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A multiscale air quality and health risk modelling system: Design and application over a local traffic management case study

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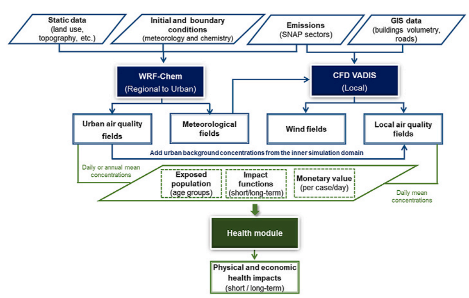
HIGHLIGHTS

- The developed modair4health modelling system is presented.
- It is able to simulate air quality and health impacts on multiple scales.
- The urban structure has a key role in flow variations and pollutant dispersion.
- Greater traffic scenario benefits are expected in areas and periods with higher NO_2.
- Integrated assessment tool to effectively support air pollution control policies.

GRAPHICAL ABSTRACT



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ABSTRACT

Air pollution is nowadays a serious public health problem worldwide, especially in urban areas, due to high population density and intense anthropogenic activity. This paper aims to present the development of a modelling tool suitable for simulating multiscale air quality and health impacts - the modair4health system, and its application to an urban case study. The modair4health system includes the online model WRF-Chem, which provides meteorological and air quality fields from regional to urban scales, and the computational fluid dynamics model VADIS, which uses the urban WRF-Chem outputs to simulate the flow and pollutant dispersion in urban built-up areas. A health module based on World Health Organization (WHO) methodologies was also integrated into the system to quantify physical and economic health impacts resulting from air quality changes.

The system was applied over a local case study, which represents one of the busiest road traffic areas of the city of Coimbra in Portugal, to assess its operationality in estimating NO_2 concentrations and health impacts, by testing two traffic management scenarios. This scenario analysis considered a 4-domain nesting approach, with the finer resolution (4 m) domain focusing on the local case study and on two simulation periods, for which short-term health impacts were estimated. Spatially, the air quality and health greatest benefits were simulated around roads, where higher emission reductions were estimated, but they were also strongly influenced by the urban structure, local weather and population affected.

The modair4health system has revealed to be an important multiscale modelling tool for integrated air quality and health assessment, able to support decision makers by facilitating the choice of cost-effective air quality and health management strategies and decisions. Moreover, its user-friendly interface allows to quickly test other

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urban air pollution control policies and the easy adaptation and application to other case studies considering regional to local atmospheric influences.

1. Introduction

The exponential population growth over the last decades, and the consequent non-sustainable intensification of the human activity, have contributed to the worsening of air pollution and its impacts on public health and the environment. From the point of view of the main pollution hotspots, particular attention should be attributed to urban areas, because more than half of the world's population lives there, and normally a dense network of emission sources is present, namely transports, industry and households (Miranda et al., 2015). However, the causes of air pollution must be analysed beyond the urban/local scales, as air pollutants are often transported across continents and ocean basins (APPRAISAL, 2013; Ramanathan and Feng, 2009; Thunis et al., 2016). Thereby, the option for emerging modelling tools as a complement to monitored data allows a more comprehensive air quality assessment, as the way monitoring networks are designed (i.e., spatial representativeness) may lead to an unbalanced checking of compliance with the air quality standards and biased population exposure assessments, given their restricted geographic and temporal coverage (Duyzer et al., 2015; WHO, 2016). For these reasons, the use of models is encouraged through environmental regulations to cover multiple scales with the following purposes:

(i) to analyse the relative importance of the main emitting sources;
(ii) to understand atmospheric and demographic dynamics that allow relating air concentrations with human exposure;
(iii) to assess health impacts resulting from short and long-term exposure to air pollutants;
(iv) to accomplish legal impositions for air quality improvement at the European Union (EU) level, in particular, those related to air pollution management strategies for the zones/agglomerations where air quality standards are exceeded.

This assessment involves the application of different types of air quality models depending on the objectives, dimension of study domains and intended resolutions. For this purpose, mesoscale and microscale models have been developed and applied, although in most cases following distinct approaches. Hence, the relationship between models, simulation domains and resolutions remains a challenging research issue (Silveira et al., 2019; Sokhi et al., 2022).

In a typical urban atmosphere, the complexity of the urban structure (e.g. buildings volumetry, road network) has a relevant role in the physical and chemical processes governing the transport, dispersion, transformation and deposition of air pollutants (Chen et al., 2011; Russo and Soares, 2014; Srivastava and Rao, 2011; Tang and Wang, 2007; Vardoulakis et al., 2003). Thus, applying air quality models at local/urban scale requires these small-scale processes to be explicitly well resolved, but also to take into account the influence of a larger scale, as the dispersion and atmospheric chemistry contribute to variations in polluted air arriving to a region from other regions and/or countries (Appraisal, 2013). However, the background and time-dependent boundary conditions provided by mesoscale modelling (i.e. physical and chemical fields), are often greatly simplified, mostly due to the nature of mesoscale-coupled urban schemes (Baklanov and Nuterman, 2009; Beevers et al., 2012; Kwak et al., 2015; Mensink et al., 2003). This is a key research area, as the proper link between mesoscale and local scale models, as well as the identification of the best parametrizations and input data, are essential requirements to decrease the uncertainties in urban-to-local modelling applications.

Another current and important challenge is to fully integrate health impacts within the air quality modelling system, moving from air pollutant levels to health indicators, and thus getting closer to the society needs (Brandt et al., 2013; Miranda et al., 2016; Pervin et al., 2008). Health impacts are highlighted by public health experts, who are aware of the impacts of air pollution in worsening morbidity (especially respiratory and cardiovascular diseases) and premature mortality (e.g., years of life lost). To quantify the extent of these adverse effects on different age groups, approaches combining air concentrations, population data, and concentration/exposure-response functions (CRF) based on epidemiological studies, have been used (Holland et al., 2005; WHO, 2013). The resulting health impacts are often converted in monetary values, allowing a cost-benefit analysis of policy options considered for air quality management (Pervin et al., 2008; Relvas et al., 2017; Silveira et al., 2016).

Based on this air quality-health framework and identified research gaps and challenges, the objective of this work is to present the modair4health modelling system, which was developed for the integrated assessment of multiscale air quality and health impacts, and to describe its application to a particular urban case study. To tackle this objective, the following activities were accomplished:

(i) an urban air pollution modelling system able to simulate atmospheric concentrations from urban to local scales was developed; this modelling system is able to bridge the gaps when crossing different scales;
(ii) the quantifiable human health effects were integrated within the multiscale air pollution modelling system;
(iii) the system was applied with high spatial and temporal resolutions and assessed for the identification of additional appropriate configurations and input data;
(iv) based on the developed modelling system capabilities, and on the analysis of different air quality management strategies and their potential health benefits, recommendations were provided for local emission reduction measures or joint pollution control with neighbouring urban areas.

The paper is organized as follows. Section 2 presents a description of the modair4health system concerning the air quality and health models used and the links among them, required input data and key simulation outputs, which are also used to feed the chain of models. In Section 3, the modelling system is applied over a local case study using the best parametrizations and previously tested input datasets to evaluate air quality management scenarios. Lastly, the main conclusions are presented in Section 4.

2. The modair4health system

The core of the modair4health multiscale air quality and health risk modelling system is composed of two air quality models, able to simulate atmospheric concentrations from regional/urban scales (WRF-Chem) to the local scale (VADIS), and a health module for estimating health impacts and damage costs caused by short and long-term human exposure to air pollutants (Fig. 1).

Details on the adopted models, recommended configurations, input data processing, and linking as a whole are presented in the following sections.

2.1. Air quality modelling

The selection and setup of air quality models to be integrated in the system was duly weighted through a critical analysis of the state-of-the-art (Silveira et al., 2019), and the performance evaluation of modelling tests aimed at finding the best parametrizations and input datasets. These tests were primarily focused on WRF-Chem applications, dictating key aspects to consider in the reference simulations, namely, including the atmospheric aerosol effect and a detailed land cover database (Silveira et al., 2021, 2022). For the VADIS simulations, different seasonal traffic emission profiles were tested.

2.1.1. WRF-Chem

For air quality modelling from regional to urban scales, the Weather Research and Forecasting model with Chemistry (WRF-Chem) was chosen, on one hand, because it is an online integrated model that allows the simultaneous calculation and consequent feedback between meteorological and chemical variables sharing the same simulation grids, physical parametrizations, transport schemes and vertical mixing; on the other hand, due its performance, as it has specific parametrizations for simulating air quality and meteorological fields at urban scale (Chen et al., 2011; Fast et al., 2006; Grell et al., 2005). WRF-Chem physical options include, for example, different schemes of microphysics, radiation, cumulus, and land surface and planetary boundary-layer representations. With regard to the chemistry, the model enables several configurations for integrating anthropogenic and biogenic emissions, and includes a set of gas-phase chemical mechanisms (e.g., RADM2, RACM, CBM-Z) and aerosol schemes (e.g., MADE/SORGAM, MOSAIC, GOCART), which can be combined using different photolysis options. The aerosol interaction with the atmospheric radiation, photolysis and microphysics routines can be tested through aerosol direct or indirect effects. As main inputs to run WRF-Chem, the following datasets are required and processed as follows:

- *Surface static data*

Within this category, a set of physical and vegetation parameters that characterize Earth's surface dynamics are included, such as topography, land cover (LC), soil type and erodibility, vegetation fraction, albedo, etc. These ready-to-use static fields can be downloaded from the WRF users webpage (NCAR, n.d.). Nevertheless, if more detailed and recent information is available, efforts to prepare these data to the required format are recommended. In that sense, after a preliminary analysis of the role, magnitude and spatial distribution of these static fields and their comparison to existing databases, it was chosen to improve the LC classification to be inputted to WRF-Chem, as it is a prevailing driver of important physical and chemical interactions within the atmospheric boundary layer, directly influencing the Earth's energy budget, and emission and deposition rates of air pollutants (Jiménez-Esteve et al., 2018; Wu et al., 2012; Xu et al., 2016). LC processing steps and its influence on air quality are presented in Silveira et al. (2018, 2022).

- *Meteorological reanalysis data*

Meteorological reanalyses are conducted from data assimilation systems using observations for model initialization and to recreate the lateral boundary conditions. These data can be retrieved from various web platforms, such as ERA-Interim (ECMWF, n.d.), NCEP/NCAR (NOAA, n.d.) and CAMS (ECMWF, n.d.). For each simulation domain, the required fields are regridded and prepared as meteorological variable through the WRF Preprocessing System (available within the WRF-Chem package).

