, 60 levels have been used, allowing us to reach a height of 300 m. This covers all the heights of the buildings in the area. In the area of the Retiro Park there are 1194 trees according to the inventory of the Madrid City Council. The predominant species is *Aesculus hippocastanum* known as European horse-chestnut. It is a species of tree of the type, broad-leaf.

Three scenarios have been simulated with the CFD PALM4U, a first reference simulation including all the information (broadleaf trees, 3D buildings, emissions, etc....) is called BAU (Business As Usual) scenario. A second scenario where we have removed the trees in the Retiro Park area and is called NOTREE simulation (without trees). The differences in the results of both simulations (BAU-NOTREE) will provide us information about the effect of the trees on the atmospheric composition of the area and thus advance in the research between the interaction between trees and the atmosphere in urban environments. Finally, in the third scenario called ND, we have completed a theoretical exercise to understand the impact on pollution in the area if the trees were all needle-leaf (ND scenario) instead of broad-leaf (BAU scenario), the differences BAU-ND will allow us to know the impact of the type of tree on the pollution. The described scenarios have been designed to analyse the influence of trees and tree type on pollution. Trees affect pollutant deposition, energy fluxes, and thermal conditions throughout the domain, as will be shown in the results. One of the objectives of the experiment is to show the high sensitivity of the modelling tool used, so that it may be seen that a simple change, such as a change in tree type or tree elimination, has important implications on the micrometeorology and thus on the urban air quality of the whole area, and that the tool is able to capture these changes.

To run the CFD domain, a multi-scale simulation has been designed to produce boundary conditions to the CFD simulation. First, a regional and urban simulation has been run with the WRF/Chem model covering the city of Madrid. The WRF/Chem modelling domains use a Lambert Conformal Projection centred at 40.478°N, 3.704°W with true latitudes of 30°N and 60°N. In the mesoscale simulation, 3 nested domains were set up. The mother domain is a horizontal spatial resolution of 25 km and covering the Iberian Peninsula. An intermediate domain with a resolution of 5 km covering the Madrid region. The final domain that provides data to the CFD simulation of 1 km is used to simulate the whole city of Madrid. All domains are centred on the city of Madrid and have dimensions of 45 × 45 grid cells horizontally. Vertically, 33 layers have been setup up to a height corresponding to a pressure of 50 hPa. The thickness of the layers close to the surface is lower than those located at higher altitudes. This domain configuration is tailored to the available computational resources and allows to simulate

the transport of pollutants on national, regional, and urban scales. The domains setup is a compromise between the computational resources available and the objectives of the study. The results of the 1 km WRF/Chem simulation is used as initial and boundary conditions for the CFD simulation. In order to perform a proper nesting between the mesoscale and the microscale model (LES), a synthetic turbulence generator has been used to generate turbulence in the CFD domain (Xie and Castro 2008; Kim et al. 2013). Unscaled turbulent motions are computed based on length scales along each direction and the amplitude tensor which in turn bases on the Reynolds stress tensor. The calculated turbulence is then added to the mean inflow data of the velocity components. The amplitude tensor depends on the Reynolds stress tensor; the required length and time scales, as well as the Reynolds stress tensor, are parametrised and the turbulence statistics at the inflow boundary are estimated; the derived turbulence statistics will depend on the height above ground but not on the horizontal location (Rotach et al. 1996). The turbulence is applied in the lateral conditions by imposing turbulent fluctuations on the boundary conditions wind data, and the amplitude of the turbulence depends on the atmospheric stability described by the WRF/Chem (mesoscale) simulation data. The PALM4U outputs in each time step are hourly time averaging.

Results

Performance analysis

Modelled results are initially compared with hourly observational data from the E. Aguirre monitoring station to evaluate the BAU simulation for O₃ and NO₂ pollutants. The model performance was analysed based on time series (Fig. 2) and statistical analysis was performed to help to determine the accuracy of the modelling results. The following statistical parameters have been calculated: Normalised mean bias (NMB); root mean square error (RMSE), and Pearson's temporal correlation (R₂). The R₂ was found to be 0.6 for NO₂ and 0.7 for O₃. The NMB values are –6% for NO₂ and –19% for O₃, and the negative values of NMB indicated an underestimation of the simulated concentration against the observational data. The resulting RMSE is below 30 µg/m³ for both pollutants. We can conclude that the BAU simulation for the NO₂ and O₃ dispersion with respect to the measured values in a specific point of the domain (5 m × 5 m where the monitoring station is located) is appropriate. It is important to highlight that the performance results of the CFD simulation is similar to the performance of the WRF/Chem simulation at 1 km spatial resolution as the surrounding concentrations have a strong influence on the local area concentrations.

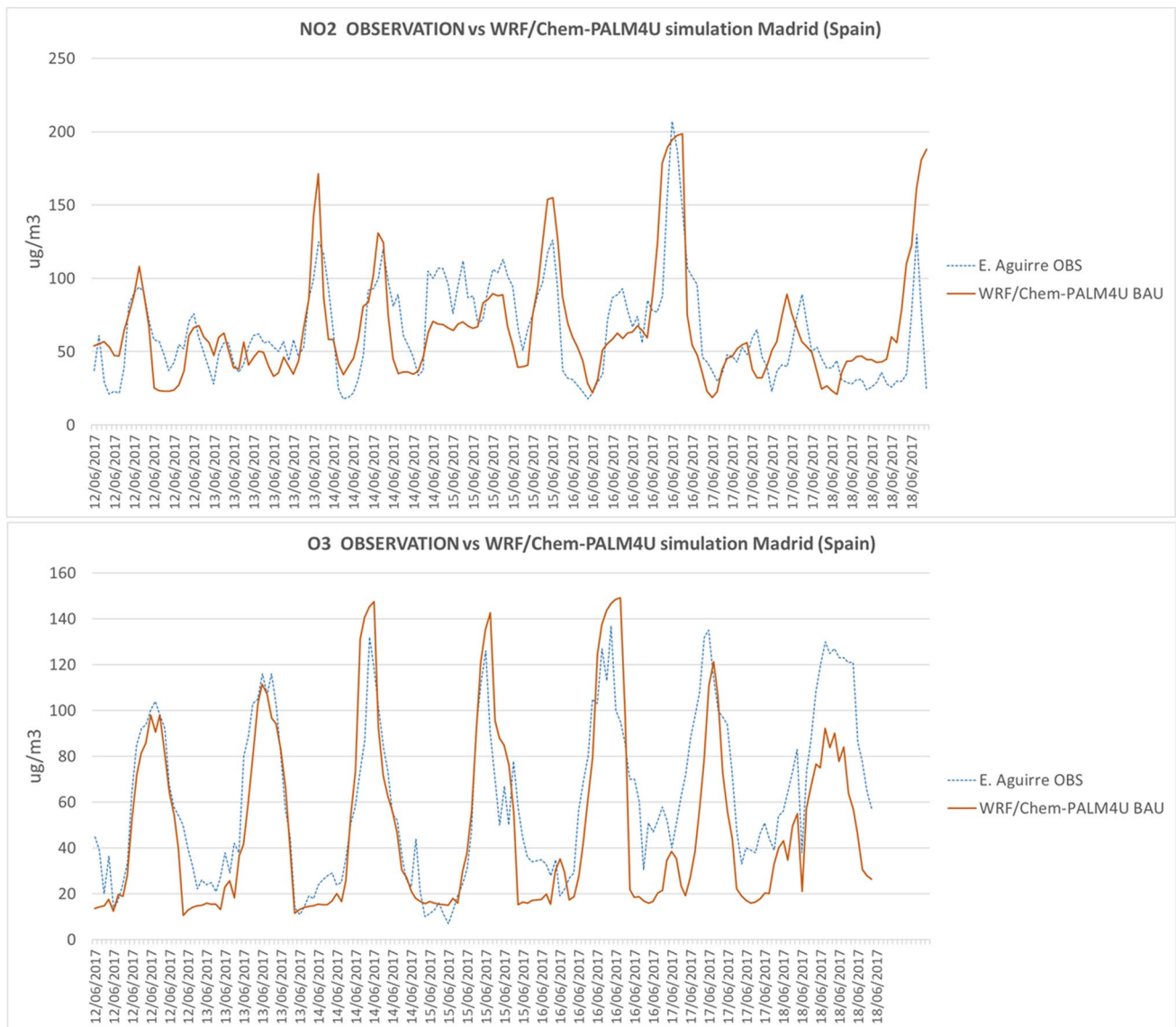


Fig. 2 Time series of observed and modelled NO₂ (top) and O₃ (bottom) concentrations

The evaluation of the simulation performance is limited, because in the current simulation domain there is only one monitoring station and due to computational limitations it has not been possible to extend the computational domain to include more monitoring stations. The authors are working on further studies to achieve a complete evaluation of the WRF/Chem-PALM4U modelling system. The aim of the current work is more focused on showing the sensitivity of the modelling system and presenting it as a possible tool for the evaluation of local strategies for pollution mitigation in cities. The calculated impact is based on the brute force method where the uncertainties are common in all simulations (BAU, ND, NOTREE).

The great variability of air pollution concentrations within a 1 km² zone can be seen in Fig. 3, as it shows the

spatial distribution of O₃ and NO₂ concentrations and wind vectors for the computational domain.