- *Chemical boundary conditions*

Chemical lateral boundary conditions are needed to account for the influence of the transboundary transport of air pollutants, and are particularly relevant for predicting longer-lived species, as ozone and carbon monoxide (Pendlebury et al., 2018; Tang et al., 2007). These time-variant chemical conditions are extracted from the global Model for OZone And Related chemical Tracers (MOZART-4/GEOS-5) and updated every 6 h with 1.9° × 2.5° horizontal resolution and 56 vertical levels using the WRF-Chem preprocessing tool mozbc (NCAR, n.d.).

- *Atmospheric emissions from anthropogenic and natural sources*

Anthropogenic emissions from the European Monitoring and Evaluation Programme (EMEP) database with a 0.1° × 0.1° horizontal resolution were used (EMEP, n.d.). This annual emission inventory (EI) is available by Gridding Nomenclature For Reporting (GNFR) including estimated emissions of classic air pollutants (e.g., NO_2, particulate matter), heavy metals and persistent organic pollutants for key activity sectors (e.g., road transport, industry). The spatial and temporal allocation of emissions to the simulation grids based on the LC, vertical distribution and application of default time profiles by activity sector, considering the seasonality, day of week and daily cycle, as well as speciation and aggregation into WRF-Chem species, are performed using the emissions interface built by Tuccella et al. (2012). In turn, biogenic, sea-salt and dust emissions are calculated online by activating WRF-Chem-coupled specific modules and preprocessing tools that create initialization fields. For computing biogenic emissions, the MEGAN (The Model of Gases and Aerosols from Nature - version 2.04) module is initialized with monthly leaf area index data, fraction by plant functional type and emission factors prepared from the bio_emiss utility (NCAR, n.d.). Further information about this MEGAN model version is

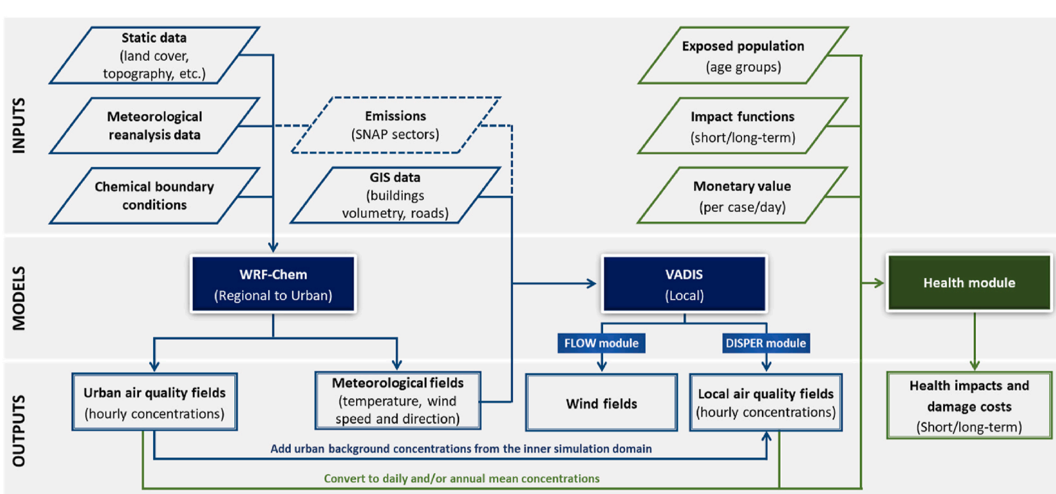


Fig. 1. Architecture of the modair4health system.

provided by Guenther et al. (2006).

2.1.2. VADIS

The downscaling to the local scale is done through the Computational Fluid Dynamics (CFD) model VADIS (pollutant DISpersion in the atmosphere under VAriable wind conditions), taking advantage of its numerical prediction capabilities and using much higher spatial resolutions to accurately reproduce turbulent flows (FLOW) and pollutant dispersion (DISPER) within the urban structure. The FLOW module is based on an Eulerian approximation for solving the Navier-Stokes equations at the atmospheric boundary layer (i.e., urban canopy), whereas the DISPER module uses 3D flows estimated by FLOW to calculate 3D concentrations of inert pollutants following a typical lagrangian approach. The numerical separation between flow estimates and pollutant dispersion modelling, whose methodological principles are described in Borrego et al. (2003), can be seen as a major advantage compared to other CFD models (e.g., ANSYS Fluent) that solve the advection-diffusion equation coupled with the Navier-Stokes equations (Vardoulakis et al., 2003). On the other hand, the VADIS capabilities to support multiple obstacles, flow fields and atmospheric emissions that vary in time, allow to more realistically evaluate maximum short-term local concentrations over complex urban geometries, especially under low wind speed conditions (Borrego et al., 2003). With this purpose, hourly meteorological fields (air temperature and wind speed and direction at a reference height) extracted from the WRF-Chem's inner domain grid cells that intersect the local domain are used as an input for the VADIS simulations (i.e., initializing the FLOW module), thus promoting the link between models (i.e., offline coupling). Besides this information, elements describing the urban geometry (buildings volumetry and streets configuration) and local emissions (point and/or line sources) are also required. For processing these inputs according to the VADIS requirements, the following methodologies and tools were used:

- *Urban geometry*

The preparation of geographic features that portray the urban structure, from their spatial representation to the format required for the VADIS simulations, is performed in two steps. Firstly, the urban area of interest (i.e., simulation domain) should be defined and, thereafter, the buildings volumetry and streets configuration with known emission rates should be drawn in parallelepiped sections, using a GIS (Geographic Information System) software. Average heights of the buildings also need to be provided. After this stage, the resulting geographic information, namely the coordinates of the vertices of each polygon and buildings height, are added to a VADIS preprocessing tool, which projects these data, aligned or in angle, under a structured mesh.

- *Local emissions*

For quantifying the pollutants dispersion over the simulation domain, local road traffic emissions are used to run the DISPER module. Thereby, the drawn streets are considered as line sources and traffic emissions are calculated for each road segment based on detailed traffic counts and fleet composition statistical data. Basically, the total emission of the pollutant p (Ep) for each road segment is estimated as follows:

$$E_p = \sum j \left[e_{pj}\ (v) \times N_j \right] \times L \qquad \text{(Eq. 1)}$$

where:

e_{pj} (v) is the emission factor for the pollutant p and vehicle category j as a function of the average speed, engine capacity, vehicle mass and emission reduction technology (v);

N_j is the number of vehicles of the category j;

L is the road segment length.

Traffic counts should be carried out seasonally considering working days and weekends. If not available, Open Transport Map data (OTM, n.d.) based on traffic volume estimates in national highways could be used and interpolated to other main roads. Regarding the fleet composition and emission factors, COPERT data (Emisia, n.d.), supported by national/regional statistics, should be used.

As a last step of the multiscale air quality modelling, WRF-Chem urban background concentrations (i.e., inner domain results) are added to the VADIS air quality estimates to account for the pollutant fraction that is not generated within the local simulation domain. Both air quality models are configured to produce hourly resolution outputs.

2.2. Health impact modelling

To quantify the health impacts of air pollution, the linear and non-linear methodologies recommended by the World Health Organization (WHO) were adopted, because these can be applied to a wide range of environmental conditions and air pollutants, as long as the resulting health effects are known (expressed as CRF), and are considered the most suitable at the city level (Brenk, 2018). Health effects of air pollution are often presented through morbidity and mortality indicators, mostly related to respiratory and cardiovascular diseases. Thereby, air quality outcomes should be incorporated in a health module that integrates the WHO methodologies, in order to estimate long and/or short-term health impacts and underlying damage costs associated to each pair pollutant p - health indicator i. Short-term exposure studies, which represent only a part of the health problem, are usually focused on exploring the high variability of acute health effects using hourly/daily time-series of pollutant concentrations; whereas long-term epidemiological evidences assess the increase in mortality risk due to chronic exposure to air pollutants, based on annual average concentrations. Both WHO methodologies use the same base formulation (Eqs. (2a) and (2b)), differing only in the calculation of the adjusted relative risk (RR). The linear RR function assumes a positive linearity between concentration and risk (Eq. (3)), whereas the non-linear method uses a RR function in which health risks tend to increase slower with increasing concentrations (Eq. (4)).

$$HI_{(p,i)} = \left(pop_{(p,i)} \times Inc_{(i)} \right) \times RR_{(p,i)} \qquad \text{(Eq. 2a)}$$

$$\boldsymbol{Costs}_{(p,i)} = \sum_{i=1}^{n} \left(\boldsymbol{HI}_{(p,i)} \times \boldsymbol{C}_{health\ (i)} \right) \qquad \text{(Eq. 2b)}$$

$$\boldsymbol{RR}_{(p,i)} = \boldsymbol{exp}\left[\boldsymbol{\beta}_{(p,i)}\ (\boldsymbol{X} - \boldsymbol{X_0}) \right] \qquad \text{(Eq. 3)}$$

$$\boldsymbol{RR}_{(p,i)} = \boldsymbol{exp}\left[\boldsymbol{\beta}_{(p,i)}\ (\boldsymbol{ln}\ (\boldsymbol{X}+\boldsymbol{1}) - \boldsymbol{ln}\ (\boldsymbol{X_0}+\boldsymbol{1})) \right] \qquad \text{(Eq. 4)}$$

According to the above equations, in addition to the estimated pollutant concentrations (X), other variables are needed to quantify the physical health impacts (HI) and corresponding costs (Costs):

- counterfactual concentration value (Xo) above which health impacts are calculated (WHO guidelines are often used);
- population size and its distribution by age groups (pop) (provided from country's population census);
- baseline mortality and cardiovascular and respiratory disease incidence rates (Inc) attributable to air pollution (usually derived from country statistics);
- β coefficient, that denotes the change in RR for unit change in concentration X - expressed as the natural logarithm of RR (derived from epidemiological studies); and
- monetary valuation of the health impacts (Chealth), individually translated to damage costs per case/day over a given health indicator i (preferentially, it should include all cost components: direct, indirect and intangible costs).