It can be seen how O₃ and NO₂ concentrations vary from one street to another, with the park area having the lowest NO₂ values (55 µg/m³) because there are no traffic emissions and the same area having the highest O₃ values (55 µg/m³). Some NO₂ hotspots (85 µg/m³) are observed in streets close to areas with high traffic density, where the gases emitted by road traffic are accumulated. Long wind arrows can be seen in the upper right-hand side, indicating that the area is highly turbulent due to the layout of the buildings. These maps show the real situation of the modelled area.

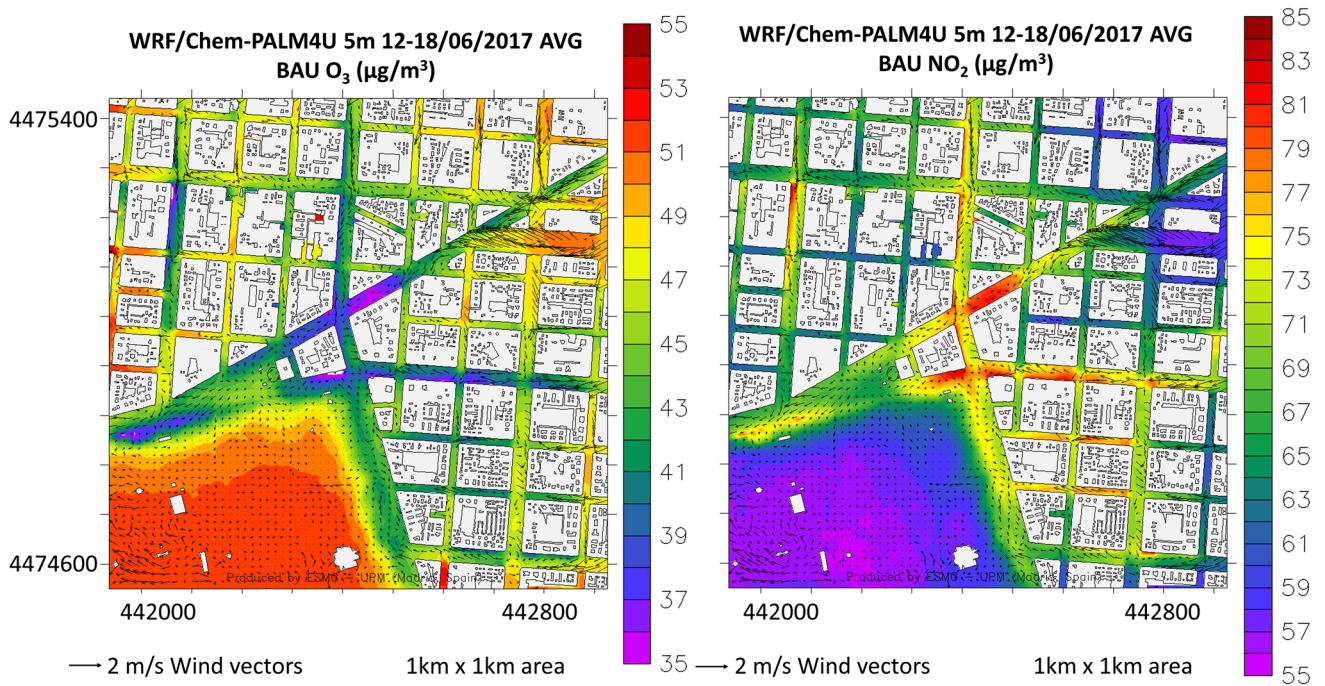


Fig. 3 High-resolution maps of O₃ (left) and NO₂ (right) hourly concentration and wind fields averaged over simulation period 12–18/06/2017 produced by the WRF/Chem-PALM4U 5 m simulation over 1 km by 1 km area of Madrid

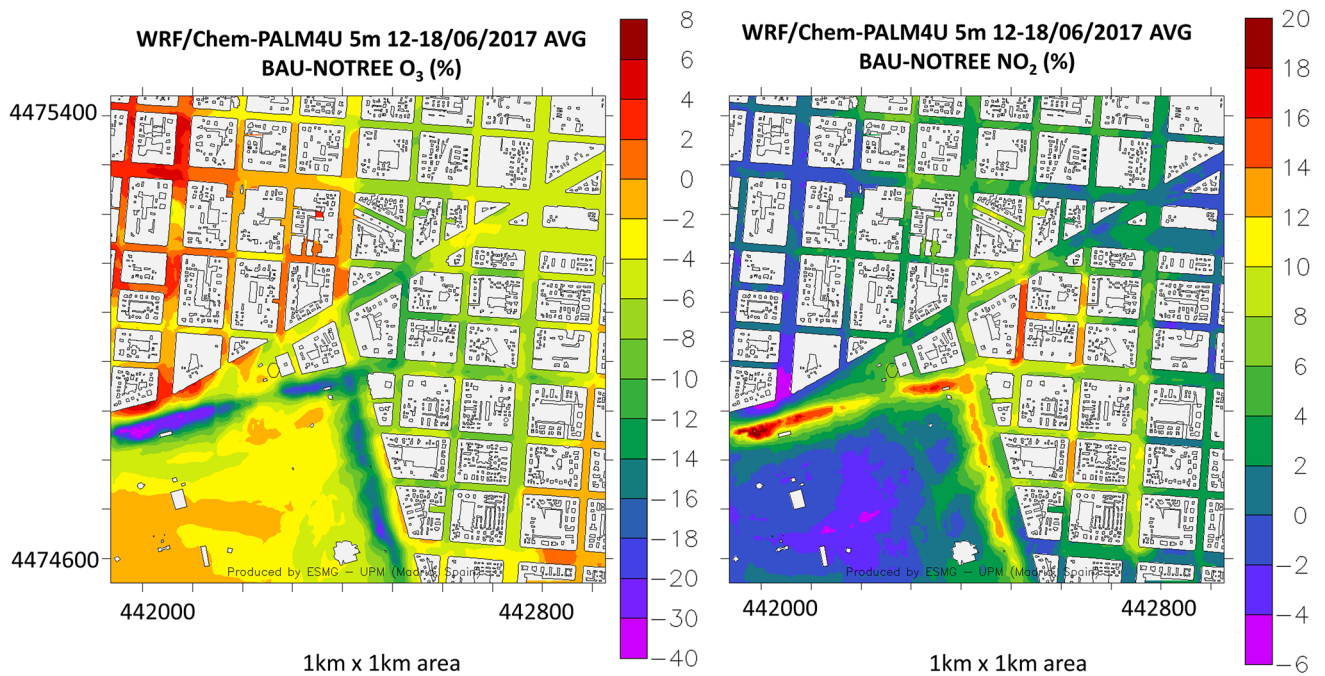


Fig. 4 Spatial distribution with 5 m spatial resolution of the effects of trees (BAU-NOTREE %) on O₃ and NO₂ hourly averaged concentrations for the period 12–18/06/2017

Impact analysis

Once validated, the BAU, NOTREE, and ND simulations are used to evaluate the effects of trees and type of trees on concentration levels of O₃ and NO₂ concentrations. Figure 4 shows the changes in NO₂ and O₃ concentrations (%) if the trees were removed from the green area (down-left). In the figure, we can see that in the streets around the green zone, the trees are increasing the NO₂ concentrations up to 20%; these increases were also seen in other narrow streets further away from the green zone. The increases in NO₂ next to the park due to the presence of trees cause large decreases in O₃ concentrations of up to 40%. In general, the presence of trees decreases the temperature of the area and reduces the O₃ concentrations; the trees decrease the concentration in 86.62% of the grid cells, with an average reduction of 4.84%, but increase the NO₂ concentrations in 70.97% of the cells, with average increases of 4.76% as the presence of the trees hinders the ventilation in the area close to the green area.

Figure 5 shows the spatial distribution of changes (BAU-ND %) in O₃ and NO₂ concentrations when changing from broad-leaf trees in the green zone to needle-leaf trees. The trees change the distribution of O₃ and NO₂ concentrations, particularly on some hotspots. The effects of type of trees (Fig. 5) are quite heterogeneous leading to decreases or increases of O₃ and NO₂ concentrations at pedestrian height.

Changing the tree type from broad-leaf to needle-leaf involves changing the minimum canopy resistance parameter (Rc_min) in Eq. 1. For broad-leaf trees (BAU), Rc_min has a value of 240 s/m and for needle-leaf trees (ND) the value changes to 500 s/m. This is the main parameter that changes from one simulation to another. Then in the ND simulation in the cells with trees, the canopy resistance (rc) is higher and therefore the latent heat flux (LE) is lower when calculated with Eq. 2 which causes an increase in temperature. This temperature increase causes O₃ concentrations to increase in 64.22% of the cells with an average increase of 1.93% and NO₂ concentrations to decrease in 90.67% of the grid cells with an average decrease of 1.69%.

$$Rc = \frac{Rc_min}{LAI} f1(R) f2(Hm) f3(e) \tag{1}$$

$$L = -\rho l_v \frac{1}{ra + rc} (q_v - q_{v,sat}) \tag{2}$$

- Rc Canopy resistance
- LAI Leaf are index
- f2 Corrector factor based on soil humidity