To evaluate the monetary losses of the estimated physical health impacts, national or regional statistics should be used. If not available, the alternative will be to use economic evaluation studies, updated for the reference year and geographic region of interest. Lastly, taking as a basis the target pollutant and exposure time, the total health costs estimated by health indicator i are added. The variable n (Eq. (2b)) represents the number of analysed health indicators.

2.3. Linking the models

After defining the methodological principles, focused on the use of the chosen air quality and health models and on the preparation of input data, the models and input-output matrices were operationalized and linked as a whole, using programming tools (python and bash shell scripting languages). This operational chain of the modair4health system was thought for research and end-user purposes. The user is guided for the choice of different system options (e.g., target pollutant, required simulation period, include or not integrated analysis, data postprocessing) and can easily adapt the baseline configurations (e.g., domains, parametrizations and input data), taking into consideration the particular case study and research objectives to accomplish. Appendix A includes the different options to run the mod4health modelling system.

3. Application of the modair4health system

The modair4health system was applied over nested simulation domains to evaluate its operability and performance as a decision-making support tool in selecting the best strategies for urban air quality and health management.

3.1. Case study

The selected case study is located within the city of Coimbra, the largest city of the Centre Region (Fig. 2) and the fourth largest urban centre of Portugal, with 99 739 inhabitants in its urban perimeter (2021 census) and a municipality area of 319.4 km^2 (INE, 2021). Coimbra plays a strategic role in connecting the north to the south, and the coast to the inland of Portugal. In the north, the landscape is typically more fragmented and complex, whereas towards the south, large homogeneous territorial units dominate. Regarding the coast-inland link, the city is near the Atlantic Ocean and the mountainous areas (approximately 50 km), thus contributing for intensifying urban/local atmospheric dynamics. These geographic nuances greatly influence the region's climate, which is affected by Atlantic and Mediterranean characteristics. The summer is typically warm and dry, with average minimum and maximum temperatures of 15 °C and 28.5 °C, respectively, reaching 40 °C or more in certain days. In winter, these values decrease to 4.6 °C and 14.6 °C, and high rainfall is recorded: total average and daily maximum precipitation for January reached 112.2 mm and 47.6 mm, respectively (IPMA - Portuguese Institute for Sea and Atmosphere, n.d.). From the point of view of urban air pollution, high levels are associated to the road traffic sector, which is the largest contributor to ambient NO_2 concentrations, representing one of the major environmental concerns and the potential cause of many diseases and premature deaths. Accordingly, to evaluate the road traffic influence, the case study was designed over one of the busiest road traffic areas of the city of Coimbra (Fernão de Magalhães Avenue) and NO_2 concentrations were estimated.

3.2. Main configurations

In terms of baseline modelling setup, the WRF-Chem mesoscale model version 3.6.1 was applied over three simulation domains (25, 5 and 1 km horizontal resolutions) in two-way nesting mode (i.e., including the feedback between domains) for the year 2015. WRF-Chem is able to capture the transboundary air pollution and, thus, to estimate urban background concentration gradients (1 km resolution Centre Region domain in Fig. 2) to the local case study. Further information on the WRF-Chem tests, the modelling setup used (domains, physical and chemical parametrizations, input data), obtained results and model evaluation are presented in Silveira et al. (2022, 2021, 2018).

The link with the local scale air quality modelling was carried out through the VADIS CFD model to reproduce the flow variability and pollutant dispersion within the urban structure. To initialize the FLOW module, WRF-Chem meteorological results for the 1 km resolution inner

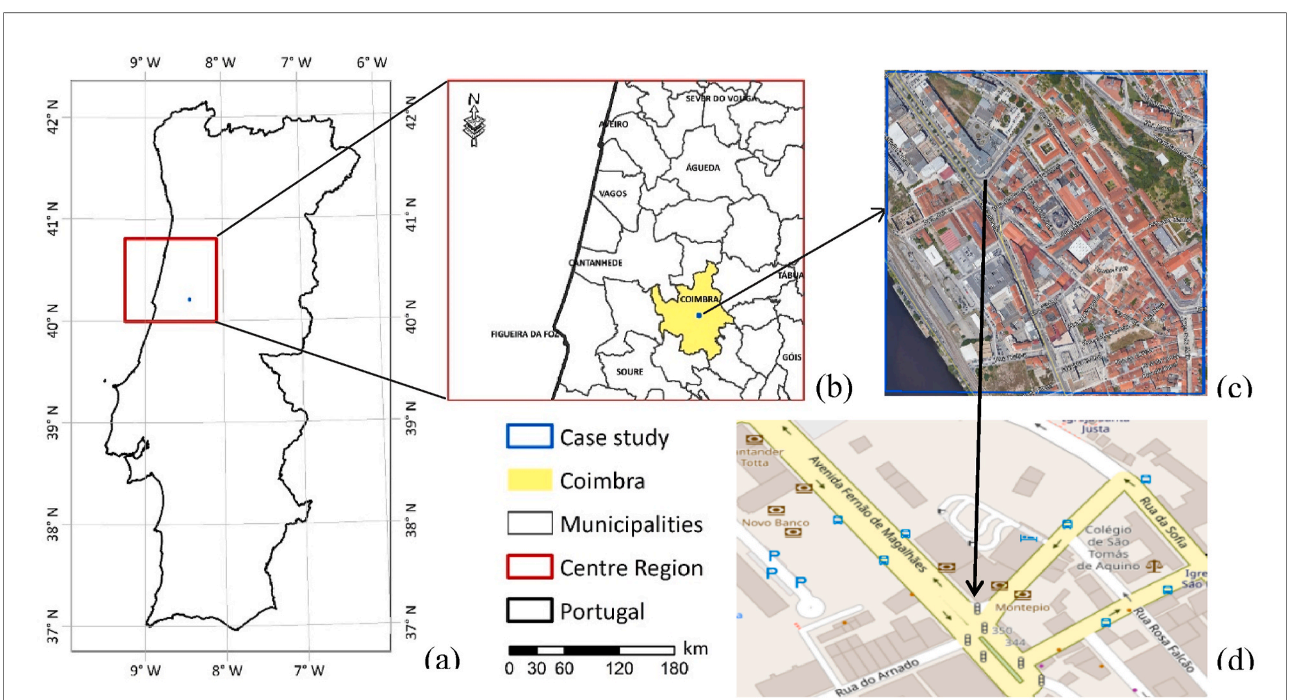


Fig. 2. Geographic location of the case study: a) Portugal, b) part of the Centre Region, c) case study domain, and d) part of the Fernão de Magalhães Avenue.

domain, namely 2 m air temperature and 10 m wind fields (wind speed and direction), were used. In turn, the impact of the road traffic activity on local NO_2 concentrations was quantified using traffic-induced NOx emissions estimated for each road segment (Eq. (1)). In order to account for the pollutant fraction that is not emitted within the case study, the WRF-Chem urban background NO_2 concentrations (1 km resolution) extracted from grid cells that intersect the local domain were added to the VADIS NO_2 results.

The local simulation domain (case study) covers an area of 600 m × 600 m where 2005 people live, and its urban structure is composed by 125 buildings and 34 road segments. These geographic features were drawn in parallelepiped sections using a GIS software (Fig. 3), and then processed for the VADIS format considering also the average height of the buildings. The tallest building, with 49 m, served as a reference for defining the urban canopy height, where atmospheric processes are solved by the CFD model.

VADIS was applied over the case study domain using a 3-D uniform grid resolution of 4 m and hourly resolution to produce NO_2 estimates for two periods:

- winter (26th January to February 1, 2015);
- summer (15th to June 21, 2015).

The simulation periods were selected taking into account the seasonality, very connected to the local weather conditions and to daily activity patterns, as well as the highest NO_2 concentrations measured in the traffic station located in the Fernão de Magalhães Avenue (marked in Fig. 3) for the year 2015, which also served to evaluate the model performance using the baseline configurations. Traffic emission profiles for each season were designed from hourly measured NO_2 concentrations during a 10-year period.

It should be noted that the definition of the domain dimensions, grid resolutions and geometric characteristics of the buildings and road segments including their orientation, was based on the COST 732 guidelines for CFD simulation of flows in urban environment (Franke et al., 2011).

To quantify the health impacts resulting from the multiscale air quality modelling (Eq. (2a), (2b)), the local case study and VADIS simulation periods were the target, considering health indicators that relate NO_2 pollution with short-term human exposure. The non-linear RR methodology (Eq. (4)) was adopted given the assumption that a simple linear extrapolation produces large overestimates of disease burden, mainly when high air concentrations are observed (Burnett et al., 2018; Nasari et al., 2016). Table 1 shows the health input metrics used to assess physical health impacts and underlying damage costs due to short-term exposure to NO_2.

3.3. *Traffic management strategies*

Given the nature of the local case study, two of the most common traffic management strategies in urban areas were selected and tested for the VADIS simulation domain and periods, in order to evaluate the system operability and the entire chain of impacts against the reference scenario (i.e., using the baseline configurations - hereinafter referred as REF):

(i) replacement of 50% of the vehicle fleet below the European emission standards (EURO) 4 (registered until the end of 2004) by electric vehicles (hereinafter referred as ELEC) that produce little local air pollution, with much more efficient engines than conventional internal combustion engines;

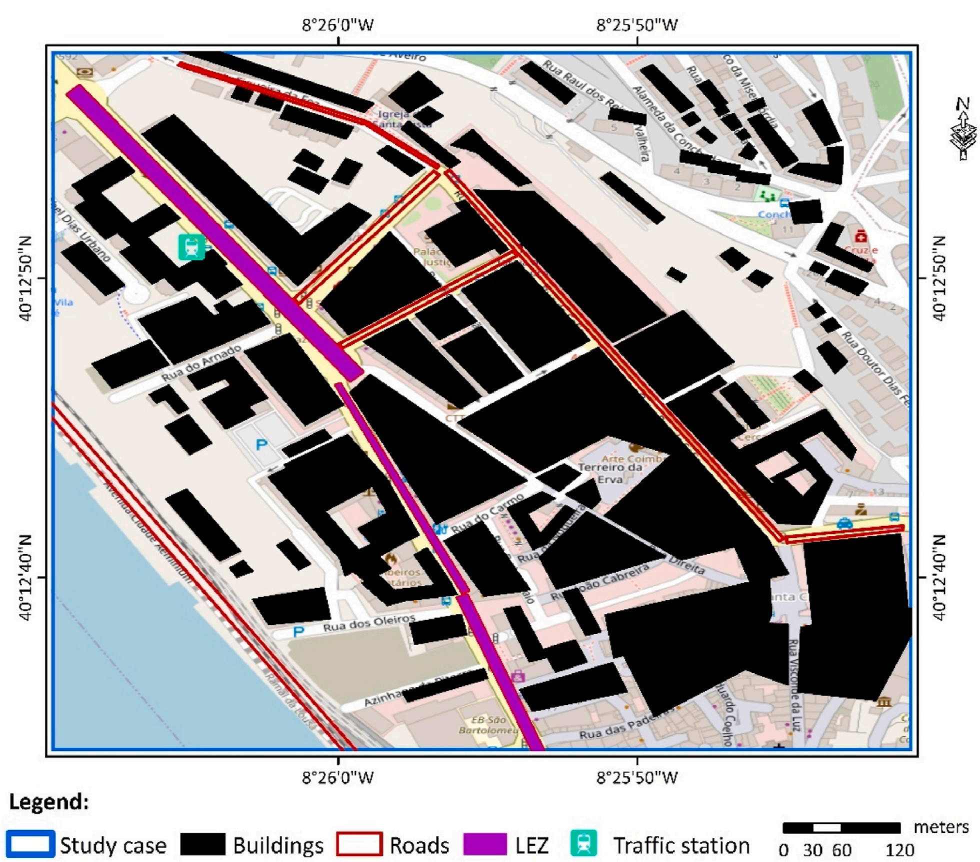


Fig. 3. Spatial representation of the local case study's urban structure considered for the VADIS simulations. The traffic influence monitoring station used to evaluate the model performance is also identified.