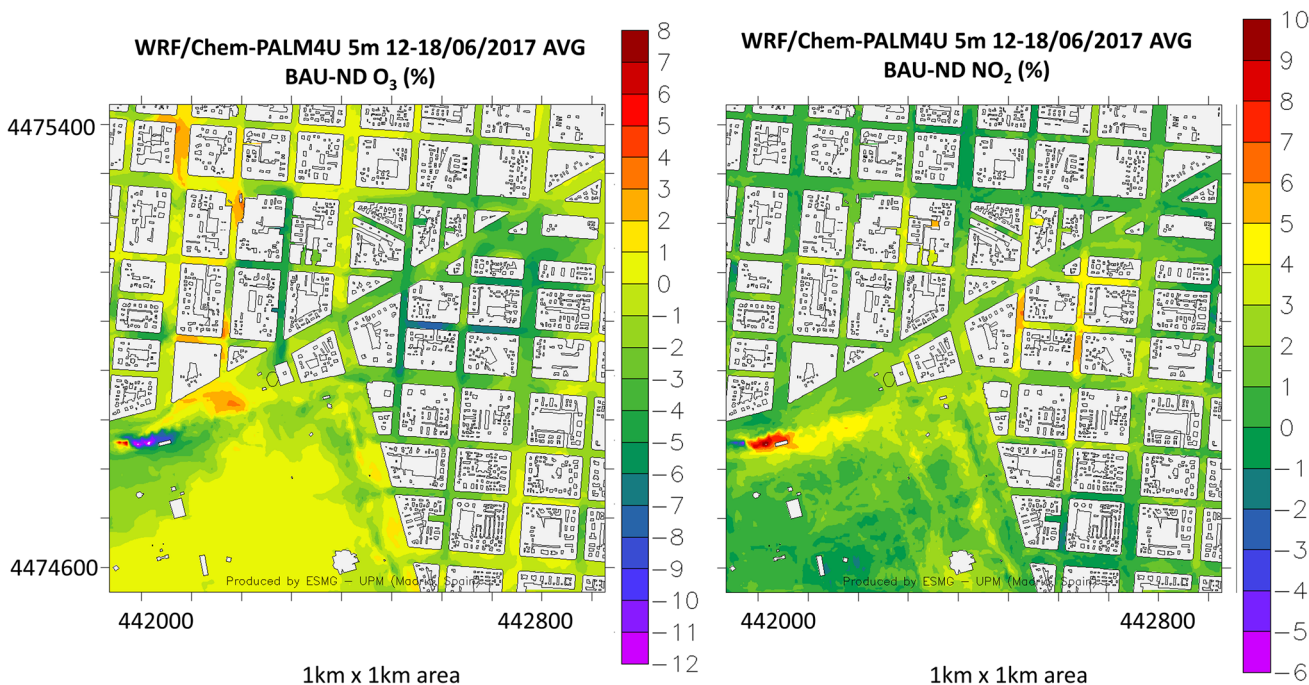


Fig. 5 Spatial distribution with 5 m spatial resolution of the effects of type of trees (BAU-ND %) on O₃ and NO₂ hourly averaged concentrations for the period 12–18/06/2017

L	Latent heat flux
Lv	Latent heat of vapourisation
Ra	Aerodynamic resistance
Rc	Canopy resistance for vegetation
qv,sat	Water vapor mixing ratio at temperature T0
Rc_min	Minimum canopy resistance
f1	Corrector factor based on solar radiation
f3	Corrector factor based on water-vapour pressure deficit
ρ	Air density. ρ : Air density
qv	Water vapour mixing ratio

Conclusions

An integrated urban air quality modelling system has been implemented. The tool includes an emission model (EMIMO), a traffic model SUMO, a pollutant transport, chemistry model (WRF/Chem), and the chemistry model CFD PALM4U (LES mode). The PALM4U 5 m simulation reproduces pollutant dispersion in the presence of boundary and top conditions supplied by the WRF/Chem 1 km simulation, real building morphology, vegetation, and hourly emissions. The results obtained allow us to confirm that the modelling tool (WRF/Chem-PALM4U) presented is capable to reproduce successfully the distribution of the concentration of pollutants over urban areas; based on the performance analysis in the location of the available monitoring station, a full evaluation performance analysis with many stations is needed to confirm the accurate of the results in other points of the city. An experiment has been ran to analyse the effects of trees and type of trees on air pollution. Three simulations were run, with broad-leaf trees (BAU), without trees (NOTREE), and with needle-leaf trees (ND) (changing the type of tree over a green area) in a 1 km \times 1 km area.