Table 1
Health input metrics used to estimate health impacts from short-term human exposure to ambient NO_2 concentrations.

Health indicator	Age group	Reference period	RR (95% CI) per 1 μg.m^{-3})	Baseline rate (%)	Damage cost	
					Price (€)	Unit
Respiratory hospital admissions	All ages	Daily maximum	0.1002 (0.0999–0.1004)	0.05	8960	Case (8-days average duration)
Mortality (all natural causes)	All ages	Daily maximum	0.1003 (0.1002–0.1004)	0.977	1844	YLL

The standard RR function selected for each health indicator determines the potentially affected age group and reference period for NO_2 concentrations to be analysed. Population data were extracted from INE (2021), whereas hourly modelled NO_2 concentrations were designed as daily maximum values.
RR is the relative risk per person and per 1 μg m^{-3} change in NO_2 concentration (source: WHO, 2013);
Baseline rate measures the probability of occurrence of a given disease (medical condition) or premature death in a population within a specified time period (sources: WHO, 2021a; 2021b);
Unit damage costs is the monetary value to pay for repairing the person's initial heath status or, at least, to remediate effects of air pollution on the health indicator (sources: Brandt et al., 2013; Maibach et al., 2008);
CI - Confidence Intervals; YLL - Years of Life Lost.

(ii) introduction of a Low Emission Zone (LEZ) in the Fernão de Magalhães Avenue (identified in Fig. 3), with an extension of approximately 830 m, where the circulation of vehicles below EURO 4 and trucks is banned.

The options for electric mobility have been expanding rapidly, leading many countries to adopt a variety of measures to encourage the change from conventional to electric vehicles (EV), such as incentives for their acquisition, and strengthening the EV's charging network and autonomy. In 2018, the global EV fleet exceeded 5.1 million, up 2 million more than in the previous year and almost doubling the number of new EV sales (IEA, 2019).

Regarding LEZs, their introduction has been regulated in many developed cities of European and Asian countries, restricting the total or partial circulation of vehicles at certain times of working days. This air pollution management strategy has low implementation and operation costs, and it is often considered as the most effective measure that local entities can take to improve the air quality of their cities (CLARS, n.d.; Wang et al., 2017).

The implementation of these traffic management strategies has also some associated drawbacks, despite the successful results in several case studies. The increase of EV in circulation contributes to a significant reduction of the air pollution levels due to a deceleration in the fossil fuel burning in the cities, but it amplifies the energy consumption, thus transferring the air pollution problem to the power generation sector. Concerning LEZs, their effectiveness to combat air pollution is often ensured locally, however, by diverting road traffic from these locations or at certain times of the day, other regions may experience anomalous air pollution levels. For these reasons, the use of multiscale modelling tools assumes a primordial role to evaluate local and transboundary contributions from different air pollution sources. However, in this work, only direct impacts of ELEC and LEZs scenarios on emissions, and consequently air quality and health, are evaluated over the case study.

3.4. *Evaluation of system performance and chain of impacts*

To evaluate the chain of impacts, which reflect the expected benefits of the implementation of the selected traffic management options, a Scenario Analysis Approach (SAA) was adopted to estimate emission, air quality and health changes compared to the REF scenario (Fig. 4).

For the air quality assessment, NO_x emissions for the traffic management scenarios (ELEC and LEZ) were calculated and, subsequently, the resulting atmospheric emissions were used to simulate the spatial and temporal changes of ambient NO_2 concentrations. The integration of health impacts aimed to: (i) assess the human exposure derived from the NO_2 concentration changes; (ii) quantify the total avoided physical health impacts with the expected air quality improvement; and (iii) value these avoided impacts (benefits) in monetary terms considering the different cost components (direct, indirect and intangible costs).

3.4.1. *Atmospheric emissions*

In urban areas, NO_x emissions are largely related to the local road traffic activity, incisively contributing to worrying air pollution hotspots. To minimize the adverse effects, over the case study and for the traffic management scenarios, NO_x emissions in each road segment were recalculated based on the following assumptions:

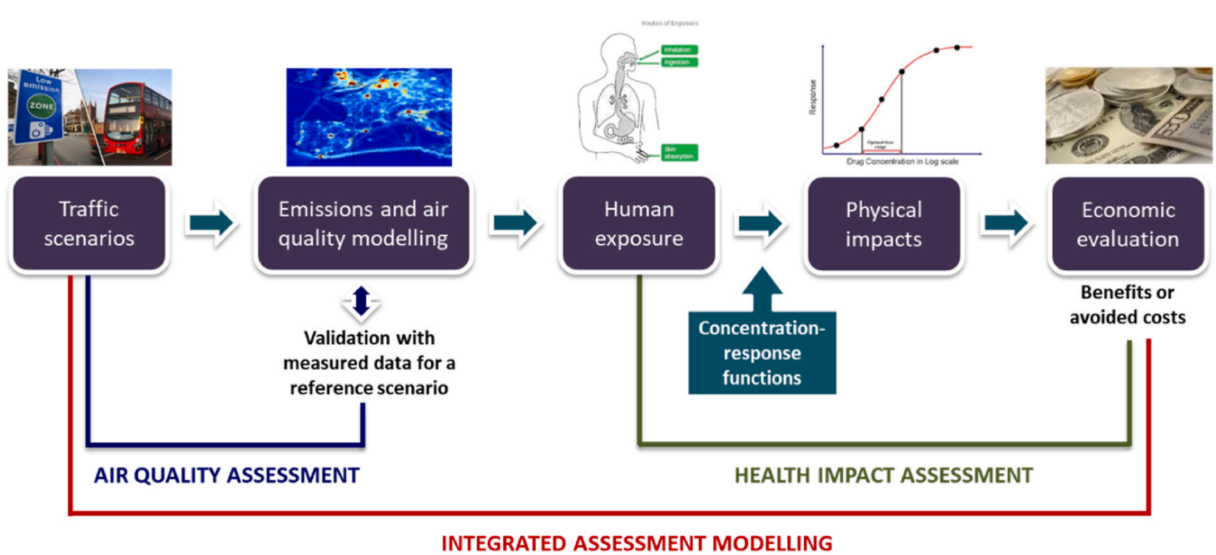


Fig. 4. Diagram of the chain of impacts associated to the selected traffic management options, to be evaluated following a SAA (adapted from Silveira et al., 2016).

(i) in the ELEC scenario, 50% of the fleet composition below EURO 4 was replaced by EV, impacting all simulated road segments;
(ii) for the LEZ scenario, fleet composition data were only changed in the road segments that correspond to the Fernão de Magalhães Avenue, banning the circulation of vehicles below EURO 4 and trucks.

As expected, larger NO_x emission reductions were obtained at the Fernão de Magalhães Avenue, due to its intense road traffic activity. For the whole simulation domain, a reduction of 17.8 (50%) and 7.8 kg d^{-1} (22%) in NO_x emissions was estimated for the ELEC and LEZ scenarios, respectively.

3.4.2. Air quality

In a multiscale perspective, i.e., taking into account the WRF-Chem urban background concentrations, the VADIS CFD model was applied to the reference and traffic scenarios to quantify the impact of NO_x emission changes on the spatio-temporal patterns of NO_2 concentrations. Fig. 5 presents the time series of hourly NO_2 concentrations modelled for the tested scenarios and for both simulation periods at the traffic station location, and of the NO_2 values measured in the same periods (OBS).

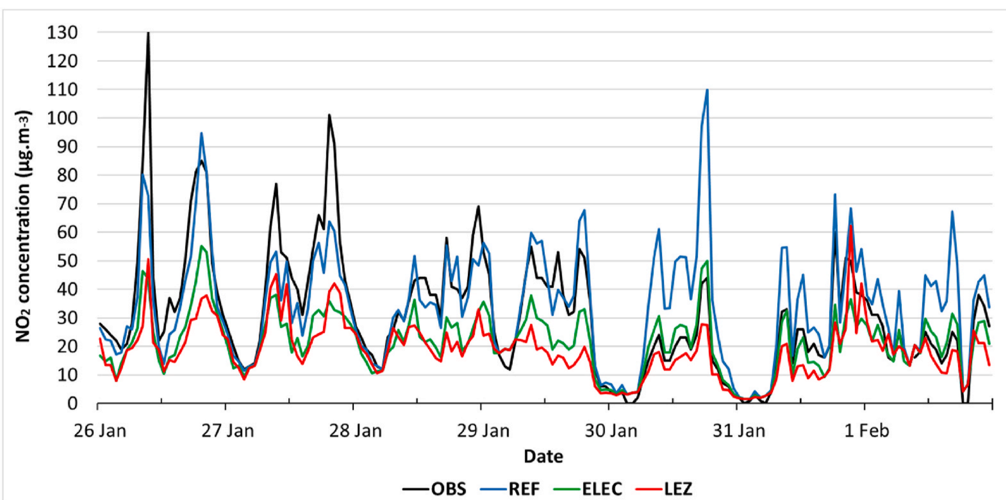
Overall, larger air quality improvements were obtained for the time periods with higher REF NO_2 concentrations, and those improvements are more evident for the LEZ scenario. In turn, small differences between REF and traffic scenarios results were estimated for lower REF NO_2 concentrations, which correspond to the times of the day with low or moderate road traffic activity (noon and night). Therefore, this hourly variability of the modelled NO_2 concentrations is closely related with the traffic emissions and the way they are disaggregated.

The daily averaged profiles of NO_2 concentrations for the same location and simulation periods (Fig. 6) allowed to identify local pollution reductions for both traffic scenarios at all hours, especially in the periods of the day associated to traffic activity peaks.

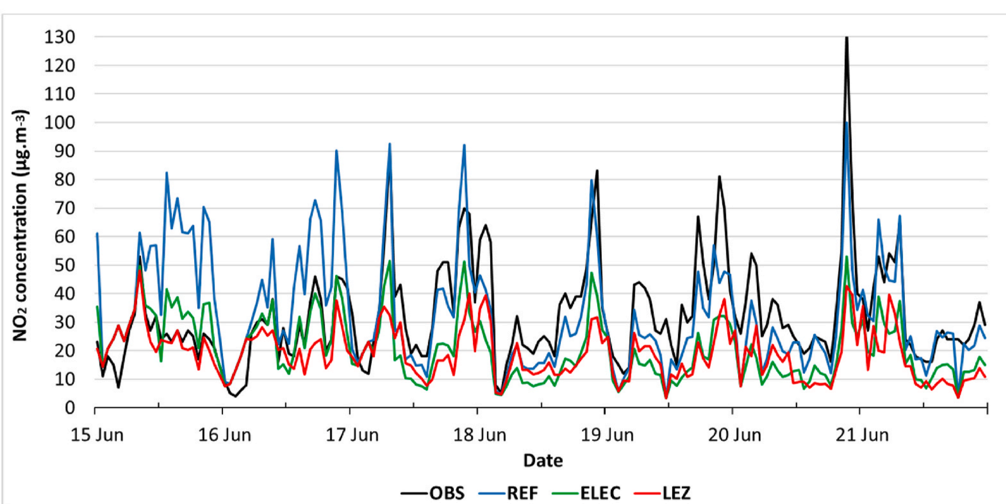
Fig. 7 presents the spatial pattern of NO_2 improvement over the case study domain, for one peak hour (higher observed and modelled NO_2 concentrations) of each simulation period.

In general, the most relevant air quality improvements in both traffic scenarios were estimated for a part of the Fernão de Magalhães Avenue (up to 100 μg m^{-3}), where REF NO_x emissions and corresponding emission reduction for the traffic scenarios were higher. Besides the emissions, these air quality estimates were also strongly influenced by the urban geometry (e.g., height and orientation of buildings), which interferes with the accumulation and dispersion patterns of NO_2 concentrations, and by local wind regimes (wind speed and direction) affecting the turbulence. From the point of view of the atmospheric flow, on January 26th at 19:00 and June 17th at 7:00, northwest and southeast prevailing winds, respectively, and slightly stable conditions were recorded.

To complement the previous analysis, the statistical performance of

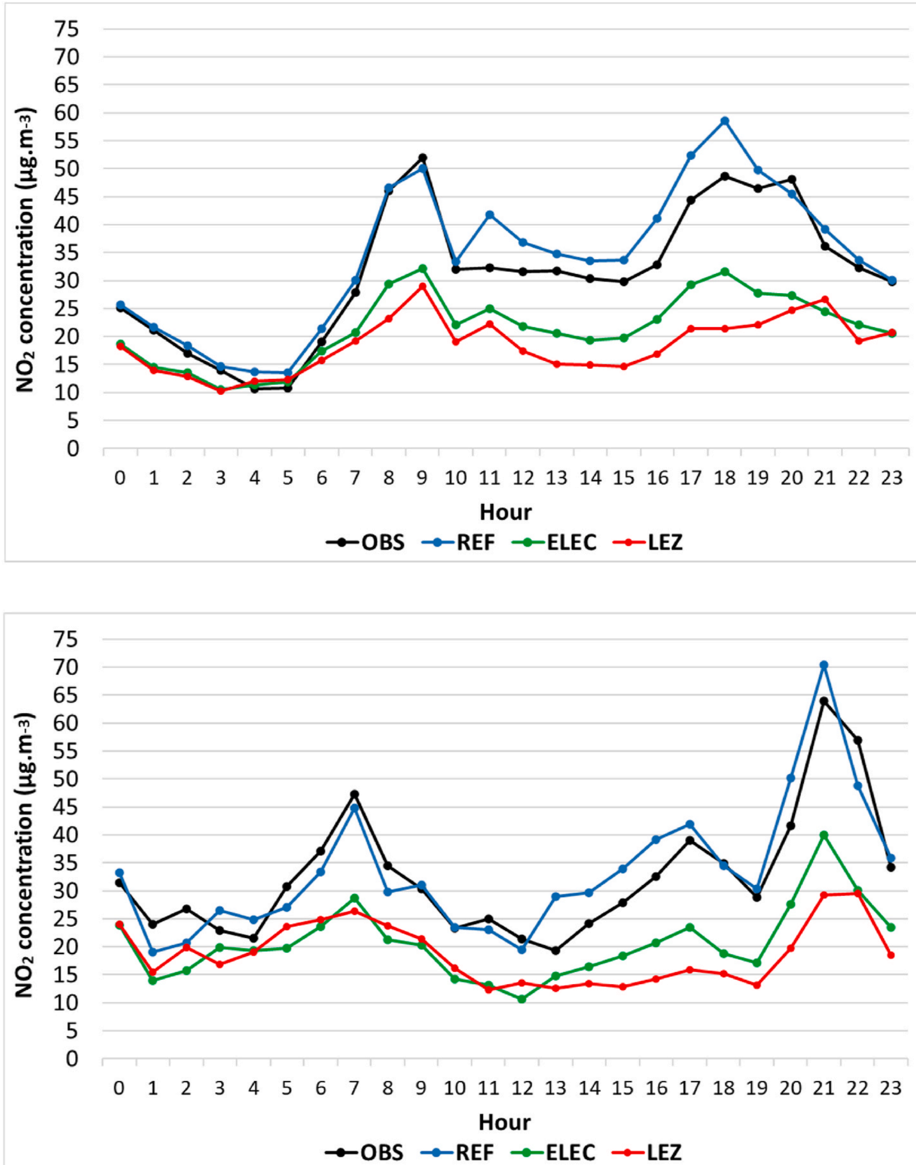


(a)



(b)

Fig. 5. Time series of hourly observed and modelled NO_2 concentrations (μg.m^{-3}) in (a) winter and (b) summer periods for the reference (REF), and for the traffic scenarios (ELEC and LEZ).



(a)

(b)

Fig. 6. Daily averaged profiles of observed and modelled NO_2 concentrations (μg.m^{-3}) in (a) winter and (b) summer periods for the reference and traffic scenarios.

the air quality modelling results was evaluated through the coefficient of determination (R^2) (Fig. 8).

The best performance reproducing local NO_2 concentrations was achieved in the winter period, slightly worsening in the summer probably due to the transport of polluted air from other regions. This potential transport of air from other regions was accounted for by adding WRF-Chem urban background concentrations to the CFD model concentration levels.

3.4.3. *Human health*

Regarding the health impact assessment (HIA) of the traffic management scenarios for the simulation periods, the non-linear WHO methodology and selected health input metrics were applied to the local case study, to quantify the avoided short-term physical health impacts and corresponding monetary savings compared to the REF scenario.

Figs. 9 and 10 present some HIA outputs, namely the spatial distribution of potential benefits or avoided costs (REF minus traffic scenario), per day, derived from the implementation of the traffic scenarios in winter and summer periods, respectively. For a better understanding of these differences, which consider the sum of the NO_2 impact on the analysed health indicators, the health damage costs estimated for the REF are mapped in Appendix B.

The comparative analysis of the daily health benefits by scenario shows that, overall, ELEC benefits cover a larger geographic area, because the ELEC scenario resulted in NO_x emission reductions in all designed road segments. Nevertheless, over the LEZ influence area, higher benefits were estimated, given the wider restrictions for the circulation of road vehicles. These outcomes show the relevance of the expected NO_x emission reductions and air quality improvement, also influenced by the urban structure and local meteorological fields. Nevertheless, the air quality improvement, by itself, does not explain the benefit, as it is combined with population data. Thus, the highest health benefits (up to 1.2 cents/day) were estimated for locations with larger NO_2 improvements and higher number of residents.

To complement this spatial analysis, Fig. 11 shows the daily total health impacts avoided in each traffic scenario for the whole domain and simulation periods.

Daily estimates indicate a higher total number of avoided cases and associated monetary benefits using the ELEC scenario. Focusing on the simulation periods, in winter, the largest total benefit in both scenarios