Results show that the effects of urban vegetation on local air quality may be very complex and have a substantial impact in local and potentially large urban areas. The trees can either decrease or increase NO₂ and O₃ concentrations over the 1 km \times 1 km domain with different impacts each day. On streets close to the green area, we found that trees can increase NO₂ concentrations by up to 20% and reduce O₃ concentrations by 30%. However, on the green area, trees can reduce NO₂ concentrations

by 5% with modest increments of O₃ of up to 2%. We found that needle-leaf trees can decrease NO₂ concentrations and increase O₃ concentrations. Trees in general and needle-leaf trees reduce latent heat flux (Rc bigger than broad-leaf trees) and increase sensible, ground heat flux, and temperature, favouring O₃ formation. The results are agreeing with other studies where deposition velocities were higher on needles than on broadleaves (Hwang et al. 2011) and that trees considerably affected the accumulation of transported pollutants (Salmond et al. 2013). The results are aligned with the conclusions found in (Vos et al. 2013); the effect of trees in air pollution is a complex issue in the real life, and trees can increment the pollution by the aerodynamic effects. To clarify, the conclusion of the study does not propose tree cutting to improve air quality in cities, trees, and vegetation since, in general terms, they have many other effects that improved/deteriorated air quality, i.e., comfort of life, noise are important parameters to take into account.

The modelling tool applied over a real 3D urban topography may provide a large amount of detailed information with high-resolution about the flow concentration fields and heat fluxes. This work demonstrates how these type of numerical simulation tools may generate information about potential mitigation actions on a scale of metres and obtaining information on their effectiveness.

Acknowledgements The UPM authors thankfully acknowledge the computer resources, technical expertise, and assistance provided by the Centro de Supercomputación y Visualización de Madrid (CESVIMA). The UPM authors thankfully acknowledge the computer resources, technical expertise, and assistance provided by the Red Española de Supercomputación.

Author contribution Both authors contributed to the study conception and design. Material preparation, data collection, and simulation were performed by Juan L. Perez. Analysis and supervision were performed by Roberto San Jose. The first draft of the manuscript was written by Juan L. Perez and both authors commented on previous versions of the manuscript. Both authors read and approved the final manuscript.

Funding Open Access funding provided thanks to the CRUE-CSIC agreement with Springer Nature.

Data availability The datasets generated during and/or analysis during the current study are not publicly available due to high volume of data but are available from the corresponding author on a reasonable request.

Declarations

Ethics approval Not applicable.

Consent to participate Not applicable.

Consent to publish Not applicable.

Competing interests The authors declare no competing interests.

Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit <http://creativecommons.org/licenses/by/4.0/>.