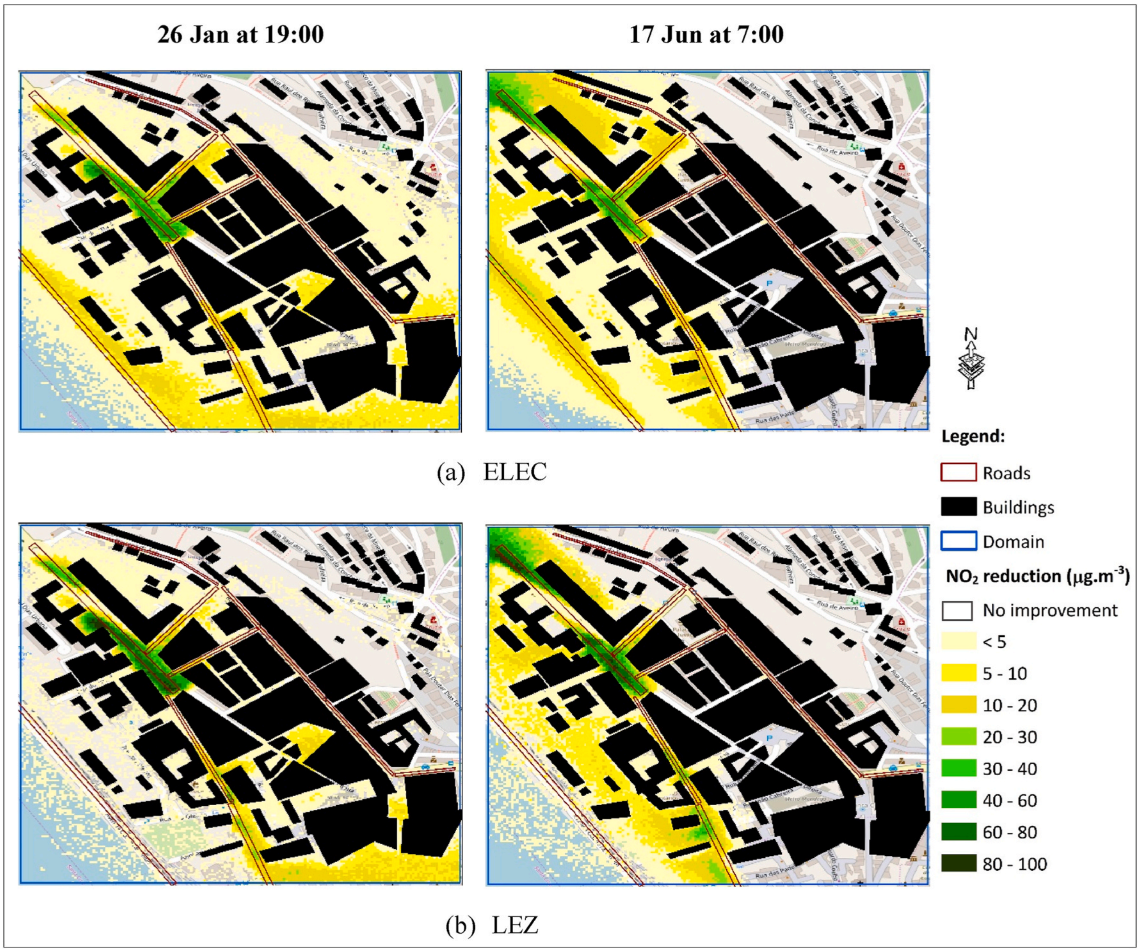


Fig. 7. Reduction of NO_2 concentrations (μg.m^{-3}) (REF minus traffic scenario) on 26th January at 19:00 (on the left) and 17th June at 7:00 (on the right) comparing the reference with the traffic scenarios: (a) ELEC and (b) LEZ.

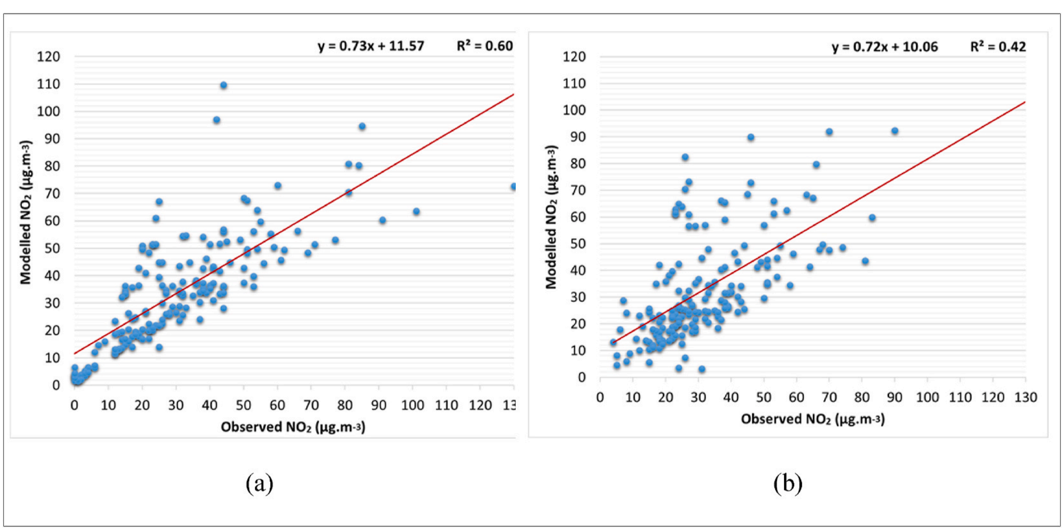


Fig. 8. Correlation between observations and hourly modelled NO_2 concentrations (μg.m^{-3}) in (a) winter and (b) summer periods.

was estimated for January 30th, being expected daily health savings of 9.9 € (0.025 avoided cases) and 7.3 € (0.018 avoided cases) for the ELEC and LEZ scenarios, respectively. The lowest impact was calculated for January 27th, with daily savings around 3 € (ELEC) and 1.4 € (LEZ). In summer, largest monetary benefits were predicted for June 16th and 18th, corresponding to 7 € in the ELEC scenario, and approximately 5 € for the LEZ. Table 2 presents the total and daily averaged health impacts, for the whole domain and for each traffic scenario, which were estimated by aggregating the obtained values per simulation period.

For both metrics, the number of avoided cases and the monetary benefit calculated for the winter period were slightly higher than those estimated for the summer. Comparing the health impacts estimated for

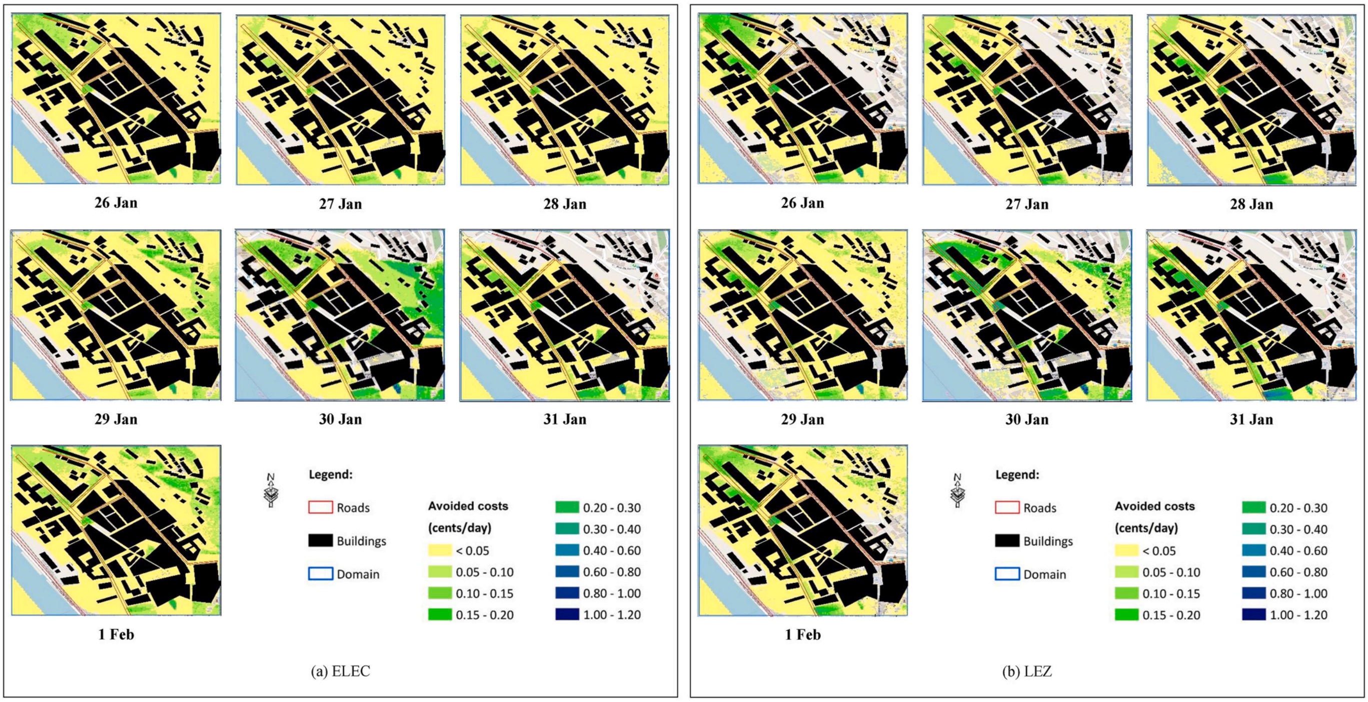


Fig. 9. Short-term health benefits (cents/day) (REF minus traffic scenario) resulting from the (a) ELEC and (b) LEZ scenarios for the winter period.

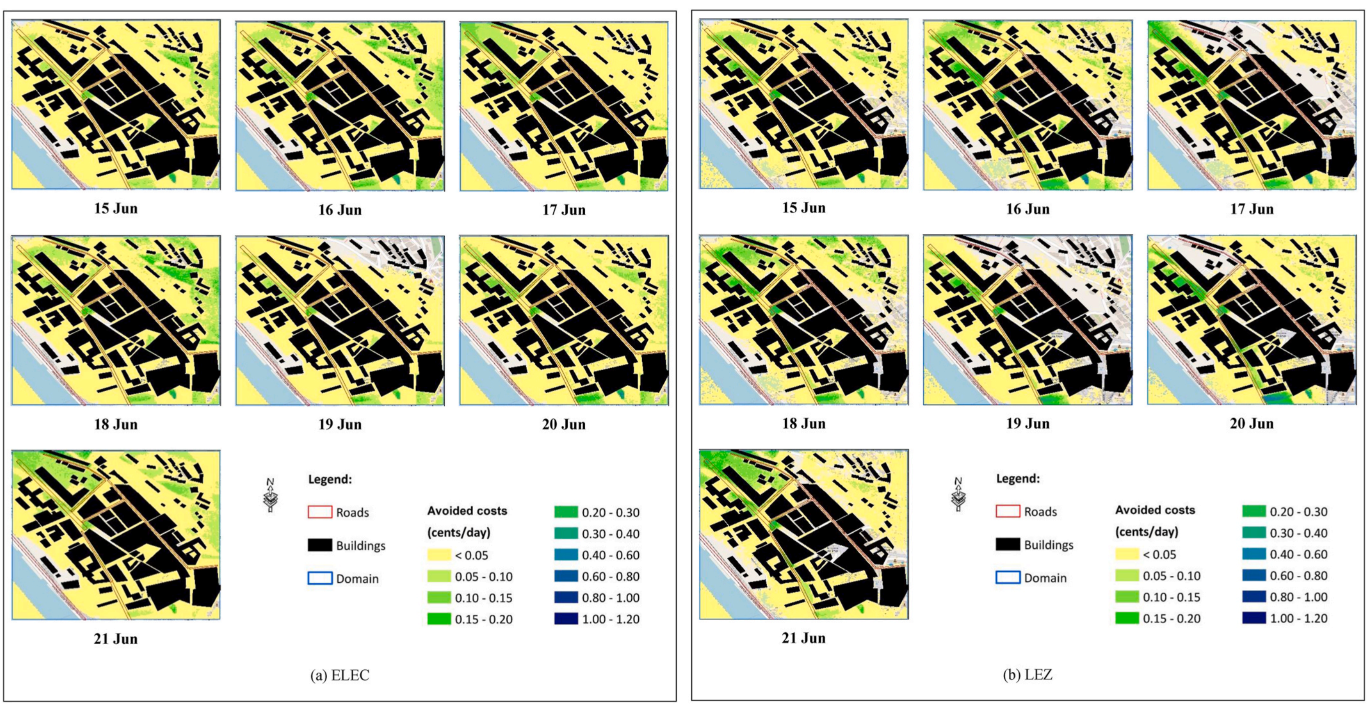


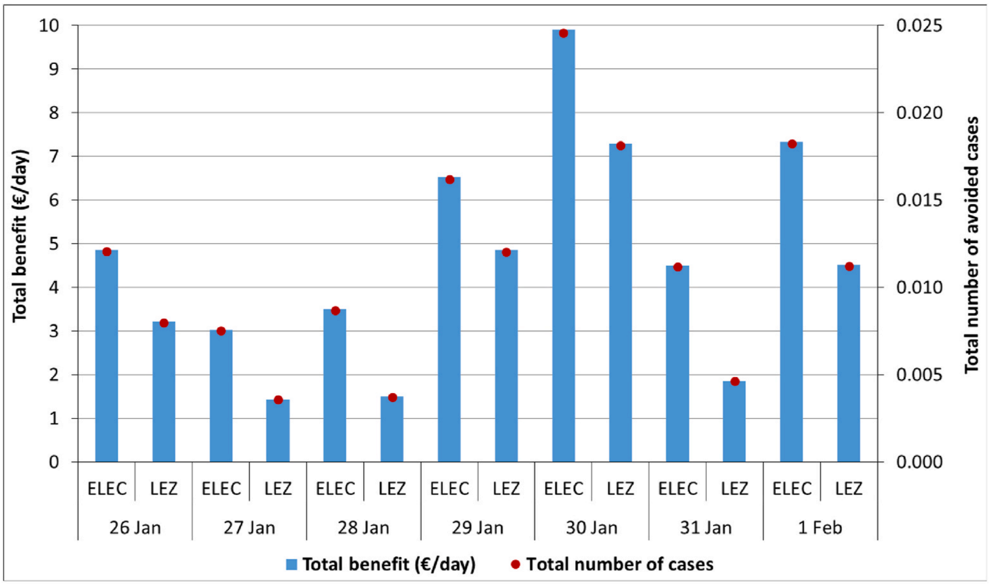
Fig. 10. Short-term health benefits (cents/day) (REF minus traffic scenario) resulting from the (a) ELEC and (b) LEZ scenarios for the summer period.

the scenarios, the results translate the values indicated in Fig. 11, where the ELEC contributes to larger health benefits.

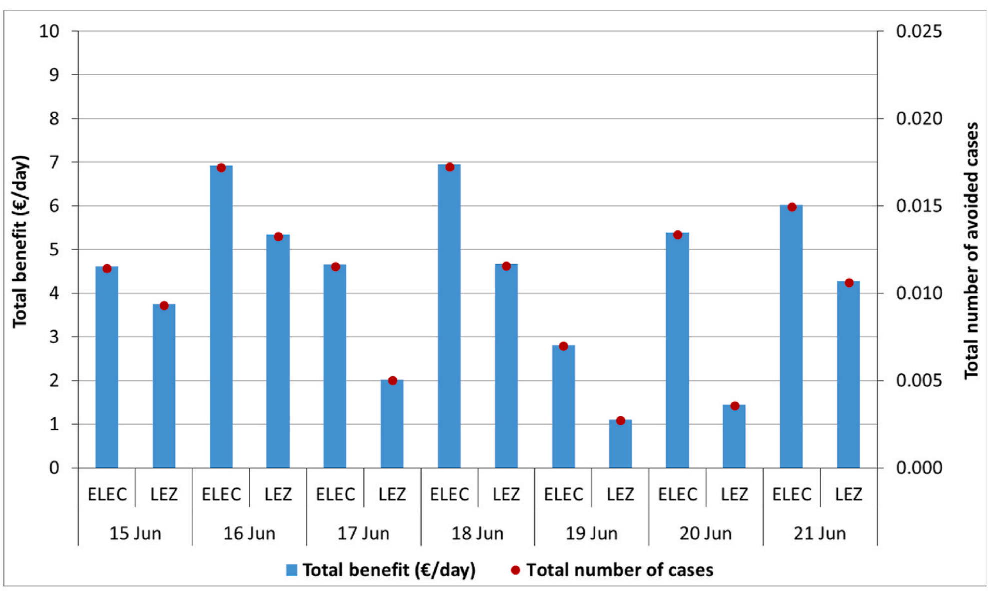
In brief, the SAA followed to evaluate the chain of impacts showed that the relatively low ambient NO_2 concentrations (Fig. 5), for the case study and simulation periods, reflect a smooth air quality improvement when applying both traffic scenarios. In turn, the monetary benefit was also reduced given the restrict number of exposed people (residents) and analysed health indicators. Envisioning the implementation of the tested traffic scenarios over a larger geographic area with NO_2 pollution problems, it will be expected a more significant air quality improvement and greater health benefits as a result of this NO_2 pollution reduction, that would benefit a higher population density. These benefits (i.e., avoided health costs) tend to be higher if new health indicators and air pollutants are included in the SAA.

4. Conclusions

Urban air pollution is increasingly a threat to public health, with the



(a)



(b)

Fig. 11. Daily total avoided health impacts for the (a) winter and (b) summer periods applying the ELEC and LEZ scenarios.

Table 2
Total and daily averaged health impacts estimated for each scenario, for the winter and summer periods and considering the whole simulation domain.

Scenario	Metric	Winter		Summer	
		Number of avoided cases	Benefit (€)	Number of avoided cases	Benefit (€)
ELEC	Daily average	0.014	5.7	0.013	5.3
	Total	0.098	39.7	0.093	37.4
LEZ	Daily average	0.009	3.5	0.008	3.2
	Total	0.061	24.7	0.056	22.6

road traffic sector being one of the major concerns and the largest contributor to NO_2 concentrations, although the influence of background chemistry must also be considered. To that end, the use of modelling tools is crucial to understand atmospheric dynamics on multiple scales, as well as to support the development of the best air quality improvement strategies.

The main purpose of this paper was to present and apply the developed modair4health system, able to simulate atmospheric concentrations and resulting health impacts in a broad spatial (regional to local scales) and temporal (short and long-term) horizon. For multiscale air quality modelling, two air quality models were selected: WRF-Chem (regional to urban scales) and VADIS (local scale). The option for the online model WRF-Chem represents an added value in atmospheric modelling, as potential meteorology-chemistry feedbacks are included. The link to the local scale was done with the CFD model VADIS, in order to accurately reproduce the spatial variability and pollutant dispersion within the urban structure. To cover the multiple spatial scales and resolutions, the models were carefully coupled (offline coupling), ensuring that the background and boundary meteorological and chemical conditions extracted from the WRF-Chem urban domain are properly assimilated by the local scale. When moving from air pollution to health impacts, the linear and non-linear WHO methodologies were integrated into the system to quantify the number of unfavourable cases per health indicator and associated damage costs due to short and long-term human exposure to air pollutants.

Focusing on the local case study, the characteristics of the urban structure (e.g., height, orientation and spacing between buildings) and meteorological conditions (e.g., wind speed and direction) strongly influenced the dispersion and accumulation patterns of NO_2 concentrations. Pollutant dispersion was favoured according to the prevailing wind directions, whereas flow dynamics perturbations induced by the obstacles tended to reduce the wind speed, leading to the formation of local air pollution hotspots. Furthermore, higher hourly concentration gradients were estimated around the main streets, where the highest traffic emissions were allocated. From the health point of view, higher adverse impacts were felt in locations with higher NO_2 concentrations and resident population. By applying the traffic management scenarios, more significant air quality improvements are expected in areas and time periods with higher NO_2 values in the reference scenario, amplifying the health benefit in more populated areas. The biggest benefit was estimated over the LEZ influence area, given the wider road circulation restrictions. In turn, the ELEC benefit covers a larger geographic area, because NO_x emission reductions were designed in all road segments. Nevertheless, it should be noted that this scenario analysis approach, which was applied to a local case study, allowed to evaluate benefits at this local scale, but the impact of the chosen emission reduction measures could go beyond the local scale, aggravating the air pollution on other areas and the health condition of the neighbouring population. Thus, as future work, a broader integrated impact assessment should be considered.

In summary, the modair4health system showed to be a powerful modelling tool for scenario analysis, providing multiscale spatial and temporal information of environmental, social and economic value to facilitate the choice of cost-effective air quality and health management strategies and decisions. Moreover, its operability allows to quickly test other urban air pollution control policies, and it can be easily adapted and applied to other case studies considering regional to local atmospheric influences.

CRediT authorship contribution statement

Carlos Silveira: Conceptualization, Methodology, Software, Formal analysis, Investigation, Writing – original draft, Writing – review & editing. **Joana Ferreira:** Conceptualization, Formal analysis, Writing – review & editing. **Ana I. Miranda:** Conceptualization, Writing – review & editing.

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.

Data availability

No data was used for the research described in the article.