References

- Abhijith K, Kumar P, Gallagher J, McNabola A, Baldauf R, Pilla F et al (2017) Air pollution abatement performances of green infrastructure in open road and built-up street canyon environments – a review. *Atmos Environ* 162:71–86. <https://doi.org/10.1016/j.atmosenv.2017.05.014>
- Bae M, Kim B, Kim H, Kim S (2020) A multiscale tiered approach to quantify contributions: a case study of PM_{2.5} in South Korea During 2010–2017. *Atmosphere* 11(2):141. <https://doi.org/10.3390/atmos11020141>
- Baik J, Kim J (2002) On the escape of pollutants from urban street canyons. *Atmos Environ* 36(3):527–536. [https://doi.org/10.1016/s1352-2310\(01\)00438-1](https://doi.org/10.1016/s1352-2310(01)00438-1)
- Beever S, Kitwiroon N, Williams M, Carslaw D (2012) One way coupling of CMAQ and a road source dispersion model for fine scale air pollution predictions. *Atmos Environ* 59:47–58. <https://doi.org/10.1016/j.atmosenv.2012.05.034>
- Binkowski F, Shankar U (1995) The regional particulate matter model: 1. Model description and preliminary results. *J Geophys Res* 100(D12):26191. <https://doi.org/10.1029/95jd02093>
- Buccolieri R, Jeanjean A, Gatto E, Leigh R (2018) The impact of trees on street ventilation, NO_x and PM_{2.5} concentrations across heights in Marylebone Rd street canyon, central London. *Sustain Cities Soc* 41:227–241. <https://doi.org/10.1016/j.scs.2018.05.030>
- Caplin A, Ghandehari M, Lim C, Glimcher P, Thurston G (2019) Advancing environmental exposure assessment science to benefit society. *Nat Commun* 10:1236. <https://doi.org/10.1038/s41467-019-09155-4>
- Choudhary H, Tarlo S (2014) Airway effects of traffic-related air pollution on outdoor workers. *Curr Opin Allergy Clin Immunol* 14(2):106–112. <https://doi.org/10.1097/aci.0000000000000038>
- Dupont S, Brunet Y (2009) Coherent structures in canopy edge flow: a large-eddy simulation study. *J Fluid Mech* 630:93–128. <https://doi.org/10.1017/s0022112009006739>
- Easter R (2004) MIRAGE: Model description and evaluation of aerosols and trace gases. *J Geophys Res* 109(D20). <https://doi.org/10.1029/2004jd004571>
- Ehrhard J, Khatib I, Winkler C, Kunz R, Moussiopoulos N, Ernst G (2000) The microscale model MIMO: development and assessment. *J Wind Eng Indust Aerodyn* 85(2):163–176. [https://doi.org/10.1016/s0167-6105\(99\)00137-3](https://doi.org/10.1016/s0167-6105(99)00137-3)
- EMEP/EEA air pollutant emission inventory guidebook (2016) Technical guidance to prepare national emission inventories. EEA Report No 21/2016. Publications Office of the European Union, Luxembourg. <https://www.eea.europa.eu/publications/emep-eea-guidebook-2016>, <https://doi.org/10.2800/247535>
- Fast JD, Gustafson WI, Easter RC, Zaveri RA, Barnard JC, Chapman EG, Grell GA, Peckham SE (2006) Evolution of ozone, particulates, and aerosol direct radiative forcing in the vicinity of Houston using a fully coupled meteorology-chemistry-aerosol model. *J Geophys Res* 111:D21305. <https://doi.org/10.1029/2005JD006721>
- Gery M, Whitten G, Killus J, Dodge M (1989) A photochemical kinetics mechanism for urban and regional scale computer modeling. *J Geophys Res* 94(D10):12925. <https://doi.org/10.1029/jd094id10p12925>
- Grell G, Dévényi D (2002) A generalized approach to parameterizing convection combining ensemble and data assimilation techniques. *Geophys Res Letters* 29(14):38–1. <https://doi.org/10.1029/2002gl015311>
- Grell G, Peckham S, Schmitz R, McKeen S, Frost G, Skamarock W, Eder B (2005) Fully coupled “online” chemistry within the WRF model. *Atmos Environ* 39(37):6957–6975. <https://doi.org/10.1016/j.atmosenv.2005.04.027>
- Hwang H, Yook S, Ahn K (2011) Experimental investigation of sub-micron and ultrafine soot particle removal by tree leaves. *Atmos Environ* 45(38):6987–6994. <https://doi.org/10.1016/j.atmosenv.2011.09.019>
- Kadaverugu R, Sharma A, Matli C, Biniwale R (2019) High resolution urban air quality modeling by coupling cfd and mesoscale models: a review. *Asia-Pac J Atmos Sci* 55(4):539–556. <https://doi.org/10.1007/s13143-019-00110-3>
- Kwak K, Baik J, Ryu Y, Lee S (2015) Urban air quality simulation in a high-rise building area using a CFD model coupled with mesoscale meteorological and chemistry-transport models. *Atmos Environ* 100:167–177. <https://doi.org/10.1016/j.atmosenv.2014.10.059>
- Miao Y, Liu S, Chen B et al (2013) Simulating urban flow and dispersion in Beijing by coupling a CFD model with the WRF model. *Adv Atmos Sci* 30:1663–1678. <https://doi.org/10.1007/s00376-013-2234-9>
- Michioka T, Sato A, Sada K (2013) Large-eddy simulation coupled to mesoscale meteorological model for gas dispersion in an urban district. *Atmos Environ* 75:153–162. <https://doi.org/10.1016/j.atmosenv.2013.04.017>
- Krajzewicz D, Erdmann J, Behrisch M, Bieker L (2012) Recent development and applications of SUMO - simulation of urban mobility. *Int J Adv Syst Measure* 5(3&4):128–138
- Kim Y, Castro I, Xie Z (2013) Divergence-free turbulence inflow conditions for large-eddy simulations with incompressible flow solvers. *Comput Amp; Fluids* 84:56–68. <https://doi.org/10.1016/j.compfluid.2013.06.001>
- Lin Y, Farley R, Orville H (1983) Bulk parameterization of the snow field in a cloud model. *J Clim Appl Meteorol* 22(6):1065–1092. [https://doi.org/10.1175/1520-0450\(1983\)022%3c1065:bpotsf%3e2.0.co;2](https://doi.org/10.1175/1520-0450(1983)022%3c1065:bpotsf%3e2.0.co;2)
- Liu S, McKeen S, Hsie E, Lin X, Kelly K, Bradshaw J et al (1996) Model study of tropospheric trace species distributions during PEM-West A. *J Geophys Res: Atmos* 101(D1):2073–2085. <https://doi.org/10.1029/95jd02277>
- Maronga B, Gryscha M, Heinze R, Hoffmann F, Kanani-Sühring F, Keck M et al (2015) The parallelized large-eddy simulation model (PALM) version 4.0 for atmospheric and oceanic flows: model formulation, recent developments, and future perspectives. *Geosci Model Dev* 8(8):2515–2551. <https://doi.org/10.5194/gmd-8-2515-2015>
- Mlawer E, Taubman S, Brown P, Iacono M, Clough S (1997) Radiative transfer for inhomogeneous atmospheres: RRTM, a validated correlated-k model for the longwave. *J Geophys Res: Atmos* 102(D14):16663–16682. <https://doi.org/10.1029/97jd00237>
- NCEP National Centers for Environmental Prediction, (2015). NCEP GFS 0.25 degree global fore-cast grids historical archive. National Center for Atmospheric Research, Computational and Information Systems Laboratory, accessed 16 August 2019, <https://doi.org/10.5065/D65D8PWK>

- Nelson M, Brown M, Halverson S, Bieringer P, Annunzio A, Bieberbach G, Meech S (2016) A case study of the weather research and forecasting model applied to the Joint Urban 2003 Tracer Field Experiment. Part 2: Gas Tracer Dispersion. *Boundary Layer Meteorol* 161(3):461–490. <https://doi.org/10.1007/s10546-016-0188-z>
- Park S, Baik J, Lee S (2015) Impacts of mesoscale wind on turbulent flow and ventilation in a densely built-up urban Area. *J Appl Meteorol Climatol* 54(4):811–824. <https://doi.org/10.1175/jamc-d-14-0044.1>
- Pope C, Dockery D (2006) Health effects of fine particulate air pollution: lines that connect. *J Air Waste Manag Assoc* 56(6):709–742. <https://doi.org/10.1080/10473289.2006.10464485>
- Pugh T, MacKenzie A, Whyatt J, Hewitt C (2012) Effectiveness of green infrastructure for improvement of air quality in urban street canyons. *Environ Sci Technol* 46(14):7692–7699. <https://doi.org/10.1021/es300826w>
- Rotach M, Gryning S, Tassone C (1996) A two-dimensional Lagrangian stochastic dispersion model for daytime conditions. *Q J R Meteorol Soc* 122(530):367–389. <https://doi.org/10.1002/qj.49712253004>
- Salmond J, Williams D, Laing G, Kingham S, Dirks K, Longley I, Henshaw G (2013) The influence of vegetation on the horizontal and vertical distribution of pollutants in a street canyon. *Sci Total Environ* 443:287–298. <https://doi.org/10.1016/j.scitotenv.2012.10.101>
- San José R, Pérez J, Balzarini A, Baró R, Curci G, Forkel R et al (2015) Sensitivity of feedback effects in CBMZ/MOSAIC chemical mechanism. *Atmos Environ* 115:646–656. <https://doi.org/10.1016/j.atmosenv.2015.04.030>
- San José R, Pérez J, Gonzalez-Barras R (2021) Assessment of mesoscale and microscale simulations of a NO₂ episode supported by traffic modelling at microscopic level. *Sci Total Environ* 752:141992. <https://doi.org/10.1016/j.scitotenv.2020.141992>
- Van Zanten MC et al (2010): Description of the DEPAC module. Dry deposition modelling with DEPAC_GCN2010, RIVM report 680180001/2010, Bilthoven, The Netherlands, 74
- Vos P, Maiheu B, Vankerkom J, Janssen S (2013) Improving local air quality in cities: To tree or not to tree? *Environ Pollut* 183:113–122. <https://doi.org/10.1016/j.envpol.2012.10.021>
- Wang K, Shallcross D (2000) A modelling study of tropospheric distributions of the trace gases CFCl. *Ann Geophys* 18(8):0972. <https://doi.org/10.1007/s005850050013>
- Williams J, Landgraf J, Bregman A, Walter H (2006) A modified band approach for the accurate calculation of online photolysis rates in stratospheric-tropospheric Chemical Transport Models. *Atmos Chem Phys* 6(12):4137–4161. <https://doi.org/10.5194/acp-6-4137-2006>
- Xie Z, Castro I (2008) Efficient generation of inflow conditions for large eddy simulation of street-scale flows. *Flow, Turbulence and Combustion* 81(3):449–470. <https://doi.org/10.1007/s10494-008-9151-5>
- Zaveri R, Peters L (1999) A new lumped structure photochemical mechanism for large-scale applications. *J Geophys Res: Atmos* 104(D23):30387–30415. <https://doi.org/10.1029/1999jd900876>
- Zaveri RA, Easter RC, Fast JD, Peters LK (2008) Model for simulating aerosol interactions and chemistry (MOSAIC). *J Geophys Res* 113:D13204. <https://doi.org/10.1029/2007JD008782>

Publisher's note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.