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Appendix A. User interface for application of the modair4health system

A.1. General options

(i) Select the air pollutant to analyse:
(PM2.5; PM10; NO_2; O_3; CO)
pollutant = NO_2

(ii) Consider Integrated Assessment Modelling (IAM):
(0 - No; 1 - Yes; 2 - Skip to the postprocessing)
IAM = 1

(iii) Select the component to run when IAM is not required:
(1 - air quality; 2 - health)
component = 1

(iv) Select the application scales to run air quality and/or health:
(1 - regional to urban; 2 - local; 3 - multiscale)
scales = 2

(v) Consider air quality and health management (AQHM):
(0 - No; 1 - Yes)
AQHM = 1
If AQHM is required, select the scenario to analyse:
(ELEC; LEZ)
scenario = ELEC

A.2. Configurations to run air quality

(vi) Select the simulation periods:
WRF-Chem (regional to urban scale; format - yyyy/mm/dd)
WRF_inidate = 2015/01/26
WRF_enddate = 2015/02/01
VADIS (local scale; format - yyyy/mm/dd_hh:00)
VADIS_inidate = 2015/01/26_00:00
VADIS_enddate = 2015/02/01_00:00
(vii) Select the traffic emission profile to run local scale air quality:
(1 - user-defined; 2 - seasonal)
emis_profile = 2

A.3. Configurations to run health

(viii) Air pollution exposure time to analyse:
(1 - short-term; 2 - long-term)
health effects = 1
(ix) Select the time period to quantify health effects (format - yyyy/mm/dd):
health_inidate = 2015/01/26
health_enddate = 2015/02/01
(x) Select the relative risk methodology to use:
(1 - linear; 2 - non-linear)
health_method = 2
A. 4. Postprocessing options

A.4. Postprocessing options

(xi) Include data postprocessing:
(0 - No; 1 - Yes)
post_proc = 1
(xii) Select the simulation domain:
(regional to urban - d01, d02, d03; local - d04)
dom = d04
(xiii) Select the time periods to analyse:
date (format - yyyy/mm/dd)
hour (format - hh; must be in 00..24)
post_inidate = 2015/01/26
post_enddate = 2015/02/01
post_inihour = 08
post_endhour = 20
(xiv) Spatial analysis:
(0 - No; 1 - Yes, only modelled data; 2 - Yes, overlap modelled and observed data)
metrics (average; minimum; maximum)
spat_dist = 2
spat_metric = average
(xv) Model evaluation:
(0 - No; 1 - Yes)
model_eval = 1
If model evaluation is required, select an air quality monitoring station or typology:
(1) insert station acronym (e.g., COI); (2) Allstations; (3) Background (Rural, Suburban, Urban);
(4) Rural; (5) Suburban; (6) Urban; (7) Traffic
post_station = COI
Validation:
Statistical metrics (observed and modelled mean, correlation, BIAS, RMSE)
(0 - No; 1 - Yes)
validation = 1
Time series:
(0 - No; 1 - Yes)
time_series = 1
Daily profiles:
(0 - No; 1 - Yes)
daily_prof = 1

Appendix B. Short-term health damage costs estimated for the reference scenario

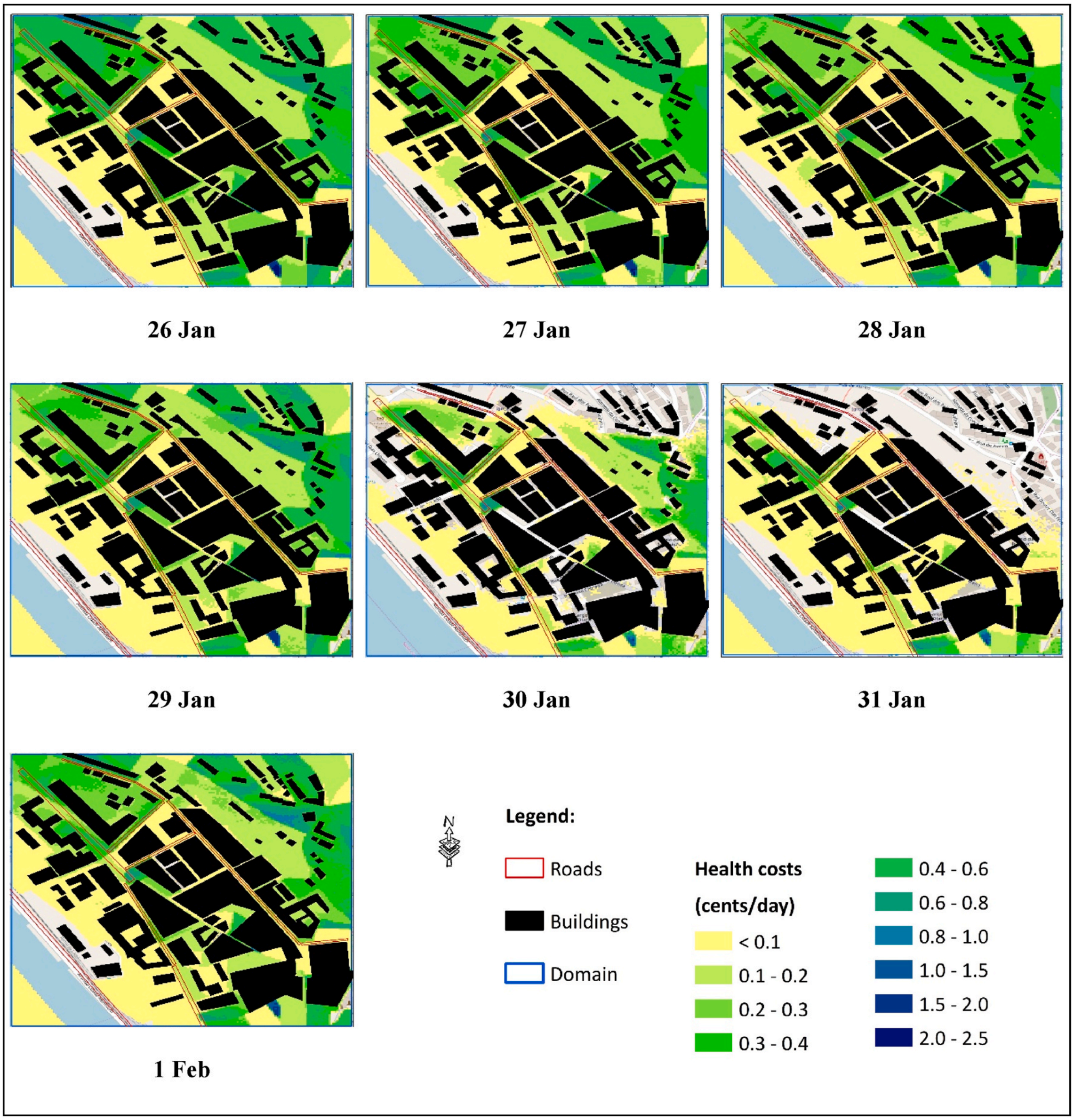

Fig. B.1. Short-term health damage costs (cents/day) estimated for the REF scenario in the winter period.

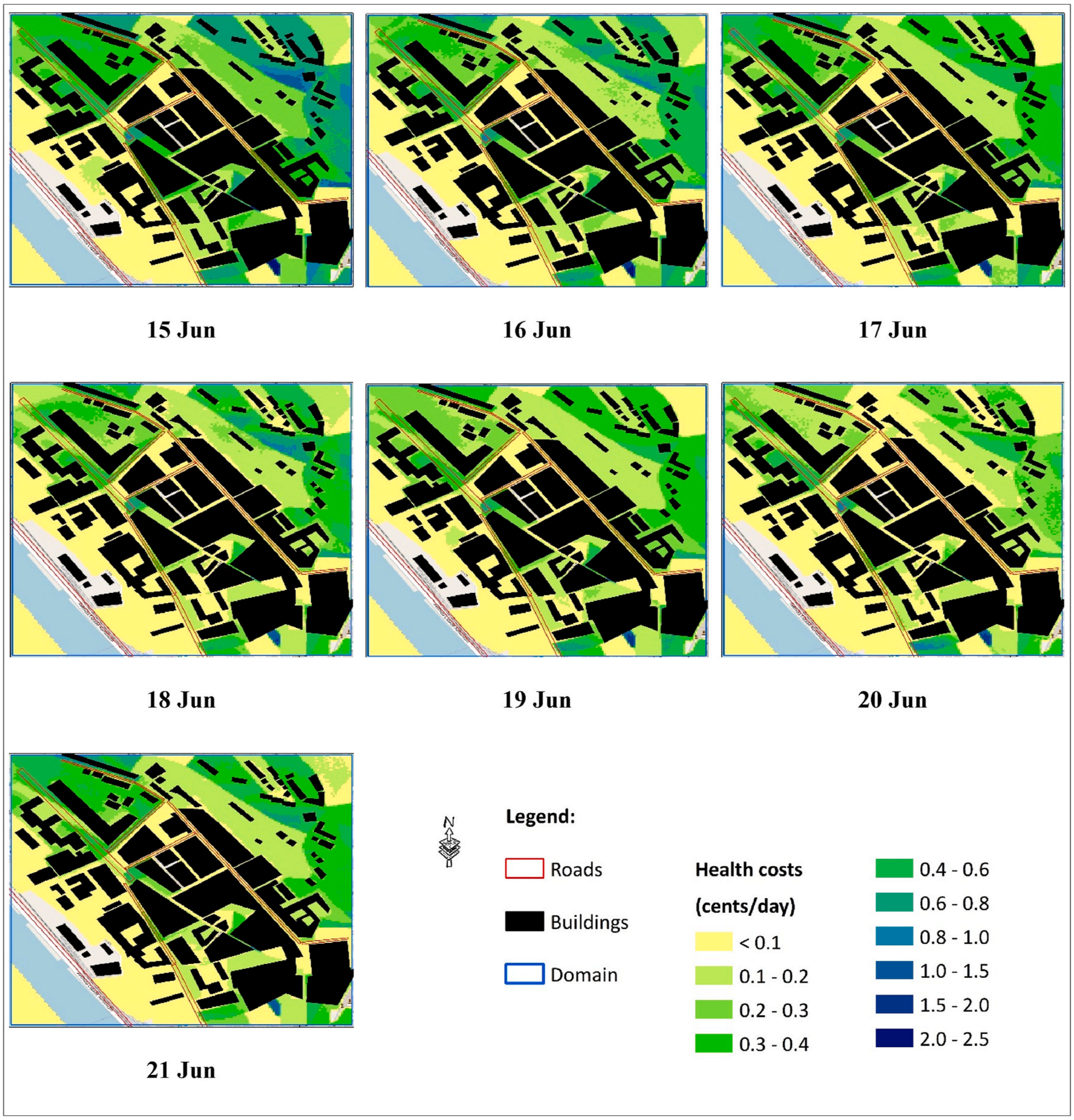

Fig. B.2. Short-term health damage costs (cents/day) estimated for the REF scenario in the summer period.

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